NEW 3D SPACE CHARGE ROUTINES IN THE TRACKING CODE ASTRA*

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Abstract

Precise and fast 3D space-charge calculations for bunches of charged particles are of growing importance in recent accelerator designs. One of the possible approaches is the particle mesh method, computing the potential of the bunch in the rest frame by means of Poisson's equation. In this, the charges of the macro particles representing the distribution of the particles of the whole bunch are distributed on a mesh. Two kinds of Poisson solvers are implemented in the tracking code Astra. One of them is the direct solution of the Poisson equation applying Fast Fourier Methods (FFT), the other is a finite difference discretization combined with an iterative multigrid Poisson solver (MG). Due to recent developments in beam dynamics studies, the simulation of high brightness electron bunches is a growing field of interest. In this paper the numerical behavior of such bunches is investigated with respect to the two different 3D Poisson solvers implemented in Astra.

INTRODUCTION

The program package Astra (A space charge tracking algorithm) has been successfully used in the design of linac and rf photoinjector systems. The Astra suite originally developed by K. Flöttmann tracks macro particles through user defined external fields including the space charge field of the particle cloud [1].

The first version of Astra allowed the calculation of space charge fields of bunches with azimutal symmetry only. A further development was the implementation of a FFT-based Poisson solver for full 3D space charge calculations with free space boundary conditions [2]. Recently, a new set of 3D Poisson solvers has been implemented in Astra by G. Pöplau. These Poisson solvers are iterative algorithms, among them the state-of-the-art multigrid Poisson solver. The first version of the multigrid solver especially developed for space charge calculations on adaptive discretizations was introduced in [9]. Further, these multigrid solvers have been developed as software package MOEVE [5]. Applications of the solvers within tracking routines can be found, for instance, in [7, 8].

In this paper, only the basic concepts of both the FFT and the iterative Poisson solvers are described. Advantages and disadvantages were discussed in [6]. Since high brightness, low emittance electron bunches have important applications in future light sources and linear colliders, the main part of this paper deals with the the numerical investigation of such bunches. In particular, the space charge calculation of bunches with uniform particle distribution poses a challenge. Results on this subject were reported, for instance, in [3, 10]. Here, cylindrical bunches with uniformly distributed macro particles will be studied with respect to space charge calculations of both the FFT and the multigrid Poisson solver.

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3D SPACE CHARGE PARTICLE MESH ALGORITHMS

A widely used method for the calculation of 3D space charge fields is the particle mesh method (PM) described e. g. in [4]. For this approach, the bunch is modelled as a distribution of macro particles. The potential φ of the bunch is determined in the rest frame by means of Poisson's equation given by

$$-\Delta\varphi = \frac{\rho}{\varepsilon_0} \qquad \text{in } \Omega \subset \mathbb{R}^3, \tag{1}$$

where ρ denotes the space charge density and ε_0 the dielectric constant. Generally, a rectangular box Ω is constructed around the bunch and a Cartesian mesh is defined inside this box. The values ρ are assigned at the grid points by a volume weighted distribution of the charge of the macro particles. Next, the potential values at the grid points are determined by a Poisson solver. In Astra two different solver types are implemented. One of these methods is the widespread FFT Poisson solver. The second approach is a fast iterative solver based on multigrid.

FFT Poisson Solver

The FFT Poisson solver is based on the direct solution of Poisson's equation by means of the Green's function G given by

$$\varphi_{i,j,k} = \sum_{i',j',k'} G_{i-i',j-j',k-k'} \cdot \rho_{i',j',k'}. \tag{2}$$

Here, $\varphi_{i,j,k}$, $G_{i-i',j-j',k-k'}$ and $\rho_{i',j',k'}$ refer to the values of the related functions at the mesh points. Applying the discrete Fourier transformation (DFT) the relation

$$\hat{\varphi}_{l,m,n} = \hat{G}_{l,m,n}\hat{\rho}_{l,m,n} \tag{3}$$

is obtained from (2) due to the convolution theorem. The circumflex denotes the DFT and (l,m,n) the harmonic wave numbers. The inverse DFT provides the potential at the grid points.

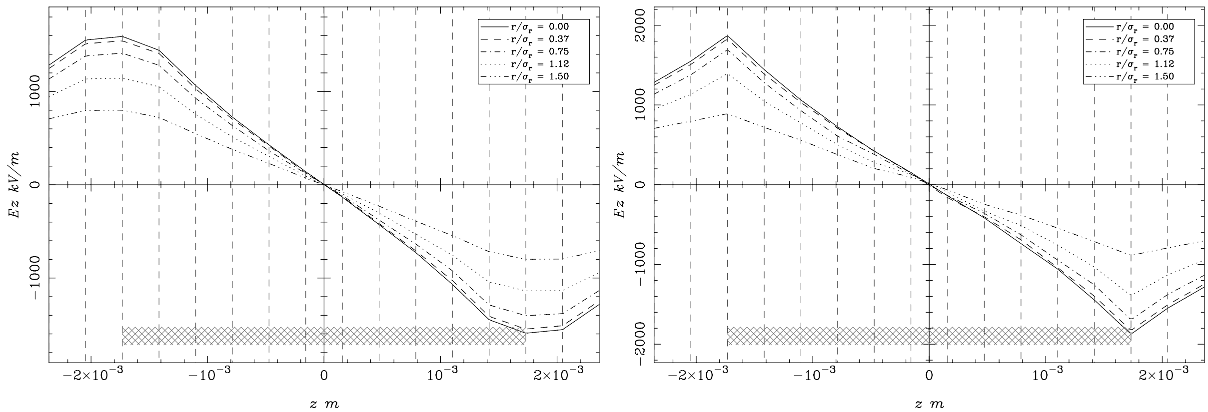

Figure 1: Longitudinal electric field of a bunch with aspect ratio 1: E_z along the z-axis calculated with FFT (left) and MG (right).

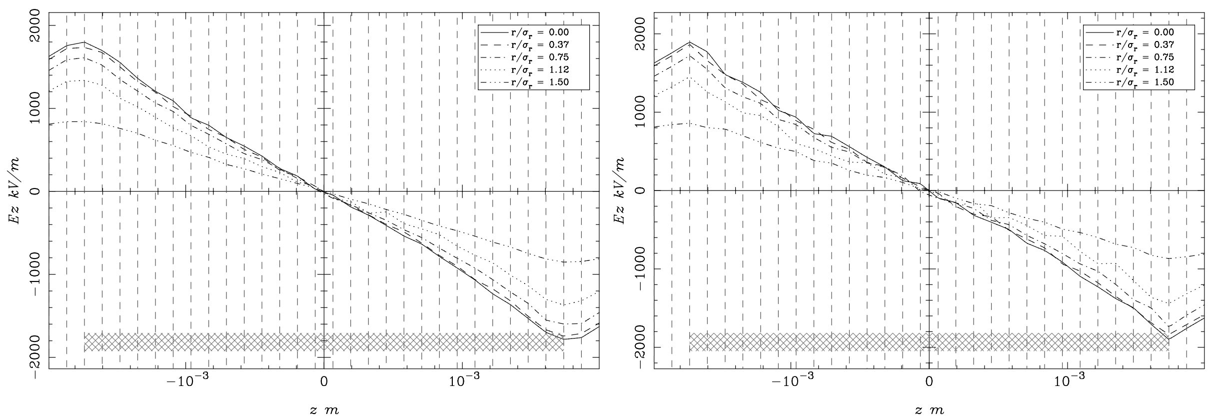

Figure 2: Longitudinal electric field of a bunch with aspect ratio 1: E_z along the z-axis calculated with FFT (left) and MG (right).

Let the computational domain Ω be defined as $\Omega = [-a_x, a_x] \times [-a_y, a_y] \times [-a_z, a_z]$. Then, the DFT of the standard Green's function is given by

$$\hat{G}_{l,m,n} = \left(\left(\frac{\pi l}{a_x} \right)^2 + \left(\frac{\pi m}{a_y} \right)^2 + \left(\frac{\pi n}{a_z} \right)^2 \right)^{-1}. \quad (4)$$

It is well-known that the DFT can be efficiently calculated by Fast Fourier Transformation (FFT) algorithms. The numerical effort of the Fourier approach in the three dimensional case is $O(M \log N)$ with the same number of steps $N = 2^t$ in each coordinate direction and $M = N^3$ the total number of grid points.

Iterative Poisson Solvers

Iterative Poisson solvers require a different approach. Firstly, the Laplacian in (1) is discretized. The discretization by second order finite differences (FD) provides a linear system of equations

$$\mathbf{A}u = f, \quad (5)$$

where u denotes the vector of the unknown values of the potential and f the vector of the given space charge density at the grid points. Since the matrix $\mathbf{A}$ is sparse, iterative solvers can be applied efficiently.

State-of-the-art is the application of a multigrid Poisson solver which has optimal convergence, i. e. the number of iteration steps to obtain a certain accuracy is independent of N. In Astra a multigrid algorithm (MG) and a multigrid preconditioned conjugate gradient method are implemented. The computational effort of the second algorithm is a little bit higher but its performance is more stable than MG. This can be advantageous for real applications.

BUNCHES WITH UNIFORM PARTICLE DISTRIBUTION

Space charge simulations of bunches with uniform particle distribution pose a problem which is caused by the jump in the space charge density at the edges of the bunch. In practice, one example of the occurrence of such particle distributions is near the cathode of a rf photo gun: the bunch is short because the electrons start at the cathode with an energy of almost zero. Furthermore, at high energies a bunch appears long stretched in the rest frame.

Recently, especially short bunches were investigated

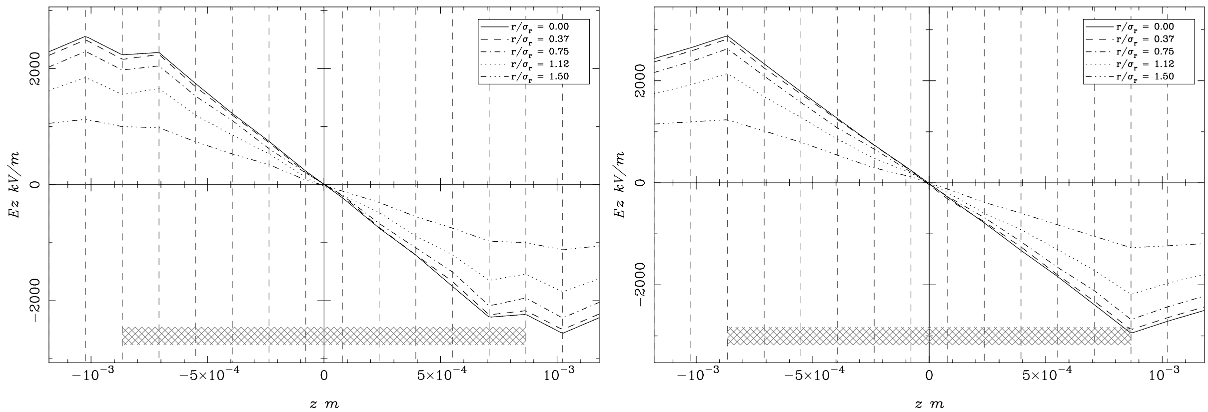

Figure 3: Longitudinal electric field of a short bunch with aspect ratio 2: E_z along the z-axis calculated with FFT (left) and MG (right).

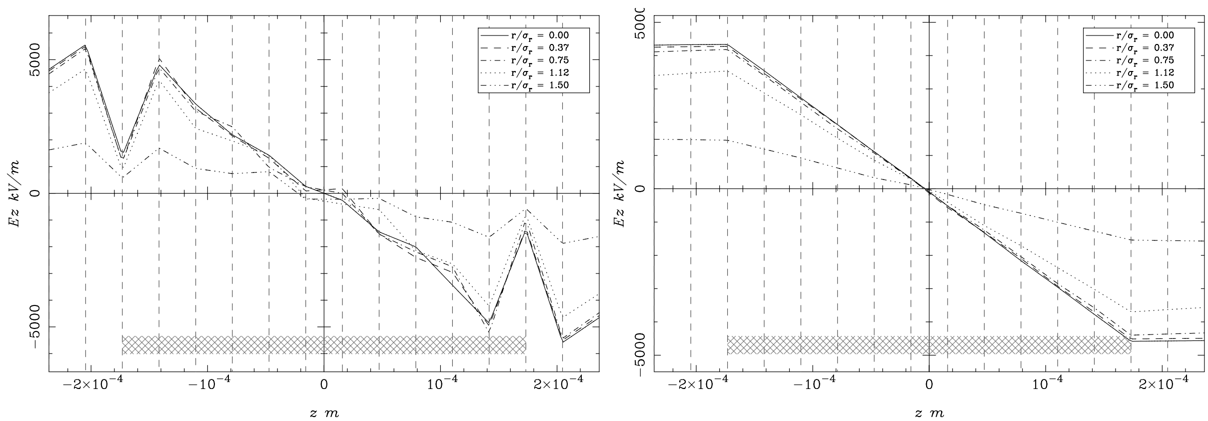

Figure 4: Longitudinal electric field of a short bunch with aspect ratio 10: E_z along the z-axis calculated with FFT (left) and MG (right).

in [10] and new Poisson solvers based on the FFT with variations of the Green's function were constructed. In the following, bunches of cylindrical shape were chosen as the model problem. All bunches contain 20,000 uniformly distributed macro particles. Further, bunches of different aspect ratios are investigated, where the aspect ratio is defined by σ_x/σ_z with $\sigma_x = \sigma_y$.

Bunch with Aspect Ratio One

The first numerical example is a cylindrical bunch with aspect ratio one in the rest frame, more precisely $\sigma_x = \sigma_y = \sigma_z = 1$ mm.

Figure 1 presents the longitudinal electric field obtained with the FFT and the MG Poisson solver, respectively. The resolution of the bounding box Ω is given by $N_x = N_y = N_z = N = 32$. While the MG solver provides a good approximation of the field at the edges of the bunch, the FFT solver smoothes the hard edges.

Figure 2 shows that a higher resolution ($N_x = N_y = N_z = 64$) reduces these edge effects. Further, the FFT solver achieves better results with respect to the inner part of the bunch: the electrical field is smoother here. The result of the MG solver can be improved by enlarging the number of macro particles.

Short Bunches

At low energy, for instance, near the cathode, a bunch has a pancake-like shape. In order to demonstrate the numerical problems with space charge calculations of pancake-shaped bunches, first a bunch of cylindrical shape with $\sigma_x = \sigma_y = 1$ mm and $\sigma_z = 0.5$ mm was chosen. The bounding box Ω was discretized by $N_x = N_y = N_z = 32$ steps.

While Figure 3 shows satisfying results for the MG Poisson solver, the FFT solver has bigger edge effects than for the bunch with aspect ratio one (compare Figure 3 and 1). In particular, the highest values of the field are not situated at the edges of the bunch but outside.

As shown in Figure 4, the edge effect related to the FFT solver becomes bigger, if the aspect ratio is enlarged. This simulation was performed with $\sigma_x = \sigma_y = 1$ mm and $\sigma_z = 0.1$ mm. Further, Figure 4 demonstrates the good approximation of the longitudinal field obtained by the MG solver. It has to be mentioned that the edge effect will be

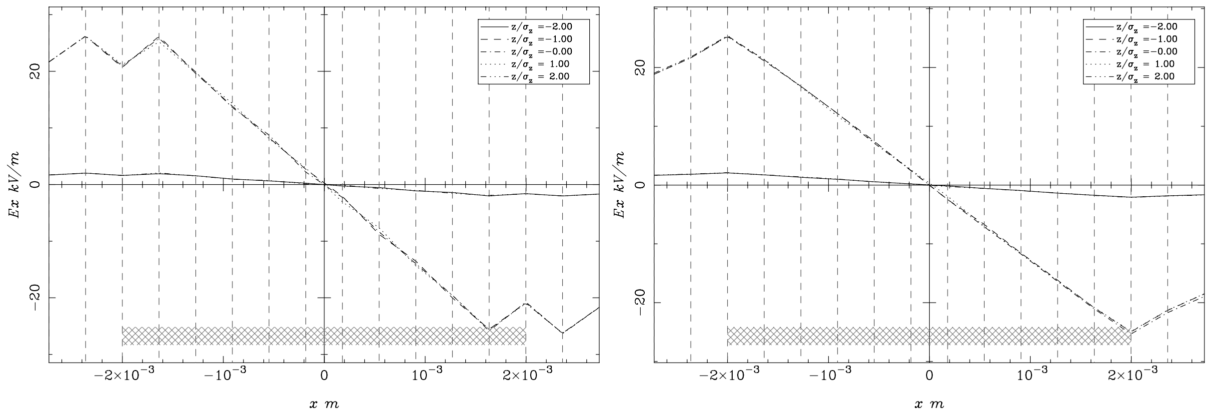

Figure 5: Transverse electric field of a long bunch with aspect ratio 0.01: E_x along the x-axis calculated with FFT (left) and MG (right).

reduced if the FFT Poisson solver is applied with a higher resolution and a larger number of macro particles.

Long Bunches

For space charge calculations a bunch appears at high energies long stretched in the rest frame. As numerical model for a long bunch a cylindrical bunch with $\sigma_x = \sigma_y = 1$ mm and $\sigma_z = 100$ mm was chosen.

The behavior of the electric field that appeared for the short bunches in longitudinal direction can now be observed transversally. Figure 5 represents E_x of the related field in x-direction (for symmetry reasons the same plot was obtained for E_y in y-direction). Here, the edge effect is not as big as for the short bunches.

CONCLUSIONS

Beam dynamics simulations of high brightness, low emittance electron beams have gained in importance over the last few years due to the application for future light sources and linear colliders. Since space charge calculations of such bunches pose a challenge to numerical procedures, the two 3D space charge algorithms implemented in Astra - the direct FFT and the iterative MG Poisson solver - were investigated concerning cylindrically shaped bunches with uniform particle distribution. It turned out that the FFT solver shows the well-known problem to approximate the field at the edges of the bunch correctly. This effect occurs for short bunches in the longitudinal and for long bunches in the transverse direction. A higher resolution reduces the edge effects. The MG Poisson solver provides good results for short as well as for long bunches. While the MG method requires a larger number of macro particles for simulations with a higher resolution, the FFT approach still achieves good results without enlarging the number of macro particles.

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