A Digital Computer Program for the Simulation of Positive or Negative Particle Beams on a PC.

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Abstract

PBGUNS, an expanded and improved version of the **SNOW2D** code for extracted ion beams will be described and demonstrated. The new code includes the electrode description and electron beam capabilities of the **SPEED** code. The new version includes positive and negative ion beam extraction systems and may include skew[1] (azimuthal energy particles) permitting the simulation of thermal effects in high energy plasmas, thermal effects in low energy electron beams, and the computation of x-x' emittance plots from axisymmetric simulations. Plasma electrons (and positive ions for negative ion beams) are simulated with background Boltzmann distributions. Electrodes are described with quadratic equations while potentials are solved by basic relaxation techniques on a rectangular array of squares. Smooth electrodes are created by extending fields into electrodes. A fine mesh covers the cathode and/or plasma-extraction region to furnish the additional accuracy required for the calculations near the particle emission surface. Axisymmetric and rectangular magnetic fields can be included in the trajectory calculations. It is written in FORTRAN 77, employing Calcomp-Versatec type plotting routines and is run on 386 or 486 IBM PC's with DOS Extenders. Generic FORTRAN 77 is used to facilitate the transfer of the program to other computers with only minor modifications.

I. INTRODUCTION

PBGUNS was originally developed from the SNOW2D and SPEED codes for the simulation of negative, sputter-source, ion beams and was then expanded to include regular plasma sources as well as thermionic and field emission relativistic and non-relativistic electron beams. The need to simulate the smooth curved emitter required for sputter ion sources required the smooth cathode routines used for electron beam simulations as well as a method of simulating the background plasma of positive ions and electrons. It was determined some time ago that a finer mesh was needed over the plasma region of an ion beam source, and recently the fine mesh was added to the SPEED program adding greater accuracy in the cathode region. The combined program is superior in accuracy and capabilities to either of its predecessors.

The 15,000 line FORTRAN program currently runs on an 80386 or 80486, IBM PC or clone, with at least 16 MBytes of memory, using DOS extenders. NDP-FORTRAN and NDP-PLOT (from Microway) are used for the compiler and the plotting capability. It will run small problems (100x50 arrays) in as little as 10 minutes, but may require several hours for very large problems (450x200) arrays, (about the limit for 16 MBytes of memory). Obviously larger memories would permit larger simulations and faster processors would require less time. All calculations are done in double precision (8 byte) arithmetic.

The potentials are solved on a two dimensional array using Poisson's equation in rectangular or axisymmetric configurations. The beam is simulated by computing representative trajectories (up to 7000) through the device. Space charge is computed from the trajectories and stored on a matrix identical to the voltage array. The cathode or plasma region for extraction problems is simulated on a second (and usually finer) matrix so that greater accuracy and resolution can be obtained, most importantly at the cathode or plasma surface. Thermal effects, which can be very important for either electron or ion extraction, can be simulated including skew (azimuthal) angular distributions.

II. THEORY

The voltages are computed by iteratively solving Poisson's Equation;

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

where V is the voltage, ρ the space-charge density, and ε_0 the permittivity of a vacuum (all in SI units). This is expressed in (second order) difference form for solution. For plasmas the space-charge term takes on the form;

$$\rho = \rho_e + \rho_{ni} + \rho_{pi} \tag{2}$$

where ρ_e is the electron space charge density and ρ_{ni} and ρ_{pi} represent the negative and positive ion space charge densities.

$$\rho = \rho_i + \rho_{eo} e^{\left(\frac{-eV}{kT_e}\right)} \tag{3}$$

Where k is the Boltzmann constant, T_e is the electron temperature and ρ_{eo} is the ion space-charge density at the injection plane. Solution of this very non-linear, and somewhat unstable problem, consists of repetitively solving Eq. 1 using the new values computed for the voltage on the left to upgrade the voltage used in the space-charge density term on the right. For negative ion beams the method of solution is similar but both the electrons and positive ions are represented by Boltzmann distributions.

The Lorentz force equation (4) or the relativistic Lagrange equation (5) can be solved in either cartesian coordinates (for rectangular configurations) or in axisymmetric-cylindrical coordinates for axisymmetric configurations.

$$F = -e(E + v \times B) \tag{4}$$

$$L = eV - e(A \cdot v) - m_0 \left(1 - \frac{v^2}{c^2}\right) \tag{5}$$

Where e is the electronic charge, m_0 the rest mass of the particle, B the applied magnetic field, **A** the magnetic vector potential, **v** the velocity of the particle, and c the velocity of light. These equations are expressed in difference form and solved for the successive points as a function of the preceding points and the electric and magnetic fields. All derivatives are expressed to second order in the equations and this seems to furnish sufficient accuracy.

Space charge limited emission is computed using Child's Law as modified by the Langmuir-Blodgett correction

$$J = \frac{4\epsilon_0}{9} \sqrt{\frac{2e}{m}} \frac{v^{\frac{3}{2}}}{x^2 \beta^2} \tag{6}$$

where x is two fine matrix square lengths in front of the cathode and β^2 Langmuir-Blodgett correction for curvature of the surface. Field emission current is calculated with the Fowler-Nordheim equation

$$J = 1.54e{-6} \frac{E^2}{W} e^{9.52\sqrt{W}} e^{\frac{6.36e9W^{1.57}}{E}} \tag{7}$$

where W is the work function in eV and E the electric field at the emission surface.

At the sputter surface a uniform emission of secondary ions in a cosine angular distribution and a sheath of several hundred Volts is assumed. The angular distribution is transformed through the sheath so that the energy distribution (normal and transverse to the surface) is preserved with the sheath voltage added. The voltage difference between the source of ions and the plasma potential is specified and is used in the transformation, but is not simulated in the voltage relaxation.

III. THE PROGRAM

PBGUNS is capable of simulating virtually any type of electron or ion beam. Ion beams can be extracted from plasma sources for positive or negative ions and sputter sources for negative ions as well as space charge limited ion sources.

The electrode configuration is described by quadratic equations which can consist of as few as 2 equations for a simple field emitter or as many as 60 equations for complex electrodes used in image intensifiers. The equations are defined by their endpoints and/or radius and center of curvature. The program relies on the fineness of the mesh to provide adequate resolution and requires electrodes to be at least one matrix square thick. The fine matrix covering the cathode or plasma region is automatically defined by the program with a resolution defined by the user.

Plots of the trajectories and equipotentials can be obtained either separately or overlaid on the same plot. Reduced annotation plots can be produced for show and tell. Current density distributions of the cathode and target are available and emittance plots can also be plotted.

IV. RESULTS

Results are in good agreement with experimental data or theory where available for comparison. The trends with negative ions have been to agree better with the data that is available as the beams seem to be more divergent than was obtained before the negative ion capability was added. The additional terms in the space charge calculation have pushed the plasma surface significantly forward over what was obtained with the positive ion simulation.

Significant efforts have been made to compare results with the experimental and theoretical data presented in the Chan[1], et al, paper. Their results indicate a beam larger than the experimental data do to their assumption of the flat emission surface from the plasma. **PBGUNS** yields quite similar results to their theoretical results *if* the parameters are adjusted so that a *nearly* flat emission surface is formed on the plasma. Their experimental emittance plot seems to indicate a significantly smaller beam than their experimental data. Reducing the background positive ion density (making the plasma surface concave) and lengthening the simulation has produced results, Figs. 1, 2, and 3 more similar to their experimental data. Figure 1 is the trajectory plot for a concave plasma surface. Figure 2 is the emittance plot obtained with a total of 25 particles injected at each point along the injection plane with 4.5 eV thermal energy in 14 degree increments. Figure 3 is the x-x' emittance computed using the same data with a technique similar, but not identical to Chan[1], et al. The results suggest that the ion temperature must be still higher and the emission may not be uniform.

V. REFERENCES

[1] Chan, C.F., et al.,"Dynamics of Skew Beams and the Projectional Emittance", *NIMPR*, A309, 112 (1991)

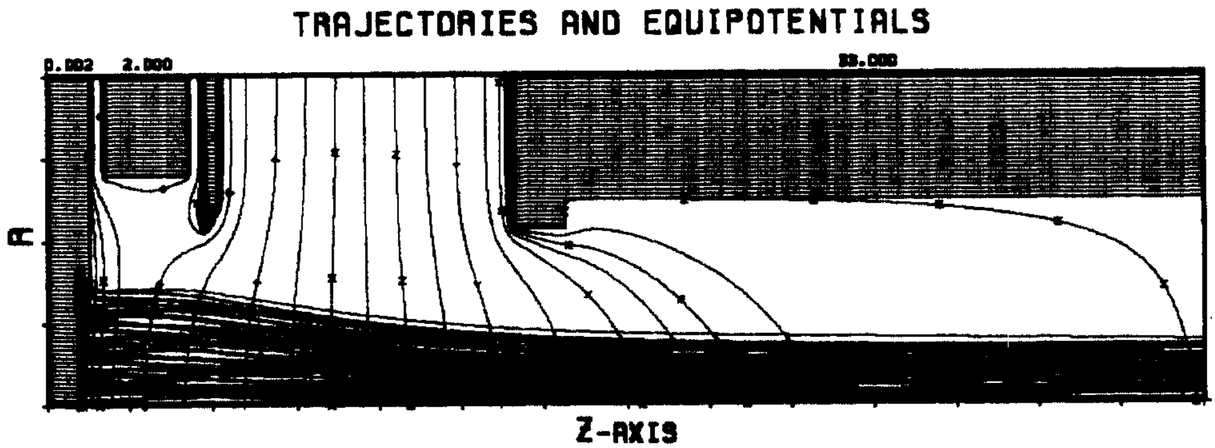
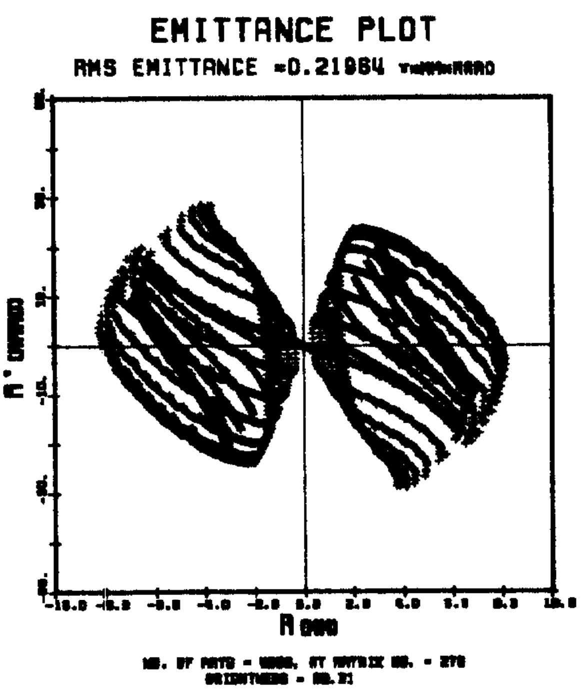


Figure 1. Sampled thermal trajectories for Chan's example with concave plasma surface.



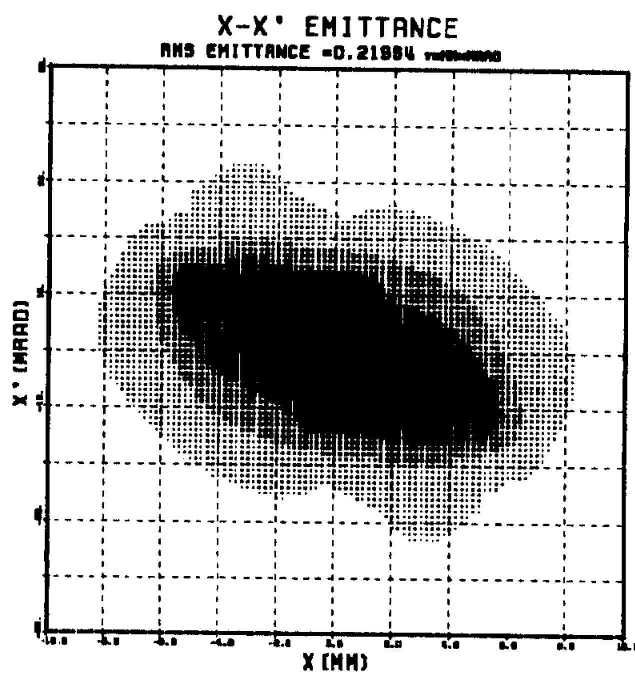


Figure 2. r-r' Emmitance plot for Example above.

Figure 3. x-x' Emittance plot for same example.