3D space charge code with the FFT method

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Abstract: Precise and fast 3D space-charge calculations have become important for high intensity hadron accelerator design. The PIC method is most frequently used due to its efficiency. This paper introduces a 3D-PIC code that computes the potential of the bunch in the rest frame by means of Poisson's equation. FFT is applied as Poisson solvers. The details and the results are presented as well as error analysis.

Key words: 3D space charge, Poisson equation, fast fourier transform

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1 Introduction

Space charge force calculation is important but time consuming, especially for low energy intense beams. Basically speaking, there are two models for calculating the space charge force: PPI (particle-to-particle) and PIC (particle in cell). The first one is scarcely used because of the large CPU time involved. Some electron accelerator tracking codes, such as GTP [1], ASTRA [2] MOEVE [3], calculate the 3 dimensional space charge with FFT and the Poisson equation in the rest frame. The ion circular code ORBIT [4], assumes that the longitudinal beam length is much larger than the transverse one, and it is the same case with the grid scale and length, which means, $\rho_{(x,y,z)}=\rho_{(x,y)}\rho_{(z)}$. It gets the 2D transverse space charge with the Laplace transform first and then the longitudinal slices. Proton LINAC codes, such as PARMILA, PARMTEQ, calculate it on the hypothesis of 2D elliptical axial symmetry and the approximation of charged rings centered in the axis, while SAS in DYNAMION uses Kellogg's formula to solve an elliptical beam [5], HERSC uses hermite functions to represent beam distribution [6]. This subroutine written in C++ is designed as part of a proton LINAC dynamic design and tracking code. It treats a beam in the beam-rest frame and the FFT serves as a Poisson equation solver. A special measure in Laplace's operator is taken to reduce the errors in discretization. The overall procedure is to generate a 3D cartesian grid and evaluate charge density at grid points, FFT to frequency domain and get corresponding potential, and then, transform it back to space domain. In this paper we shall introduce the steps for getting the field in rest frame and evaluate the errors.

2 The 3D space charge model

Take 1D condition as an example. The overall sequence is given in Fig. 1 [7].

In the beam-rest frame, the Maxwell equation to be solved becomes electrostatic problem. The generation of grid is shown in Fig. 2.

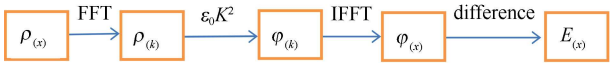

Fig. 1. Overall steps of the code for 1D condition.

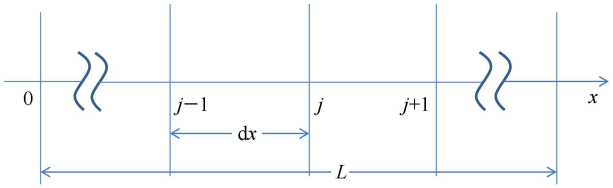

Fig. 2. The source grid $X_j=j\times$dx where the potential, charge density only distributed on the grids, and the field grid are equally spaced at the source grid intervals.

Where L is the length of NG points. There is no strict limit between periodic and nonperiodic FFT. When the grid scale is long enough compared with the beam size, a periodic transform becomes nonperiodic. Then the distribution in k space becomes continuous and can be represented by points in its envelope. This is just as

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what periodic FFT does. The charge density is calculated in grids and $\rho_{(x)}$ at N points is obtained. FFT transform can be used. $\rho_{(x)}$ has Fourier transforms $\rho_{(k)}$ where k is wave vector in Fourier transform, $k=n\times 2\pi/L$ Then, the Poisson equation in one dimension becomes $\partial^2/\partial x^2=-k^2$, it means:

$$\phi_{(k)}=\frac{\rho_{(k)}}{\epsilon_0 k^2}. \tag{1}$$

In a discret FFT problem, the forward transform is

$$\rho_{(k)}=\Delta x\sum_{j=0}^{N-1}\rho_{(X_j)}\mathrm{e}^{-\mathrm{i}kX_j}, \tag{2}$$

and the inverse transform of the potential is:

$$\phi_{(X_j)}=\frac{1}{L}\sum_{n=-N/2}^{N/2-1}\phi_{(k)}\mathrm{e}^{-\mathrm{i}kX_j}, \tag{3}$$

where $k=n\times 2\pi/L$.

2.1 Discretization of differencing operatiors

The deviation operator, a local one in continuous space, is changed to a finite difference operator. When modeling a continuous system with a discrete system, it is desirable to retain local information.

$$\nabla^2\phi_{(j)}=\frac{(\phi_{j+1}-\phi_j)-(\phi_j-\phi_{j-1})}{\Delta x^2}. \tag{4}$$

According to FFT,

$$\nabla^2\phi_{(k)}=k^2\times\left|\frac{\sin(\Delta x\times k/2)}{\Delta x\times k/2}\right|^2\phi_{(k)}. \tag{5}$$

2.2 Expression in a 3D Cartesian coordinate system

Similarly, in a 3D Cartesian coordinate,

$$\nabla^2\phi_{(\boldsymbol{k})}=K^2\times\phi_{(\boldsymbol{k})}. \tag{6}$$

where

$$\begin{aligned}K^2 &= k_x^2\left|\frac{\sin(\Delta x\times k_x/2)}{\Delta x\times k_x/2}\right|^2\\ &+k_y^2\left|\frac{\sin(\Delta y\times k_y/2)}{\Delta y\times k_y/2}\right|^2\\ &+k_z^2\left|\frac{\sin(\Delta z\times k_z/2)}{\Delta z\times k_z/2}\right|^2,\end{aligned} \tag{7}$$

and the Poisson equation becomes

$$\phi_{(k)}=\frac{\rho_{(k)}}{\epsilon_0\times K^2}. \tag{8}$$

Taking the boundary condition into consideration, let the potential in transverse edges be const.

3 Results and comparison with the ideal theoretical value

Take a uniform charge distribution in a ball as an example. The radius of the ball equals 0.2 cm. The isopotential line in any plane is a circle or polygon that centers in the charge center as shown in Fig. 3.

The results are related to the grid intense and scale as shown in Fig. 4.

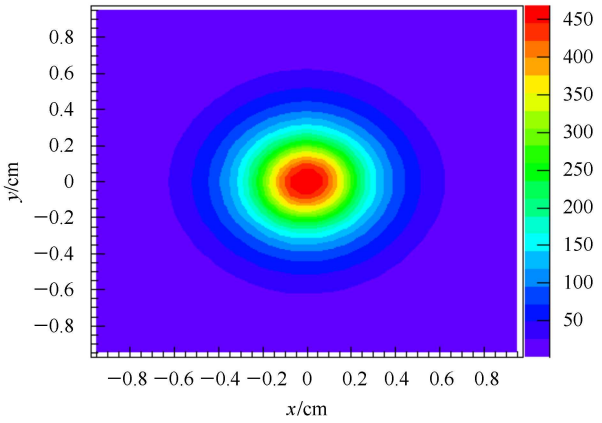

Fig. 3. The potential distribution in any 2D plane. The equipotential lines are similar circulars. The grid number is 40^3, and the grid intense is 0.05^3.

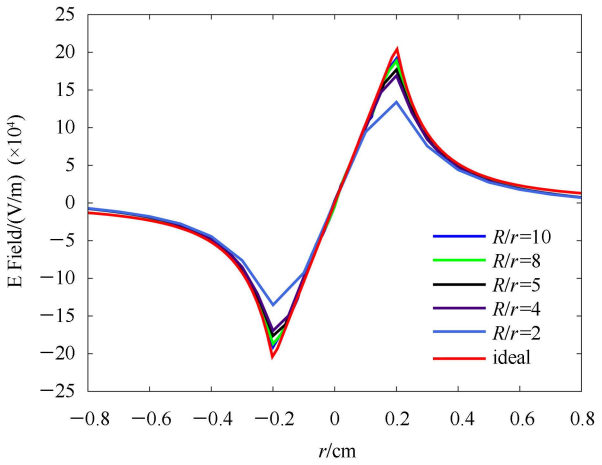

Fig. 4. The space charge field distribution with r in different grid densities. The red one is analytic solution in a uniform-ball charge distribution. The data above is obtained on the condition that the grid scale is $(1\ \mathrm{cm})^3$. R is the beam radius and r is the grid length.

As the grid becomes more intense, the numerical field solution is closer to the ideal. But when the grid number in charged radius scale is greater than 4, the difference is very small. Considering the CPU time consumption, $R/r>=5$ seems to be reasonable. Taking the condition $R/r=5$, Fig. 5 shows that the field corresponds to a different ratio of grid scale to beam scale.

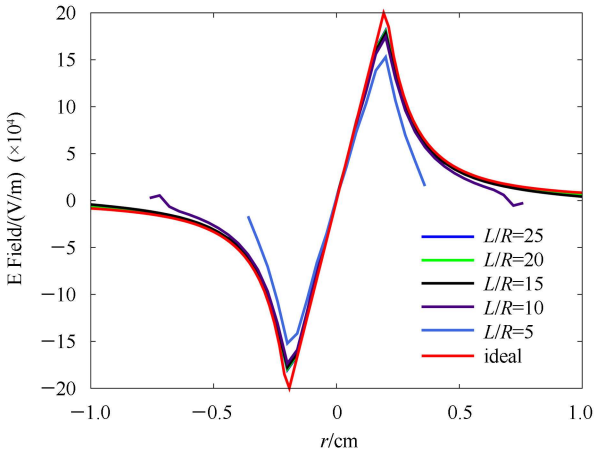

Fig. 5. Space charge field versus r for different grid scale. R/r=5. Curves end in different points because of the different field scales.

When the grid scale L is 10 times larger than the beam radius R, the error is small.

4 Error analysis

Errors are unavoidable in any models. Here are some important reasons leading to errors.

1) Errors caused by the following reasons: when continuous space becomes discrete, discrete charged representation, derivation operator changed to a finite-difference operator, difference of potential to get an electric field, all of these result in errors, which has a strong relation with grid length and numbers [8].

2) Computer round off errors. Also related to grid information. The error can be evaluated according to the Gauss theorem with the function

$$g=1-\frac{\oint \boldsymbol{E}\mathrm{d}\boldsymbol{S}}{\int_V \frac{Q}{\epsilon_0}\mathrm{d}V}. \tag{9}$$

Pictures in Fig. 6 show the relationship of g versus the particle number, the grid size, the grid number, and the position from the beam center. Take the integration outside of the charged ball. Then Q is the exact total electric quantity, that is not related to numerical errors. The error from the Gauss theorem in radius=0.2 cm, and the grid 40^3, 0.02^3, is about 0.1. The number decreases as the radius enlarges, and the grid becomes finer or the gird number enlarges.

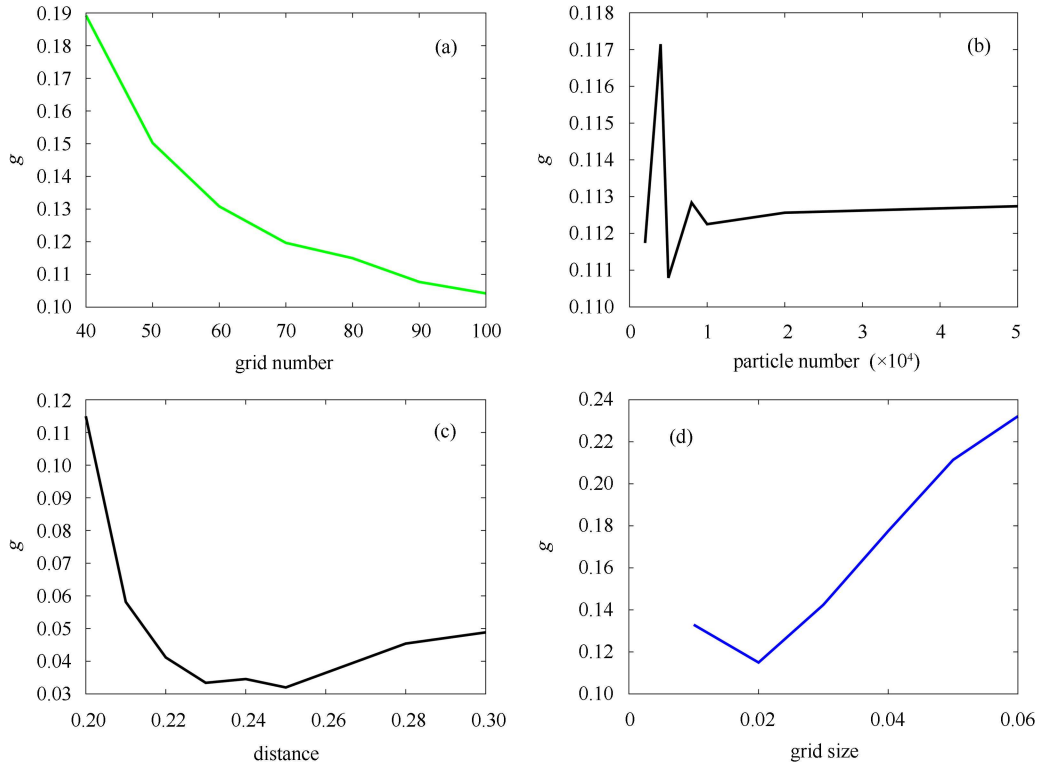

Fig. 6. The error parameter g has little relationship with particle numbers. g goes small as the measured ball goes bigger in some scale, or the grid number becomes larger, or the grid size becomes finer. The auto set of the grid is 40^3, 0.02^3, the distance is 0.2 cm, and the particle number is 2×10^4. Pictures are obtained on the condition that just the corresponding parameter changes, the others are equal to the default.

5 Conclusion

3D space charge calculation is important but time consuming. By using the FFT method acting as the Poisson solver to obtain the space charge field is available and reliable. When the grid size is less than one fifth of the beam the size and the grid scale is as large as five times of the beam size, the method will reflect the real field very well.

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