

# SPACE CHARGE MODELS FOR PARTICLE TRACKING ON LONG TIME SCALES\*

J.A. Holmes, S. Cousineau, A. Shishlo, ORNL, Oak Ridge, TN, 37830, USA  
R. Potts, University of Tennessee, Knoxville, TN 37996, USA

## Abstract

In order to efficiently track charged particles over long times, most tracking codes use either analytic charge distributions or particle-in-cell (PIC) methods based on fast Fourier transforms (FFTs). While useful for theoretical studies, analytic distribution models do not allow accurate simulation of real machines. PIC calculations can utilize realistic space charge distributions, but these methods suffer from the presence of discretization errors. We examine the situation for particle tracking with space charge over long times, and consider possible ideas to improve the accuracy of such calculations.

## INTRODUCTION

Space charge physics has been successfully incorporated into numerous computational particle-tracking studies of linacs, accumulator rings, and rapid cycling synchrotrons. These space charge models have allowed the successful simulation of phenomena that would have been impossible otherwise. Particle-tracking simulations for these machines all involve following particle distributions over short to moderate time scales. With the emergence of ever-higher beam intensities, it is now necessary to incorporate space charge effects into simulations of storage rings [1]. Calculations for storage rings require tracking beams for far longer times than those in linacs, accumulator rings, or rapid cycling synchrotrons. These long time scales place severe requirements on the speed and accuracy of the physics models and call for innovative methods of solution. For example, Lie Algebraic methods have been used with great success in single particle tracking to provide fast symplectic high order maps for storage rings. Although it is difficult to conceive of full turn maps for collective effects, such as space charge, advances will be necessary to incorporate this physics reliably into storage ring applications.

The problems of simulating space charge over long times arise partly from simplifications in the physics required to obtain a computational model and, more seriously, from the numerical properties of the model so obtained. From the physics perspective, a beam consists of many identical indistinguishable particles interacting quantum mechanically with each other and with their surroundings. In order to perform tracking studies, we make a series of approximations to arrive at a picture in

which we treat the beam as a collection of distinguishable particles moving and interacting with each other and their surroundings primarily according to classical physics. Within this picture, space charge is the inter-particle Coulomb force, and its evaluation requires the solution of Poisson's equation.

Thus, even at the outset, space charge models represent a very simplified picture of reality. Their success in predicting and describing the physics of accelerators on short to intermediate time scales is some testimony to the validity of these approximations. However, for extension to long time scales, we must keep in mind that many other effects, such as lattice imperfections and nonlinearities, wake forces, neutral gas ionization and scattering, electron cloud interaction, intrabeam scattering, beam loss, and others may be important. These effects may be relatively unimportant at short or intermediate time scales, but critical at longer times. To study them in the presence of space charge, it is necessary understand and to mitigate the numerically induced noise and errors in the space charge models. The challenge of simulating space charge over long times lies in the representation of the beam distribution and the discretization of the problem.

## CHOICE OF PHYSICAL MODEL

The first issue in space charge modeling is to determine what type of model contains physics sufficient to your needs. One criterion is the dimensionality of the model. 1D longitudinal models are used in longitudinal beam dynamics codes and also in conjunction with 2D transverse space charge calculations in 3D tracking codes. 2D transverse models, including bunch factor effects, are the most widely used for calculation in rings. If transverse properties vary longitudinally or transverse impedances are of interest, 2.5D models are necessary. These consist of a series of 2D model slices along the longitudinal direction that are connected by a common boundary condition. 2.5D models provide both the longitudinal and transverse space charge force components. All the above models are valid only for long bunches in which the bunch length greatly exceeds the beam pipe radius. Finally, there are full 3D space charge models. These are essential for short bunches, where the longitudinal and transverse dimensions are comparable, and are widely used in linac studies. Computational requirements rise steeply with the dimensionality of the model, so it is important to adopt the simplest model that contains the necessary physics.

\* ORNL/SNS is managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725

## REPRESENTATION AND DISCRETIZATION

Important issues that limit the applicability of space charge models are their representation of the beam distribution and the numerical discretization of the problem. Because the space charge forces depend on the charge distribution in the beam, the representation of the beam distribution in a simulation is very important. One simple class of space charge models, called envelope or particle core models, represents the space charge distribution as a uniform ellipsoidal core that propagates according to the envelope equation. The tracked particles feel the space charge force due to the propagating core. This force is linear inside the core. Envelope models are computationally fast and easy to apply. They have been used to study halo generation by mismatched beams and also the approach to the half integer resonance. One limitation of such models is that a constant emittance is specified in the envelope and thus constrains the evolution of the core. Accordingly, envelope models are simple, but far from realistic.

Conceptually, the opposite approach is to use the numerical distribution of tracked particles to provide the space charge forces. The implication in using this approach is that the tracked beam distribution realistically describes the actual beam distribution, which may require tracking many particles. Such methods, often called particle-in-cell (PIC) methods because of the techniques employed to evaluate the collective forces, are much more computationally intensive than envelope models and, as we shall see, they introduce discretization at more levels.

An intermediate class of methods for handling space charge involves the use of analytic or smoothed distributions for space charge evaluation, where the parameters of the smoothed distribution are fitted to those of a tracked beam consisting of particles. Such hybrid methods can, in principle, enjoy the speed and simplicity of envelope models while having parameters that evolve with the tracked beam distribution. A disadvantage could be that, depending on the details of chosen analytic representation or smoothing function, important features of the tracked distribution may be lost.

Any numerical space charge model will suffer from discretization error, but some methods are subject to more error than others. Time discretization is a feature of any space charge simulation, regardless of beam representation. While space charge forces act continuously in classical dynamics, simulations apply them as impulses, separated by single particle transport. If the time between impulses is too large, accuracy is lost. For example, nearby particles may become anomalously close in the single particle transport step. At the very least, it is necessary to include many space charge evaluations per betatron or synchrotron oscillation.

An additional level of discretization occurs when using the tracked particles directly to provide the charge/current distribution. Real accelerator bunches typically have  $10^8 - 10^{14}$  particles, while accelerator simulations may use  $10^4 -$

$10^9$  macroparticles, with the lower end of this range being typical on workstations or small clusters. The impacts are an increased graininess of the force distribution and an increased potential for large binary collisions. Both of these effects introduce noise, or diffusion, into the particle evolution. The problem of the enhanced binary collisions is often handled by introducing into the inter-particle force Green's functions artificial smoothing parameters that reduce the force at close range.

A final source of discretization in many PIC methods relates to the use of spatial meshes. The straightforward direct evaluation of pairwise forces between  $N$  particles requires  $O(N^2)$  computational work. Faster  $O(\sim N)$  methods have been developed. The most popular of these methods involve the distribution of the particle charges to a selected set of mesh points. This is followed by the solution of the resulting potential or forces at the mesh points, and then the interpolation of the forces back to the particle locations. Computational meshes are used in multigrid methods and also in algorithms using fast Fourier transforms (FFTs). Many of these are described in Refs. [2] and [3]. The approximations in distributing the charges to the mesh points and then interpolating the resulting forces from the mesh points back to the particles introduce additional noise into the space charge calculation that can be seen in the motion of individual particles. This is illustrated in Fig. 1, where the horizontal motion of three particles, initially at  $(x,y) = (3,0)$ ,  $(0,0)$ , and  $(0,3)$  mm, selected from a cylindrical constant density beam of radius 7 mm in a uniform focusing channel, is plotted over 1000 betatron oscillations at the bear tune. The space charge tune reduction here is about one third. The space charge solution is carried out using a 2D FFT-based PIC solver. Without discretization noise, the amplitudes would remain constant. However, even with 400000 particles in a 2D problem, the effects of noise in diffusing the individual particle orbits are soon apparent.

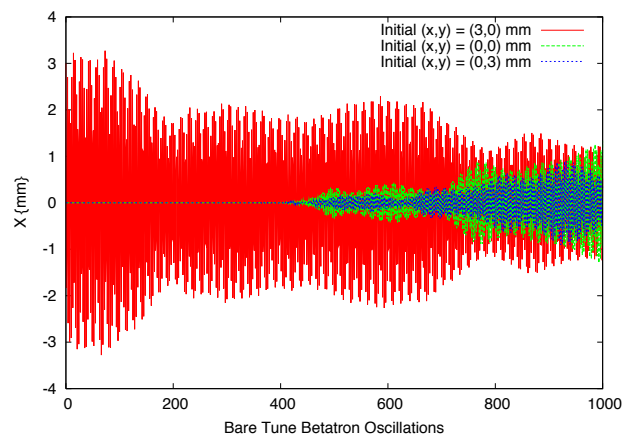


Figure 1. Horizontal motion of three particles in a uniform focusing channel with constant space charge, calculated using an FFT-based PIC algorithm. Without discretization noise, the amplitudes would remain constant.

Within the realm of fast grid-based methods, techniques have been devised to reduce the noise by using the grid for evaluating the forces of distant particles and calculating the forces due to nearby particles pairwise [2].

Another fast method that uses pairwise force evaluations for nearby particles eliminates grid-based discretization errors completely. The fast multipole method [4] expands the individual particle potentials as multipoles at the centers of a collection of square gridded cells containing the particles. These expansions are then shifted and accumulated through a hierarchy of coarser “parent cells” and the resulting totals are converted to Taylor series expansions as they are shifted backwards through the hierarchy of “child cells”. The result is a set of local Taylor series expansions for the potential and force within each starting cell. This method solves the N-body force evaluation to machine precision when enough terms are retained in the multipole and Taylor series expansions. Even so, the discretization effects of the time step and the numerical particle distribution remain.

### OPTIONS FOR LONG TIME SCALES

Given the problems of properly representing the beam distribution and reducing the discretization noise, the question remains: What steps can be taken to extend space charge calculations reliably to long time scales? One possibility is the sledgehammer approach. It is possible to use smaller time steps, more particles, and finer meshes to reduce the level of noise due to discretization. This is feasible to some extent with the help of modern computer technology: clusters, GPUs, etc. Still, this approach is expensive and only delays the inevitable effects of the numerical noise. Another approach to reduce noise from discretization is to eliminate the discretization. At present, FFT-based methods are extremely popular for solving Poisson’s equation. The fast multipole method can eliminate grid discretization errors associated with FFTs. However, the effects of the graininess of the particle distribution and discrete time steps are still present. Another approach with grid-based methods is to study different binning or smoothing algorithms for distributing space charge from the numerical particle distribution to the grid. Like low pass filters, such methods can alleviate noise due to gridding and the particle representation. One example is the template method of Vorobiev (presentation in Ref. [1]) in which the binned point charges on the grid are replaced by smoothed elements. Simplified or analytic distributions, based on statistically calculated parameters of the macroparticle distribution, are also worth exploring. For example, Figure 2 shows the evolution of the vertical beam size in three different tracking calculations through the SNS MEBT. Two of the calculations were carried out using grid-based 3D space charge models (PICNIC and SCHEFF) in the Parmila code, and the third utilized a uniform ellipsoid with parameters taken from tracking a distribution with 10% as many particles as in the 3D calculations. The RMS beam sizes from the three methods are virtually identical, although the ellipsoidal calculation required only 20% as much computer time as PICNIC and

40% as much as SCHEFF. Of course, these linac calculations are for short times, but similar hybrid models should be explored for calculations at long times.

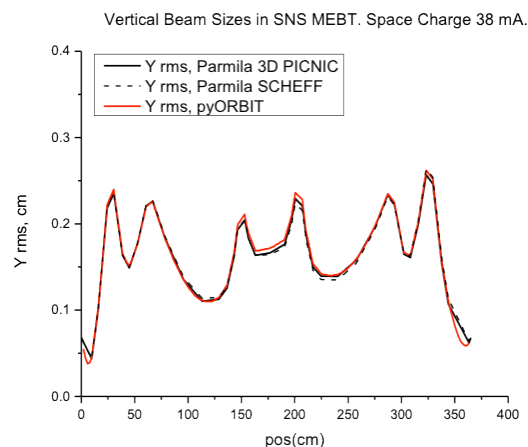


Figure 2. Vertical beam sizes from particle tracking calculations in the SNS MEBT. Space charge models include 3D PICNIC and SCHEFF PIC solvers and an ellipsoidal uniform density model with parameters set to those of a tracked distribution.

We are exploring all of these approaches in the ORBIT Code. At present, we have completed writing and are now testing a fast multipole method package. The intent is to compare the speed and numerical noise of this method with those of our existing FFT-based PIC solvers. In the future we plan to develop a number of fast hybrid models for long time scale calculations. All of these methods must be compared through careful benchmarking. As a final remark, we note that an excellent set of benchmark tests for space charge has been developed by Giuliano Franchetti, and can be found on-line [5]. These provide a thorough set of tests for space charge models, including some that involve long time scales.

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