IBSIMU: A three-dimensional simulation software for charged particle optics[a]

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A general-purpose three-dimensional (3D) simulation code IBSIMU for charged particle optics with space charge is under development at JYFL. The code was originally developed for designing a slit-beam plasma extraction and nanosecond scale chopping for pulsed neutron generator, but has been developed further and has been used for many applications. The code features a nonlinear FDM Poisson's equation solver based on fast stabilized biconjugate gradient method with ILU0 preconditioner for solving electrostatic fields. A generally accepted nonlinear plasma model is used for plasma extraction. Magnetic fields can be imported to the simulations from other programs. The particle trajectories are solved using adaptive Runge–Kutta method. Steady-state and time-dependent problems can be modeled in cylindrical coordinates, two-dimensional (slit) geometry, or full 3D. The code is used via C++ programming language for versatility but it features an interactive easy-to-use postprocessing tool for diagnosing fields and particle trajectories. The open source distribution and public documentation make the code well suited for scientific use. IBSIMU has been used for modeling the 14 GHz ECR ion source extraction and for designing a four-electrode extraction for a 2.45 GHz microwave ion source at Jyväskylä. A grid extraction has also been designed for producing large uniform beam for creating conditions similar to solar wind. The code has also been used to design a H^- extraction with electron dumping for the Cyclotron Institute of Texas A&M University. *© 2010 American Institute of Physics.* [doi:10.1063/1.3258608]

I. INTRODUCTION

Numerical simulation is a standard way of designing ion optical devices in the field of ion source and accelerator physics. Many two-dimensional[1,2] (2D) and three-dimensional[3,4] (3D) computer programs with long histories exist for modeling these problems. Still, new codes are being developed for various problems that cannot be solved using existing programs with limited features. The development of ion beam simulator (IBSIMU) started from such a need at LBNL in 2004. The code was used for designing a slit-beam plasma extraction and nanosecond scale chopping for pulsed neutron generator.[5] Later on the development of the code has been continued at the University of Jyväskylä, Department of Physics (JYFL) with a drive to making the code modular and suitable for many different types of problems. The code has been documented and released with an open source license, which makes the code well suited for use in the scientific community.[6] This paper provides an overview of the code. The versatility of the software is highlighted by describing the recent applications it has been used for.

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II. CODE OVERVIEW

The general-purpose ion optical code IBSIMU is capable of solving electric fields in one-dimensional, 2D (planar or cylindrical symmetry), or full 3D simulation geometries. The definition of solids is done using mathematical description, AutoCAD DXF-file import (2D only), or constructive solid geometry. The simulation domain is discretized with a rectangular mesh with constant step size.

Electrostatic potential calculation is based on solving Poisson's equation using finite difference method (FDM) on the nodes of the mesh. To achieve smooth electric fields on the solid edges, the edge nodes within the solids are adjusted to virtual potentials using subnode information about the geometry. On the edges of the simulation domain, the solver supports Dirichlet and Neumann (first and second order approximations) boundary conditions. The calculation can also include the generally accepted nonlinear plasma model for positive ion extraction,[7] where thermal background electrons of the plasma are modeled analytically in Poisson's equation,

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0}, \tag{1}$$

where $\rho = \rho_{\text{ion}} - \rho_{e0} \exp[(\phi - \phi_P)/(kT_e/e)]$. The model parameters are plasma potential ϕ_P and electron temperature T_e. Ion charge density ρ_{ion} is calculated from beam current density and electron charge density ρ_{e0} is set to ρ_{ion} at plasma potential.

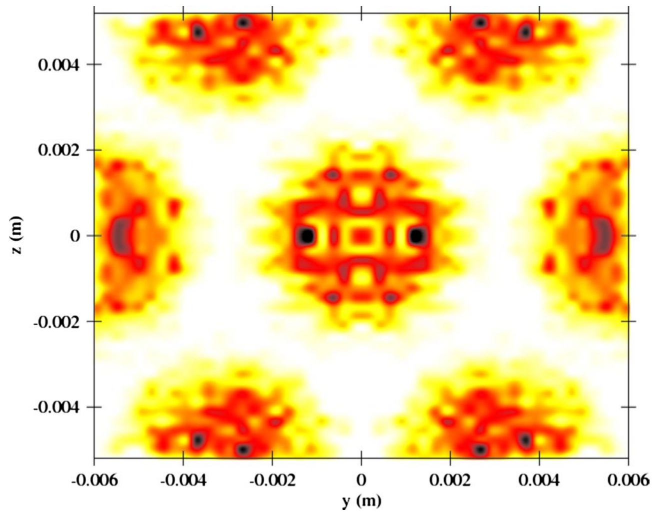

FIG. 1. (Color online) Profile plot of the beam extracted through the grid extraction at $x=0.018$ m.

The code has several nonlinear solvers for calculating the electrostatic potential. The primary solver for 3D is based on iterative stabilized biconjugate gradient (BiCGSTAB) method[8] with ILU0 preconditioner. For 2D fields, the most efficient solver is direct LU decomposition solver UMFPACK.[9] A classic successive over-relaxation solver exists for reference purposes.

Particle tracer of the code works by integrating the equations of motion, derived from Lorentz force, with an embedded Runge–Kutta Cash–Karp (fourth and fifth order) method featuring automatic step-size adjustment for required trajectory accuracy. The implementation of the Runge–Kutta method is used from the GNU Scientific Library.[10] The particle tracer is multithreaded for high efficiency calculation on modern multicore CPUs. The particle tracer algorithm finds all the mesh squares the trajectory passes through and deposits the charge of the particle on the four (eight in 3D) surrounding mesh nodes. The same procedure checks for collisions in the mesh square.

The electric field needed for particle trajectory calculation is obtained by numerical differentiation and interpolation of potential using 9 closest neighboring mesh nodes (27 in 3D). Special measures are adopted close by to the solids and simulation boundaries to achieve continuous electric field everywhere in the geometry, which is a prequisite for smooth trajectory distributions inside beams. Magnetic fields can also be imported from other programs.

The simulation sequence for self-consistent beam optics starts with an initial guess. Typically the starting point is solved from Poisson's equation with $\rho=0$. In plasma extraction problems there is also an initial plasma volume with potential fixed to ϕ_P. The simulation proceeds with calculating particle trajectories and space charge density. The space charge is used in Poisson's equation to solve a new potential map. This sequence is repeated until the solution converges to required precision.

IBSIMU is not distributed as a precompiled binary contrary to commercial software. It is used as a computer library through a C++ programming interface. The code is well structured into separate modules, which enables a wide range of problems to be solved. The built-in modules can be replaced if customization is required or the modules can be integrated into other codes. Programming interface also enables batch processing and automation of simulations. Even though the code is rich in features, it is simple to use. It contains many ready-made diagnostic tools for particle and field data. Data exporting and visualization can be performed using an interactive tool.

IBSIMU has been successfully benchmarked with 2D and 3D electric field and particle problems against PBGUNS,[1] SIMION,[4] and analytical cases. The plasma extraction calculations have been verified by comparing to PBGUNS in 2D (planar and cylindrical cases). Also the benchmarking described in Ref. 11 has been performed successfully.

III. APPLICATIONS

The code has been used for several applications at JYFL, including the modeling of the 14 GHz electron cyclotron resonance (ECR) ion source extraction. The simulations suggest that the problems in the original extraction design for the ion source is one of the reasons for the beam quality issues we are experiencing on the injection beam line of the cyclotron. Improved extraction designs are being simulated.[12]

A new 2.45 GHz microwave ion source is under development at JYFL. The test bench extraction system consists of four electrodes in a configuration with extraction diode and a

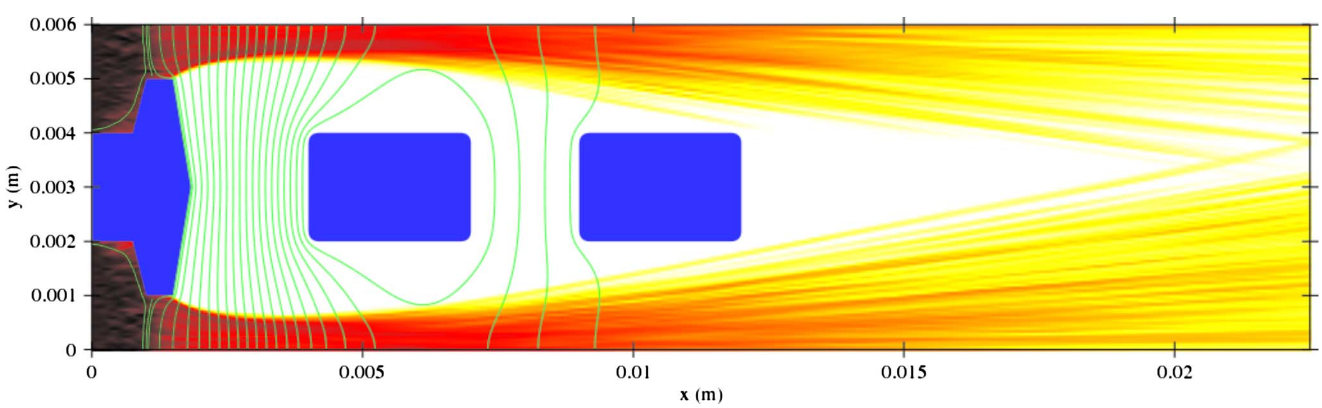

FIG. 2. (Color online) Simulation of the center of the grid extraction with space charge compensation starting from $x=0.013$ m.

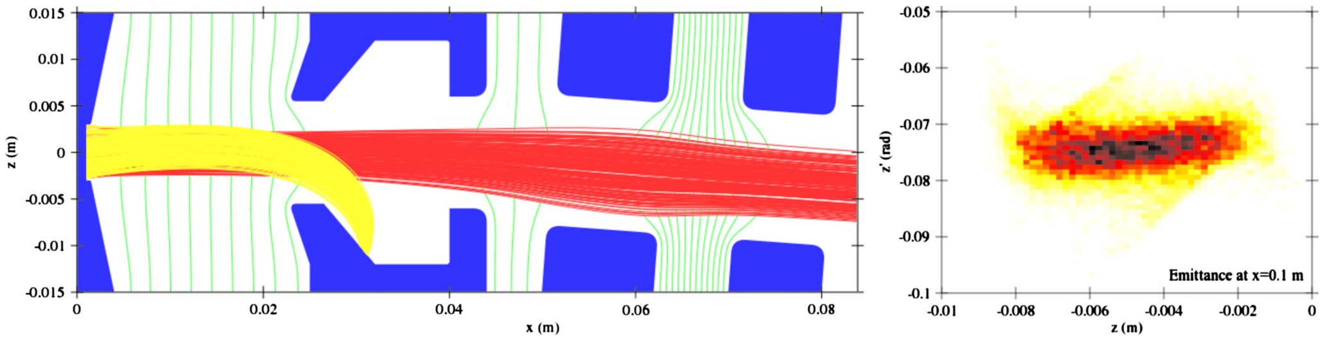

FIG. 3. (Color online) 3D simulation of H^- LEBT with 12 keV final beam energy. The coextracted electron beam is deflected into a water-cooled electron dump by a magnetic filter at the energy of 6 keV. The ion beam is symmetric and has little aberrations at the end of the simulation.

decelerating Einzel lens. The design base line is 5 mA beam extraction from a ∅3 mm aperture. The extraction has been designed to be versatile and easy to match to different plasma densities. The solenoid magnetic field of the ion source has been taken in account in the simulations.

An alternative grid extraction was developed for the microwave ion source for producing large uniform beam for creating conditions similar to solar wind in laboratory. The solar wind, which consists mainly of protons and electrons, has speed in the range of 300–600 km/s (500–1900 eV for protons) close by to earth. The extraction was chosen to be designed for H^+ beam with a final energy of 1 keV. A triode extraction was selected to enable space charge compensation starting right after the electrodes, which is necessary for the application. The grid is formed by 2 mm diameter extraction holes (4 mm holes in puller and ground electrodes) packed hexagonally with center-to-center spacing of 6 mm. The total beam size is ∅75 mm with about 150 beamlets. The simulation of the extraction cannot include as many beamlets when run on a desktop computer. Therefore the study was separated into examination of center part and the boundary of the beam area. The beamlets merge starting from 2 cm from the extraction. The divergence of each beamlet is about 150 mrad. See Figs. 1 and 2 for simulation results.

The code has also been used in designing a H^- low energy beam transport (LEBT) for 1 mA beam with final energy varying from 5 to 15 keV for the Cyclotron Institute of Texas A&M University. The LEBT was designed and optimized in 2D with PBGUNS as IBSIMU does not have negative ion plasma extraction capability. The optimal geometry was found to be the one shown in Fig. 3. The puller electrode is at a fixed 6 kV potential with respect to the source. The decelerating Einzel lens is adjusted with required final energy. The geometry was modeled in 3D with IBSIMU by starting the beam from a solid surface with a shape of the plasma meniscus determined from the 2D simulations. The beam definition in 3D was adjusted to get a similar beam as in 2D at 5 mm from the plasma meniscus. In 3D, the simulations included a combined magnetic field of the filter magnets inside the H^- ion source and the uniform dipole magnetic field with a peak strength of 32 mT inside the puller electrode. The electrons are deflected by the magnetic field from the ion beam into a water-cooled dump inside the puller. The field also deflects the ion beam and therefore, the ion source and the puller electrode have to be tilted with respect to the beam line. The required angle of tilt varies from 4.1° to 4.9° with changing final beam energy because the dipole field is still nonzero at the Einzel lens. The variation of the tilt is so small that the tilt was made fixed. The beam deflection can be corrected by a slight adjustment of the puller electrode potential. The designed LEBT provides a compact extraction with electron removal, which meets the design goals and provides a clean, symmetric H^- beam. Experimental results have confirmed the simulations.

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