THE PERFORMANCE OF 3D SPACE CHARGE MODELS FOR HIGH BRIGHTNESS ELECTRON BUNCHES*

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Dedicated to Professor Manfred Tasche on the occasion of his 65th birthday

Abstract

Precise and fast 3D space charge calculations for high brightness, low emittance electron beams are of growing importance for the design of future accelerators and light sources. In this paper we investigate the performance of the 3D space charge models implemented in the tracking code Astra. These are the FFT-Poisson solver with the integrated Green's function and iterative Poisson solvers from the software package MOEVE. The numerical tests consider the performance of the solvers for model bunches as well as the performance within a typical simulation for the XFEL.

INTRODUCTION

The design of future light sources and colliders requires increasingly precise 3D beam dynamics simulations. The program package Astra (**A** **s**pace charge **tr**acking **a**lgorithm) has been successfully used in the design of linac and rf photoinjector systems [2]. 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. Since efficient space charge calculations gained in importance, the 3D algorithms in Astra have been further developed. Actually, two different types of Poisson solvers for 3D space charge calculations are implemented. One Poisson solver is a new FFT method based on the integrated Green's function. This concept was proposed in [8, 9] and has been only recently implemented in Astra. Another set of solvers consists of several iterative solvers among them the geometric multigrid technique. These solvers have been developed by G. Pöplau for space charge calculations and implemented in the software package MOEVE (**M**ultigrid for n**o**n-**e**quidistant grids to sol**v**e Poisson's **e**quation) [5].

In this paper the performance of the MOEVE and the FFT Poisson solvers is investigated, in particular, for large numbers of mesh points. Furthermore the behavior of the Poisson solvers within the particle tracking Astra is tested with the simulation of the first $14.5\ \mathrm{m}$ of the XFEL. The numerical investigations were performed with the typical restrictions of the FFT method (e.g., equidistant mesh, rectangular box as computational domain). However, the application of iterative solvers offer much more possibilities for simulations which are considered elsewhere, e.g., in [6, 7].

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MODEL FOR 3D SPACE CHARGE SIMULATIONS

All algorithms for space charge calculations described here have been developed for the particle-mesh method [3]. It is assumed that the bunch is modelled by means of a distribution of macro particles. Generally, a rectangular box, in the following denoted as Ω, is constructed around the bunch. Then, a Cartesian grid is defined inside the box and the values of the space charge density ϱ are assigned at the grid points by a volume-weighted distribution of the charge of the macro particles. Next, the potential φ is calculated by means of Poisson's equation given by

$$\begin{aligned} -\Delta\varphi &= \frac{\varrho}{\varepsilon_0} \quad \text{in } \Omega \subset \mathbb{R}^3, \\ \varphi &= 0 \quad \text{on } \partial\Omega_1, \\ \frac{\partial\varphi}{\partial n} + \frac{1}{r}\varphi &= 0 \quad \text{on } \partial\Omega_2, \end{aligned} \tag{1}$$

where ε_0 denotes the dielectric constant and r the distance between the center of the bunch and the boundary. The application of a Poisson solver provides the potential φ at the mesh points. Usually, the domain Ω is a rectangular box constructed around the bunch. On its surface $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$ ($\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$) perfectly conducting boundaries ($\partial\Omega_1$) or open boundaries ($\partial\Omega_2$) can be applied. For space charge calculations within a beam pipe the domain Ω is assumed to be a cylinder with elliptical cross section.

While the FFT approach solves the Poisson equation with open boundary conditions directly, equation (1) is discretized by means of second order finite differences in order to apply a MOEVE Poisson solver on the resulting system of equations [7].

PERFORMANCE OF 3D POISSON SOLVERS

In this section the performance of the 3D Poisson solvers implemented in Astra is investigated. These are a selection of the MOEVE Poisson solvers and the new FFT Poisson solver with the integrated Green's function.

Performance of MOEVE Poisson Solvers

In MOEVE, different iterative solvers are implemented: multigrid (MG) and multigrid pre-conditioned conjugate gradients (MG-PCG); a pre-conditioned conjugate gradient method (PCG) with Jacobi pre-conditioner; (mainly for comparison reasons) the successive over relaxation (SOR);

and (for the solution of Poisson's equation within an elliptical shaped beam pipe [4]) biconjugated gradients (BiCG) and BiCGSTAB as a stabilized version of BiCG.

The implementation of the methods PCG, SOR, BiCG and BiCGSTAB is simple but these algorithms suffer from the drawback that the number of iterations grows with $\mathcal{O}(N^2)$. Here, N denotes the number of mesh lines in each coordinate direction. The state-of-the-art is the application of a multigrid method as Poisson solver. This offers optimal performance, i.e. in general the number of iteration steps to obtain a certain accuracy is independent of N. Consequently, the numerical effort grows only linearly with the total number of mesh points. This is proven for model problems, where $N = 2^t + 1$. The MG solvers of MOEVE are constructed such that this optimal behavior is also achieved if $N \neq 2^t + 1$ (see Figure 1). Details of these algorithms can be found in [6, 7] and citations therein.

The objective of this subsection is to investigate the performance of the MOEVE Poisson solvers MG, MG-PCG and PCG for a large number of grid points up to more than 3 millions. The parameters of the model bunch were taken from the simulation of the XFEL (see next section): 0.07 m after the cathode the bunch has an extension of $\sigma_x = \sigma_y = 1.36$ mm and $\sigma_z = 1.7$ mm at an energy of 2.5 MeV. Thus, for the numerical tests, the bunch was assumed as ellipsoid with the half axes $a = b = 1.4$ mm, $c = 8.5$ mm in x-, y- and z-direction, respectively. Further the ellipsoid had a uniformly distributed charge of $Q = -1$ nC, i.e. the influence of the macro particles were neglected. The algorithms MG, MG-PCG and PCG were applied with Dirichlet and open boundary conditions, respectively. The discretization was chosen to be equidistant. All algorithms were performed until the maximum norm of the relative residual had reached a value of less than 10^{-2}. This accuracy value seems to be rather large, but further iterations would not improve the numerical error, because the source term ϱ is discontinues in general.

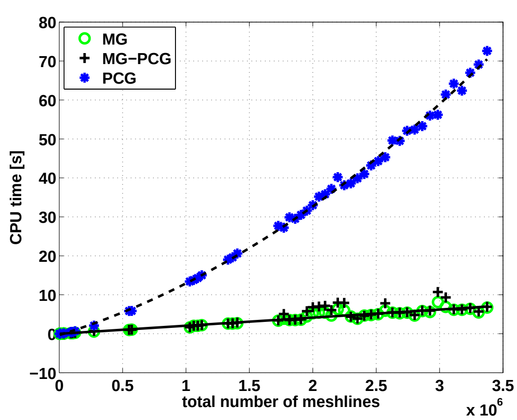

Figure 1: Performance of selected MOEVE Poisson solvers for Dirichlet boundary conditions.

Figure 1 shows the performance of the solvers for the Poisson equation (1) with Dirichlet boundary conditions: the numerical effort grows linearly for the MG solvers and quadratically for the PCG method with the number of unknowns. The results for open boundary conditions are presented in Figure 2. The performance of PCG grows again quadratically with the number of unknowns. The behavior of the MG solvers is linear in general but there are some exceptions. The red markers indicate the runs, where the maximum norm of the relative residual doesn't achieve a value of less than 10^{-2}. The worst performance was observed with 1,331 million grid points. Here, the maximum norm of the relative residual achieved only a value of 0.136 for MG and 0.176 for MG-PCG, respectively. These problems with open boundaries occur because the matrix of the linear system of equations becomes numerically singular with increasing number of mesh points (see [4] for the structure of the matrix).

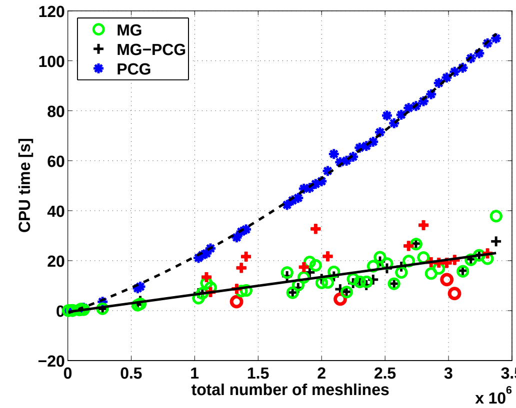

Figure 2: Performance of selected MOEVE Poisson solvers for open boundary conditions.

Performance of FFT and MOEVE Poisson Solvers in Astra

The FFT Poisson solver recently implemented in Astra is based on the integrated Green's function proposed in [8, 9]. It aims to overcome the problem which the simple Green's function has with the approximation of the field of short or long bunches [6].

In this subsection, the performance of the FFT algorithm and the MOEVE Poisson solvers is investigated in the Astra environment. The routine *fieldplot* was used in order to get the CPU-time of a single space charge calculation. Here, the particle distribution for the simulation includes 500,000 macro particles, otherwise it has the same parameters as given in the previous subsection. Since the FFT method is restricted to $N = 2^t + 1$ we performed the tests with the following total number of grid points $N_p = N^3$: $N_p = 33^3 = 35,937$, $N_p = 65^3 = 274,625$ and $N_p = 129^3 = 2,146,689$.

Table 1 represents the CPU-times of a single space charge calculation. In general the effort is comparable for MG, MG-PCG and FFT. MG applied on Poisson's equation with Dirichlet boundary conditions is a little bit faster

Table 1: Performance in Astra: CPU-times of MOEVE Poisson solvers and the FFT Poisson solver.

N_p	MG	MG-PCG	PCG	FFT
	Dirichlet boundary conditions			
35,937	0.12 s	0.15 s	0.24 s	0.12 s
274,625	0.91 s	1.30 s	5.07 s	1.08 s
2,146,689	8.26 s	11.20 s	74.60 s	9.11 s
	open boundary conditions			
35,937	0.14 s	0.15 s	0.95 s	0.12 s
274,625	1.46 s	1.45 s	14.77 s	1.08 s
2,146,689	11.46 s	16.62 s	244.00 s	9.11 s

than FFT, while MG with open boundaries is slower than FFT.

XFEL SIMULATION

In this section the performance of the Poisson solvers is investigated within a tracking simulation with Astra. Our test scenario includes the first 14.5 m of the XFEL [1]. Since the 3D space charge models do not yet take into account the cathode, the first 0.07 m were simulated with with the 2D space charge model of Astra which assumes a cylindrically symmetric bunch. Then, the particle distribution at 0.07 m was taken as the initial distribution for the further simulation with the 3D space charge algorithms. All space charge calculations were performed on an equidistant mesh with $N_p = 65^3 = 274,625$ grid points. The bunch contains 500,000 macro particles.

Table 2: Performance time for the tracking procedure for different Poisson solvers.

Poisson solver	CPU-time
FFT, integrated Green's function	5 h 25 min 6.36 s
initial guess = 0	
MG	5 h 28 min 15.18 s
MG-PCG	5 h 21 min 21.34 s
PCG	6 h 11 min 58.45 s
initial guess = solution of previous time step	
MG	5 h 32 min 55.45 s
MG-PCG	5 h 16 min 45.47 s
PCG	5 h 21 min 2.39 s
other method	
2D, cylindrical symmetric model	8 h 27 min 36.47 s

Table 2 represents the CPU-times of the tracking simulation with the different Poisson solvers. It turns out that the simulation with MG, MG-PCG and FFT takes nearly the same CPU-time each. Since the MOEVE Poisson solvers are iterative methods, the solution of the previous time step of the time integration can be taken as initial guess for the space charge calculation. As shown in the second part of Table 2 especially the PCG algorithm profits from this approach. The reason is that in the present simulation MG and MG-PCG needed half of the iteration steps with the initial guess from the previous time step (for instance 1 or 2 steps instead of 3 or 4 with initial guess=0) while PCG could save up to 3/4 or more of the iteration steps.

The tracking simulation performed 9814–9816 time integration steps (4th order Runge-Kutta scheme) for the MOEVE Poisson solvers and 9835 time integration steps for the FFT method, both with 524 space charge calculations.

CONCLUSIONS

In this paper the performance of the 3D space charge routines – partly only recently – implemented in Astra was tested. A model bunch was considered as well as a tracking scenario including the first 14.5 m of the XFEL. It turned out that the multigrid solvers of MOEVE and the FFT solver with the integrated Green's function have comparable performance. Nevertheless the MOEVE Poisson solvers permit a greater variety considering the choice of boundary conditions and the number and distribution of mesh points.

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