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Recent Improvements to the ASTRA Particle Tracking Code

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Abstract

The Astra simulation code has been successfully used in the design of linac and rf photoinjector systems utilizing beams with azimuthal symmetry. We present recently implemented changes to Astra that allow tracking of beams in beamlines without the assumption of any symmetry. The changes especially include a 3D mesh space charge algorithm and the possibility to import 3D electromagnetic field maps from eigensolver programs.

INTRODUCTION

Program description

The computer program Astra (A space charge tracking algorithm) originally developed by one of us (K.F.) has been extensively used in the framework of photoinjector designs [1] and benchmarking of experimental data [2]. The program executables are freely available on various operating systems (Linux, Mac X, Solaris and Windows) from the world wide web page http://www.desy.de/~mpyflo/Astra. The Astra suite of programs consists of the particle tracking code together with an input distribution generator and several graphical user interface post-processors based on the PGPLOT library [4]. Astra tracks point-like macroparticles (currently possible species are electrons, positrons, protons and hydrogen ions) through a user defined external fields taking into account the space charge field of the particle cloud. The tracking is based on a Runge-Kutta integration of the fourth order with fixed time step. The beamline elements are set up w.r.t. a global Cartesian coordinate system. The program is a three-dimensional code, but its first version allowed the calculation of the space charge field only for round beams on a cylindrical grid and all the external fields (apart from quadrupoles) were cylindrical symmetric.

Note on particle emission

The dependence of the charge emission on the electric field at the cathode surface due to the Schottky effect can be simulated. At any time step during the emission, the charge of the macroparticles is calculated according to the relation: $Q_{\text{Macroparticle}} = (Q_{\text{Total}} + Q_{\text{Shottky}}E_{\text{acc}})/N_{\text{Particles}}$ wherein $E_{\text{acc}}$ is the actual accelerating field (including both RF and space charge) in the center of the cathode, $Q_{\text{Shottky}}$ is a user defined parameter, $Q_{\text{Total}}$ and $N_{\text{Particles}}$ is the bunch charge and number of macroparticle used to model the bunch. Thus a self-consistent emission is simulated. The linear parameterization w.r.t. the accelerating field is motivated by measurements performed on Cs$_2$Te photocathodes reported in Ref. [3].

3D CAVITY ELECTROMAGNETIC FIELD

In the case of cylindrical-symmetric field, the radio-frequency field for a standing wave accelerating structure (TM modes) are described by the on-axis longitudinal electric field $E_z(z, r = 0)$ the radial electric and azimuthal magnetic fields are then computed from $\nabla E = 0$ and $\nabla \times B = dE/dt$ respectively.

To accommodate more general problem, e.g. simulation of deflecting mode cavity or asymmetric rf-field, arbitrary external fields defined on a three-dimensional mesh can directly be loaded into Astra. Such field are generally obtained from electromagnetic eigensolvers. Given the six components of the electromagnetic field vector $[\Re(E), \Im(B)](x_1, y_1, z_1)$ tabulated on a grid node $(i, j, k)$, the field experienced by a particle with coordinate $x \approx (x, y, z)$ is obtained via a tri-linear interpolation of the tabulated field, and the time dependence is introduced following

$$\begin{bmatrix}
E \\
B
\end{bmatrix}(x; t) = \begin{bmatrix}
\Re(E) \sin(\omega t + \varphi) \\
\Im(B) \cos(\omega t + \varphi)
\end{bmatrix}(x),$$

wherein $\omega/(2\pi)$ and $\varphi$ are respectively the frequency of the rf-structure and the phase of the electric field. Practically, each of the field components is given in a separate ASCII file whose header describes the mesh geometry. Such a description enables the user to defined the different field components not a fortiori on the same mesh.

Since Astra allows the overlap of cavity fields onto the same position, the simulation of traveling wave structures described by 3D fields is straightforward if included as a superimposition of two standing wave fields with the proper phase and amplitude relations [5].

An example of application of the 3D rf-field map option has been the simulation of the beam dynamics in the L-band rf-gun cavity used at TTF 1 and FNPL facilities. This 1+1/2 cell cavity has an input power coupler that induces rf-field asymmetry in the full cell; the 3D electromagnetic field map has been simulated using HFSS [6] and was used in ASTRa to study the impact of the induced asymmetry. In Fig. 1, we compare the vertical phase space obtained...
after tracking the particle distribution in the case of (1) a cylindrical symmetric field and (2) the HFSS 3D field map.

**3D SPACE CHARGE PARTICLE-MESH ALGORITHM**

We have implemented a 3D space charge algorithm to handle beam distributions without the assumption of azimuthal symmetry. The algorithm does make the usual assumptions: that no dipole or bending magnet element exists along the beamline, so that the geometry is essentially Euclidean; that conducting walls are located far from the beam, so that free space boundary conditions apply in all directions; and that the velocity distribution in the beam rest frame is non-relativistic, so that an electrostatic approximation is valid. With these assumptions, the underlying Poisson equation is solved by a simple, volume-weighted particle-mesh (PM) algorithm. The PM algorithm is well known [7]. We use a variant of the field solver that is based on Fourier expansion, convolution with a grid Green function, and Fourier synthesis to determine the electrostatic potential on the grid nodes [7, 8]. The rest frame electric field components are calculated by second-order differencing, and tri-linear interpolation calculates the field values at the individual particle locations. The resulting electric and magnetic fields (neglecting the longitudinal B-field component) are applied in the laboratory frame with the remainder of the external fields.

This algorithm is known to suffer from errors due to aliasing effects from the use discrete Fourier transforms. There are several known methods for dealing with this error. The issue may be successfully handled with the brute force technique of using very large meshes and correspondingly large number of particles. By ensuring that fine details in the beam distribution vary over at least several mesh cells, the highest frequency error components are excluded. Widely used [7, 9] is the method of truncating the Green’s function at the edge of the first Brillouin zone, or otherwise introducing a cutoff mechanism in the frequency domain to remove these high-frequency errors. We employ a similar technique by applying a charge-conserving smoothing kernel to the mesh nodes after the charges have been distributed onto the grid. We also apply a technique where the solution for the scalar potential is then differenced twice to obtain the charge distribution. This ‘new’ distribution is compared with the original one. The difference is computed and fed back into the field solving algorithm with the original charge distribution to counter the errors. In effect we are executing the field solver twice (or more, if addi-
tional iterations are warranted). However, the Astra particle tracking engine utilizes an algorithm that rescales the solution to Poisson’s equation, and need not execute the complete field solver at every time step.

In Figure 2 we compare the phase spaces calculated with the 2-d and 3-d mesh algorithm for the case of a cylindrical symmetric beam; the agreement between the two algorithms is good.

**OUTLOOK**

The 3D space charge algorithm will be released in a forthcoming new version of Astra. In a close future we also plan to introduce the dipole magnet element to enable simulation of magnetic bunch compression systems and analyzing spectrometers.

**REFERENCES**


[4] The PGPLOT library is freely available from the world wide web: http://astra.caltech.edu/~tjp/pgplot


