

## PARTICLE-IN-CELL NUMERICAL SIMULATIONS OF PARTICLE DYNAMICS IN BEAMS AND ECR SOURCES

G. Shirkov, V. Alexandrov, V. Shevtsov, JINR, Dubna, Russia

### *Abstract*

Finite particle methods allow studying the detailed beam and plasma characteristics, the distribution function of particles, the nonlinear self and external fields. A particle-in-cell method is one of finite particle methods and it is the most effective for simulations in physics of plasma and charged particle beams.

The basement and recent development of the particle-in-cell method are presented. Two examples illustrate the application of the particle-in-cell method in beam dynamics and plasma physics.

### INTRODUCTION

Mathematical modeling and numerical simulation of beam dynamics and multicomponent plasma with consideration of space charge effects are of great important in the connection with modern trends of investigations in the physics of particle accelerators and ion sources. These problems belong to the electrostatics of continuous medium.

The distribution of particles in the phase space of coordinate and velocities is described by the distribution function. In consideration of the particles' space fields and of impact processes that take place in ion sources and beams, the motion of charged particles is described in a generalized form by a system of self-consistent kinetic equations completed by Maxwell equations.

Finite particle methods are the most powerful methods for the numerical simulation of motion of continuous medium, gas and plasma dynamics, dynamics of charged particle beams. These methods allow studying the detailed characteristics of continuous medium, taking into account the distribution functions of particles (spatial, velocity and energy distributions), real self and external fields, particle-particle interactions and many other effects.

The most of finite particle methods are Euler or Lagrange methods [1]. In the Euler method for a continuous medium the physical system is considered at definite mesh points which coordinates are independent variables. In time course, the mesh points pass various parts of the medium. In the Lagrange method, the motion of particles is observed. The entirety of phase trajectories of these particles give the complete information about considered process. Particle numbers or their initial phase coordinates are used as independent or Lagrange variables. It is assumed, that the initial and actual phase space coordinates directly connected with the trajectory equations. The combination of both methods is the most effective for simulations in the physics of plasma or charged particle beams. In the particle-in-cell methods, for example, the motion of particles is described in Lagrange variables and, simultaneously, the particle densities, currents and fields are determined in a stationary mesh or in Euler variables.

The modern particle-in-cell schemes have two or three dimension (2D or 3D) geometries. All the volume of particles is divided by a set of mesh cells and an every point of the considered space belongs to one of existing cells of a mesh. The fixed and time independent set of cells is usually used for this tasks. A number of finite particles presents the continuous medium of plasma or beam. Each finite particle has a mass, charge state and coordinates in the phase space of motion. In order to describe atomic processes and effectively calculate Coulomb interactions among the charged particles the best way is to have densities of each type of physical particle in the mesh. A sufficient number of finite particles of each species should be in each cell for this purpose.

The electrostatic potential  $U$  for the medium simulation is described by the Poisson's equation. Double Fourier transformation is the most effective way to solve the Poisson's equation on the grid of cells.

Self-consistent description of medium is provided by simultaneous solution of equations of particle motion in the field, obtained from Poisson's equation at every integration step. The Cauchy-Dirichlet problem should be formulated to solve these equations.

Particle-in-cell model was successfully applied for the simulations of multicomponent beam and plasma dynamics of electron synchrotron resonance (ECR) ion source.

### BEAM DYNAMICS

A program library based on the particle-in-cell method (MCC code) [2] was applied for simulations of transverse dynamics of an argon ion beam in the beam line from the 18 GHz ECR Ion Source to the linear RFQ accelerator of the RIKEN Beam Factory. The line consists of an Einzel lens (EL), a horizontal bending magnet (BM) with poles, Faraday cup (FC) and a solenoid (SRFQ).

The results of numerical simulation of the multicomponent ion beam dynamics in this channel were published in [3]. It was shown that EL is not effective for multicomponent low energy ion beam. A new beam line with a solenoid S2 instead of EL is proposed, simulated and optimized.

The simulation and optimization of ion beam dynamic was carried out for the beam of argon ions of 5 species:  $\text{Ar}^{6+}$ -  $\text{Ar}^{10+}$ . The experimental charge state distribution of the ion beam after BM, ion beam emittance  $100 \text{ mm } \Delta \text{ mrad}$  and momentum spread  $\Delta p/p = 0$  were used as initial data. Particles in the phase planes were generated according to the micro-canonical distribution. The kinetic energy of ions was 11 Z keV (here Z is the ion charge). The magnetic field in BM corresponds to the equilibrium orbit for  $\text{Ar}^{8+}$ .

It was shown that secondary electrons are accumulated in the beam if there is no any external transverse magnetic or electric field in the beam line [3]. These electrons reduce space fields and improve the beam transmission in the channel. A factor of neutralization  $FN$  was introduced in simulations for taking into account the influence of secondary electrons on the beam transmission.

The optimization of S2 parameters (location and magnetic field) was carried out to achieve the maximum capture of beam current into the RFQ acceptance. The dependence of accepted current on the neutralization factor  $FN$  was studied. The magnetic field induction was varied in the limits: 0.15...0.3T in S2 and 0.25...0.35T in SRFQ. The results of optimization for  $I_{ext} = 6mA$  are presented in Figs. 1 and 2.

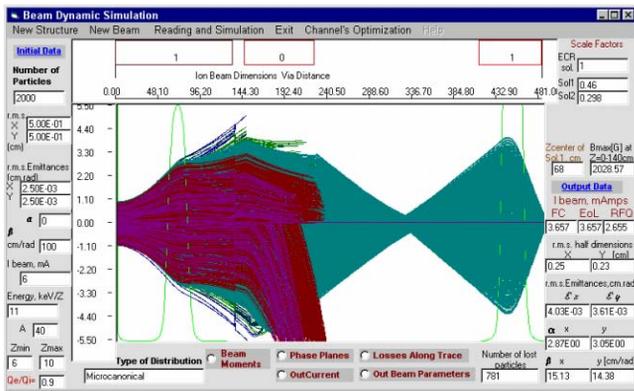


Figure 1. Beam trajectory after optimization.

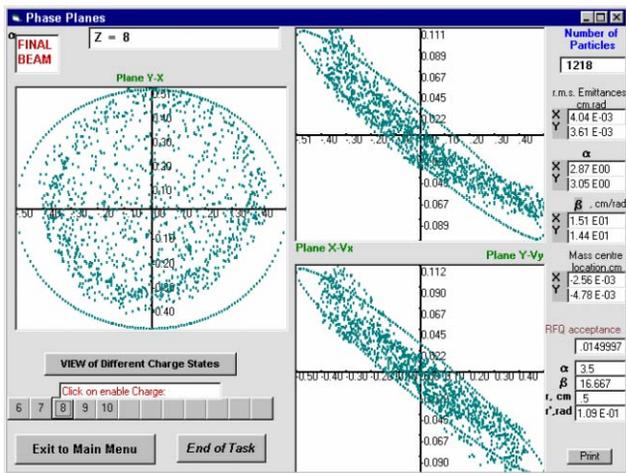


Figure 2. Beam cross section and phase planes

Beam line simulation and optimization have shown:

- € numerical simulation with  $NF \sim 0.9$  of the beam are in the best coincidence with experimental data;
- € maximum acceptance of ion beam current into the RFQ is about 70-80% of the beam current on FC.
- € maximum beam current into the RFQ acceptance can be provided by the beam with double waist envelope in FC region of line.
- € solenoid instead of Einzel lens is able to increase the beam current at the RFQ in a factor of 2.5 - 3. The first test of S2 without any optimization has improved the beam current in a factor of 1.6.

## PLASMA OF ECR ION SOURCE

The project "Numerical simulation and optimization of ion accumulation and production in multicharged ion sources" was fulfilled in 1999 – 2001 at International Science and Technology Center (ISTC). This project was carried out in the frame of Beam Factory at RIKEN. The physical substantiation of the ISTC project was prepared and published in 1997 [1].

A goal of the project is the creation of a new generation 3D model and codes for the numerical simulation based on the particle-in-cell method.

### Physical and mathematical models [4].

The difference of electron and ion velocities is 2 – 3 orders of magnitudes due to their different masses and energies in the plasma. The integration of the equations of motion for the electron component requires a time step of about  $10^{-12}$ – $10^{-11}$ s. This is the main limitation for computer simulation of ion accumulation in plasmas with a time scale of 10 ms.

The electron motion consists of fast Larmor rotation with frequencies of about  $10^{10}$  Hz and relatively slow drift of the electron trajectory in the magnetic trap of the ECR source. The Larmor rotation does not determine peculiarities of slow rate processes of ion production and accumulation in the ECR source. Therefore, it is possible to exclude fast rotation of a particle around a small Larmor circle from the equations of motion, with the aim to sufficiently increase the integration step of the problem to be solved. The theory of “guiding center approximation” of averaging of fast electron rotation in the magnetic field [5], was developed and applied for simulation of the ECR plasma.

Electrical and magnetic fields are created by a system of coils, permanent magnets and special electrodes in the ECRIS. These fields can be calculated analytically or numerically, or can be fixed as an experimental data table. A quadratic interpolation is used to calculate fields in every point inside of cells.

The physical model is based on differential equations of motion for the charged particles and the Poisson equations for the self and external fields [1]. The self (space) fields of particles is obtained from direct solution of Poisson's equation for an electrostatic potential at every time step, in a cylindrical system of coordinates with Dirichlet boundary conditions at the conductive surface, and with Neumann conditions at the axis. The double Fourier transformation is used to solve the Poisson's equation. The procedure of quadratic interpolation is used to calculate the values of self-fields in every point of every particle position. The density distributions of every plasma component are calculated at every integration step on these mesh cells, in order to provide self-consistent solutions of equations of particle motion and fields in the plasma.

Particles of all masses and charge states are available in the consideration: ions of all charge states of all elements, different kinds of neutrals, electrons. Basic inelastic atomic processes providing the change of a charged

particle distribution are: ionization of neutral atoms and ions by electron impact; charge exchange of ions with neutral atoms; recombination among ions and electrons.

The following model conceptions of ECR plasma components are used in consideration [6, 7]:

- € the electrons have a few components: cold primary electrons of tens or hundreds of eV; a main electron component of keV energy which produces highly charged ions and, according to the experimental data, a component of superhot electrons of tens or hundreds of keV;

- € electrons undergo the RF heating on a surface with ECR conditions in the magnetic field;

- € the ECR plasma is neutral or quasi neutral in every point of the volume.

- € all ion components have Maxwellian energy distribution with a common temperature in the plasma due to intensive elastic Coulomb collisions.

*Testing of the library of computer codes.*

The code library with the name EPC (ECR source Particle Code) to simulate ECR sources has been prepared. First tests of the library are presented in Figs. 3 and 4. These figures show results of a model simulation of nitrogen ion production and accumulation during about  $50\sigma_s$ , have been taken from the computer screen and can give some impressions of the user interface: numbers of macro particles, items of the user menu, charge states of ions etc. The initial data for this numerical experiment for the 18 GHz ECR source were as follows:

- € density of nitrogen neutrals  $2 \cdot 10^{10} \text{ cm}^{-3}$ ;
- € average initial energies of electrons and neutrals 10 eV and 0.03 eV correspondingly,
- € longitudinal magnetic field with trap longitudinal configuration ( $B_z = 0.47\text{T}$  at the center of chamber  $Z = 0$  and  $B_z = 1.5\text{T}$  at  $Z = \partial 12\text{cm}$ ) and magnetic field of permanent sextupole were used in computations,
- € initial amount of macro particles 50000,
- € mesh sizes on X-, Y- and Z- axes 4mm x 4mm x 8mm.

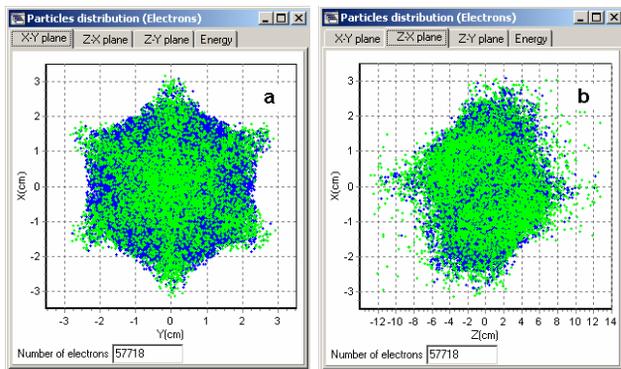


Figure 3. XY (a) and XZ (b) distributions of electrons.

Spatial distributions of two electron components are shown in Fig. 3: (a) XY and (b) XZ planes. The blue colour of macro particles corresponds to a low energy electron component and the green colour corresponds to high energy species. Fig. 4 presents the ionization dynamics of  $N^{1+} - N^{7+}$  ions and neutrals (red colour line).

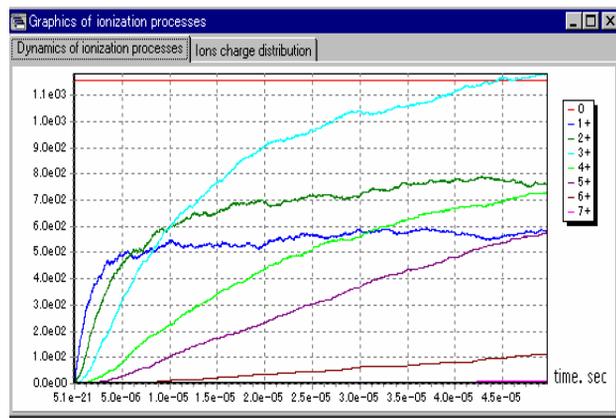


Figure 4. Ionization dynamics of nitrogen ions

Simulations of ECRIS plasma have shown:

- € detailed and exhaustive spatial description of fields and particle motion and interaction in the ECR source plasma requires a full-scale 3D task to be solved;
- € computer executing time of simulation is mostly determined by the time step of integration ( $\sim 10^{-10}$  s) of electron equations of motion and by the number of macro particles for the electron component representation;
- € time range of production and accumulation of heavy highly charged ions is about 1 – 10 ms and it requires about  $10^8$  time steps of simulation;
- € 2D task requires at least  $2-3 \cdot 10^5$  and full-scale 3D task requires at least of  $3-5 \cdot 10^6$  macro particles in the simulation;

The most significant difficulty of 3D problems is a large computation time. High power multiprocessor computers with parallel computation only are able to satisfy the requirements of a 3D simulation. The development and adaptation of numerical methods and computer codes for parallel computations at a multiprocessor computer are necessary for the full-scale 3D task. **REFERENCES**

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