Comparison of the PIC model and the Lie algebraic method in the simulation of intense continuous beam transport*

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Abstract Both the PIC (Particle-In-Cell) model and the Lie algebraic method can be used to simulate the transport of intense continuous beams. The PIC model is to calculate the space charge field, which is blended into the external field, and then simulate the trajectories of particles in the total field; the Lie algebraic method is to simulate the intense continuous beam transport with transport matrixes. Two simulation codes based on the two methods are developed respectively, and the simulated results of transport in a set of electrostatic lenses are compared. It is found that the results from the two codes are in agreement with each other, and both approaches have their own merits.

Key words PIC model, Lie algebraic method, intense continuous beam

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1 Introduction

Nowadays intense beam accelerators have received increasing interest, but the space charge effect is still a complicated problem facing us. Because of the space charge effect, especially in the low energy transport lines, much more charged particles may be lost, and then the transport rate is reduced. In order to design and optimize the transport systems of the intense beam accelerators, many kinds of simulation codes have been developed, such as TRACE-3D[1], BEAMPATH[2], but there are few of them simulating the transport of intense continuous beams. Both the PIC model and the Lie algebraic method can be used to simulate the transport of intense continuous beams, and two simulation codes are developed based on the two methods respectively.

In this article, the application of the two methods in the simulation of intense continuous beam transport is introduced respectively, and then the calculated results of intense continuous beam transport in a set of electrostatic lenses are compared.

2 PIC model

The first method discussed is the PIC model. According to the PIC theory, thousands of macro particles which have the same charge-to-mass ratio as real charged particles are needed to calculate the space charge field and then simulate the trajectories of charged particles in the optic elements. In order to improve the precision, the optic elements are usually divided into several small segments, and the macro particles are transported through the segments one by one. In a segment the field acting on the charged particles is supposed to be constant. Three steps will be completed orderly in one segment.

Divide the region which the charged particles occupy, with a set of uniform rectangular meshes, and then distribute the charge of the particles in the mesh to the four nearest node points. As shown in Fig. 1, the contribution to the charge density at the node point a from the macro particle o is

$$\rho_a = \frac{Q}{\Delta x \Delta y}\left(1-\frac{|x_o - x_a|}{\Delta x}\right)\left(1-\frac{|y_o - y_a|}{\Delta y}\right), \quad (1)$$

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where Q is the charge of the macro particle, and $\Delta x, \Delta y$ are the mesh sizes, (x_a, y_a), (x_o, y_o) the coordinates of the node point a and the macro particle o respectively. In the same way, the charge of macro particle o is distributed to the other three node points.

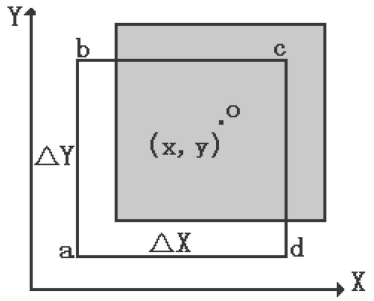

Fig. 1. Charge distribution (The rectangle abcd is a mesh, and the shade one represents the macro particle o).

Having assigned the charge density to all the node points, the Poisson's equation is solved by the Green's function to calculate the space charge potential as well as the self electric field at the node points

$$G(x,y,x',y') = \ln\left(1+\frac{(x^2+y^2-R^2)(x'^2+y'^2-R^2)}{R^2((x-x')^2+(y-y')^2)}\right), \quad (2)$$

where (x', y') are the coordinates of the source point, and (x, y) the coordinates of field point. R is the inner radius of the optic element. If $x = x'_i, y = y'_j$, $G = 1$. Since the Green's function is adopted in a closed space with the boundary conditions properly set, the influence of the image charge has been taken into account. The potential at a node point is

$$\phi(x,y) = \frac{\Delta x \Delta y}{4\pi\varepsilon}\sum_{j=1}^{N_y}\sum_{i=1}^{N_x} G(x,y,x'_i,y'_j)\rho(x'_i,y'_j)\ , \quad (3)$$

where ε is the vacuum permittivity, and N_x, N_y are the numbers of the node points along the x and y directions respectively.

The space charge field acting on each particle is obtained by interpolation from the field of the nearest four node points[3]. With the combination of the external and self fields, the force on the particles can be calculated, as well as the motion of them.

One important advantage of the PIC model is that the calculated results are self-consistent. But in order to improve the precision, one has to use much more macro particles and much smaller meshes. So enormous calculations must be completed, and much more CPU time and computer storage are required.

3 Lie algebraic method

The Lie algebraic method is to calculate the transport matrixes, and then simulate the transport of intense continuous beams. As mentioned above, the optic elements are also divided into several small segments and four steps will be finished in order to obtain the transport matrixes.

Calculate the particle's Hamiltonian H in the phase space (x, p_x, y, p_y, z, p_z) with the independent variable time t,

$$H = (m_0^2c^4 + p_x^2c^2 + p_y^2c^2 + p_z^2c^2)^{1/2} + Q\psi\,, \quad (4)$$

where $\psi = \psi_e + \psi_s$, and ψ_e is the external potential and ψ_s the space charge potential, m_0 the mass of the charged particle, and c the light velocity.

Convert the Hamiltonian H into a new one with the longitudinal coordinate z as the independent variable,

$$K = -[(p_t + Q\psi)^2/c^2 - p_x^2 - p_y^2 - m_0^2c^2]^{1/2}\,, \quad (5)$$

where $p_t = -H$[4].

Perform the canonical transformation[5]:

$$x = x,\ p_x = p_x,\ y = y,\ p_y = p_y,$$
$$\tau = t - z/c\beta, \quad p_\tau = p_t - p_t^0, \quad (6)$$

where β is the relative velocity of the reference particle, and p_t^0 is the value of p_t for the reference particle

$$p_t^0 = -m_0c^2\gamma\,, \quad (7)$$

where $\gamma = 1/\sqrt{1-\beta^2}$. The new Hamiltonian in the new phase space $(x, p_x, y, p_y, \tau, p_\tau)$ is

$$H = -[(p_\tau + Q\psi - m_0c^2\gamma)^2/c^2 - p_x^2 - p_y^2 - m_0^2c^2]^{1/2} - (p_\tau - m_0c^2\gamma)/\beta\,. \quad (8)$$

Expand the new Hamiltonian H into the power series about the reference orbit

$$H = \sum_{n=0}^{\infty} H_n\,. \quad (9)$$

In the linear approximation, the first three terms are kept

$$H = H_0 + H_1 + H_2\,, \quad (10)$$

where H_0 is constant and H_1 zero, so they can be neglected.

Substitute H_2 into the Lie map

$$\varsigma_i = \exp(-L:H_2:)\varsigma_{\varsigma=\varsigma_0}\,, \quad (11)$$

where $\xi = (x, p_x, y, p_y, \tau, p_\tau)$, and L is the length of a segment, ξ_0, ξ_i are the coordinates of the particles in the new phase space at the entrance and exit of the segment respectively.

Using the Lie algebraic method, the transport matrixes of intense continuous beams are calculated. When calculating the space charge potential, it is supposed that the distribution function of the charged particles is Gaussian distribution. In fact the distribution of the charged particles will change in the transport. However, comparing the results from the Lie algebraic method with those from the PIC model, it can be concluded that this approximation is valid. In the simulation, only several thousand macro particles are sufficient, and the calculations are much simpler than those based on the PIC model. So much more CPU time is saved as well as the computer storage.

4 Comparison of calculated result

Two simulation codes are developed based on the PIC model and the Lie algebraic method respectively. The simulation results of the intense continuous beam transport in a set of electrostatic lenses are compared with each other. As shown in Fig. 2, the proton beam extracted from the ion source is focused by two three-tube lenses, and then injected into the next optic element. The focusing potentials of the two three-tube lenses are 8.0 keV, and the current of the beam 2.0 mA, the energy of the beam 25.0 keV.

In Fig. 3, the envelope is the calculated result of the code based on the PIC model. In the simulation, one hundred thousand macro particles and 128×128 meshes are used. In Fig. 4, the envelope is the result of the program based on the Lie algebraic method. Only three thousand macro particles are adopted. Comparing the two envelopes, it can be seen that the simulated results by the two codes are in agreement with each other.

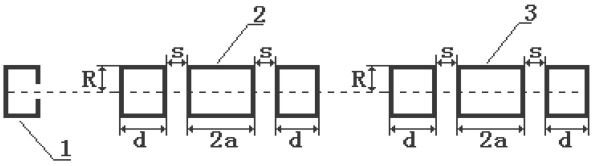

Fig. 2. Transport line (1: ion source. 2, 3: three-tube lens. $R = 2.0$ cm, $d = 5.0$ cm, $s = 1.0$ cm, $a = 4.0$ cm).

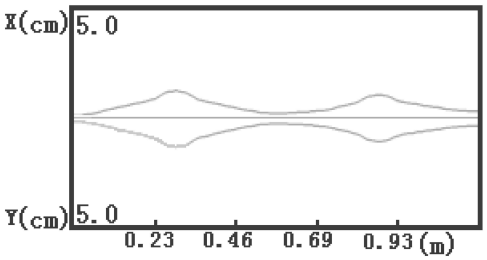

Fig. 3. Envelope-a (simulated by the PIC model).

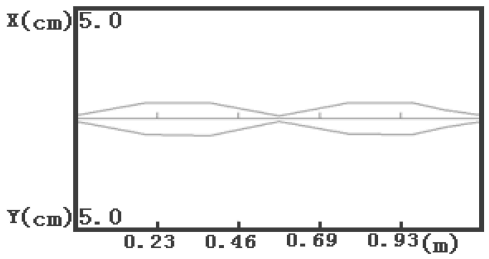

Fig. 4. Envelope-b (simulated by the Lie algebraic method).

5 Conclusion

Both the PIC model and the Lie algebraic method are used to simulate the transport of intense continuous beams. Because in the code based on the Lie algebraic method the linear approximation is made, the results are a little different from those from the PIC model.

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