

# DEVELOPMENT OF A 3D-GUN CODE BASED ON A CHARGE CONSERVING ALGORITHM

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## Abstract

A charge conserving algorithm for the simulation of Space Charge Limited emission from conducting surfaces is proposed. The method is based on a subcell resolution approach, which allows of imposing accurate charge conservation on emission boundaries. The paper concentrates on the simulation of three dimensional structures with curved emission surfaces, for which the application of the presented method is particularly useful. Validation studies are performed for a cylindrical diode and for an emission strip of finite width. As an application example, the simulation of an electron gun of Pierce type is given.

## INTRODUCTION

Space Charge Limited (SCL) emission is a basic mechanism of electron injection in high-power microwave devices and particle accelerators. The interest on the of space charge field effects upon the emission process is related to the actual efforts in the development of high current electron sources, such as modified Pierce guns and field emitter arrays, involving complex, fully three dimensional geometries. While the basic SCL regime in one dimension is analytically described by the Child-Langmuir law, the 3D-characterization of the limiting current, however, remains accessible only to numerical simulation tools.

A typical simulation of SCL emission consists of the coupled computation of the particle equations of motion and that of the electromagnetic fields on a computational grid. Orthogonal mesh discretization techniques seem to provide a better simulation framework than finite-element and boundary-element discretizations, because of their capability of handling a large number of unknowns and to the efficiency of particle tracking algorithms involved. The principal difficulty on applying orthogonal mesh discretization, however, is related to the modeling of curved emission boundaries. Most of the simulation codes avoid dealing with boundary charges and fields by introducing a virtual diode of finite width, for which the one dimensional Child-Langmuir law is locally applied [1]. Unless the gap width associated with the virtual diode is very small, this approach may fail to converge to the right solution when strongly curved emission surfaces and emission corners are involved. The problem is thus stated as, how to provide for accurate emission currents for arbitrary source geometry, while preserving the simulation efficiency of the orthogo-

nal mesh discretization. In this paper a boundary conformal subcell resolution technique is applied on emission cells for imposing charge conservation in the presence of emission currents. The method avoids completely the need for a virtual diode and the treatment of curved emission surfaces and emission corners is naturally embedded into the charge conserving algorithm.

## PROBLEM STATEMENT

SCL emission occurs when the charge density of electrons extracted from a conducting emission surface by an externally applied electric field becomes sufficiently large to drive the total field on the emission surface to zero. The process depends itself on the applied fields, since the electron paths are determined by the electromagnetic field forces. The equations of motion of an ensemble of  $N$  particles is given by

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = e \left( \mathbf{E}_i + \frac{\mathbf{p}_i}{m} \times \mathbf{B}_i \right), \quad (1)$$

for  $i = 1 \dots N$ , where  $e$  is the electron charge,  $m$  is the electron mass, and  $\mathbf{r}_i$  and  $\mathbf{p}_i$  denote the electron positions and momenta, respectively. The electric and magnetic fields,  $\mathbf{E}_i$  and  $\mathbf{B}_i$  evaluated at the position of the  $i$ -th particle, contain the contribution of external field sources as well as that of the space charge distribution. Introducing a scalar potential  $\varphi$ , the equations for the space charge field in the electrostatic approximation become,

$$\mathbf{E} = -\nabla\varphi, \quad \nabla(\varepsilon\nabla\varphi) = -\frac{1}{\varepsilon_0} \sum_i^N e\delta(\mathbf{r} - \mathbf{r}_i), \quad (2)$$

where  $\varepsilon$  is the relative permittivity of the medium. The set of coupled equations is completed by specifying boundary conditions for the electrostatic field and initial conditions for each of the electron trajectories. When SCL regime is established, both, tangential and normal field components on the emission surface must vanish. Applying these boundary conditions directly to the solution of (2) for an arbitrary charge distribution, however, leads to an overdetermined set of differential equations. Therefore, a particular space charge distribution must be selected so that, imposing either of the boundary conditions to the solution of (2), implies vanishing of the total field on the emission surface. In other words, the solution of the SCL problem consists in selecting appropriate initial conditions for the emitted electrons in (1) such that a solution of (2) with vanishing electrostatic field on the emission boundary exists.

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## NUMERICAL PROCEDURE

Equations (2) are discretized in space using the Finite Integration Technique (FIT) [2]. The technique uses an orthogonal doublet of staggered grids, with grid potential values  $\Phi_i$  defined on the primary grid nodes. Denoting,  $\widehat{\mathbf{d}} = (\widehat{\mathbf{d}}_1, \widehat{\mathbf{d}}_2, \dots)^T$  the vector of electrostatic fluxes through each of the elementary facets of the dual cells, the discrete equations counterpart to (2) read,

$$\widehat{\mathbf{d}}_i = - \iint_{\Delta A_i} \varepsilon (\nabla \varphi) \cdot \mathbf{dA}, \quad \mathbf{S} \widehat{\mathbf{d}} = \mathbf{q}, \quad (3)$$

where  $\mathbf{S}$  is the discrete div-operator,  $\mathbf{q}$  is the vector of total charge contained in each of the dual cells and  $\Delta A_i$  is the area element corresponding to the  $i$ -th dual cell facet. The flux integrals appearing in (3) are evaluated using a boundary conformal approach [2], which accounts for the exact shape of the boundary surface within inhomogeneously filled cells containing material transitions.

Given the solution of (3) for the space charge fields on the grid, a solution of the equations of motion (1) can be found by integrating the trajectories of a set of computational particles using a standard PIC method. The resulting charge distribution is then used for updating the electrostatic field in (3). Self-consistent space charge fields and particle trajectories are obtained by repeating this procedure in a coupled manner as described in [3].

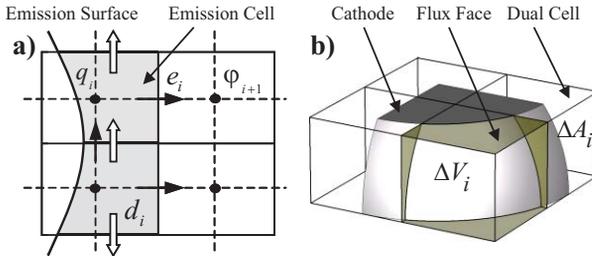


Figure 1: Layout of papers.

The challenge of the SCL emission modeling, however, consists in assigning appropriate charge and initial velocities to the emitted particles as they are injected into the computational domain. Since the equations of motion (1) are completely determined by the initial conditions of the particles, if a SCL solution exists, there will be a unique set of such initial conditions which correspond to this solution. The algorithm proposed here, determines the charge of the emitted particles by imposing conservation of charge within the partially filled, dual grid cells adjacent to the emission surface (c.f. Fig. 1). Integrating Gauß' law over the volume of such a cell yields,

$$\frac{1}{\varepsilon_0} Q_e = \sum_i \widehat{\mathbf{d}}_i - \frac{1}{\varepsilon_0} \sum_p q_p. \quad (4)$$

The space charge considered in (4) is composed of the particle charges  $q_p$  already resident in the cell volume, and of

an additional term,  $Q_e$ , corresponding to the charge emitted from the surface during an iteration step in the simulation. Since by virtue of the SCL emission condition, the normal field component on the emission surface vanishes, only grid fluxes  $\widehat{\mathbf{d}}_i$ , defined on the faces of the emission cell contribute to the total flux in (4). Assuming that,  $\widehat{\mathbf{d}}_i$  are the flux solutions with vanishing tangential field components on the emission boundary, Eq. (4) can be interpreted as the determining condition for the emission charge  $Q_e$ , such that also the normal field component vanishes, as required by the SCL condition.

Note, that exact area and volume elements are employed in the implementation, thus, exact charge conservation in the boundary cells is achieved. The accuracy of the method is, therefore, completely determined by the accuracy of the discrete field solution. In particular, no approximation to the geometry of the emission surface needs to be done, as opposed to the virtual diode technique where a piecewise planar emission surface is assumed.

Two more remarks regarding the accuracy of the above algorithm compared to the virtual diode approach are in order. First, the application of the method is independent of the geometry of the emitting surface. As special but important cases consider the SCL emission from corners and emission tips. Here, the 1D-Child's law used in the virtual diode technique does not apply even for very thin diode gaps. Second, since the algorithm only predicts the emitted charge, there is a freedom of choice in initializing particles with arbitrary velocity. This is particularly important in the modeling of hot cathodes, where the current enhancement resulting from the particle thermal velocities can be easily accounted for in the numerical simulation.

## VALIDATION AND EXAMPLES

### Cylindrical Diode

As a first validation example, the 3D-simulation of SCL emission in a cylindrical diode is considered. The analytical solution for the current density at the cathode is given by,  $J_c = 2.336 \cdot 10^{-6} V_a^{3/2} / (R_a R_c \beta_c^2)$ , where  $V_a$  is the diode voltage,  $R_a$  and  $R_c$  are the radii of anode and cathode, respectively. The corrective term  $\beta_c = \beta(R_c)$  is obtained by the solution of the differential equation,

$$3\beta^2 r^2 \frac{d^2 \beta}{dr^2} + r^2 \left( \frac{d\beta}{dr} \right)^2 + 7\beta r \frac{d\beta}{dr} + \beta^2 - 1 = 0, \quad (5)$$

which can be evaluated with a symbolic mathematical package. Similar expressions can be written for the potential and charge density in the diode gap (c.f. [4]).

Numerically computed curves for the charge density in the diode gap, with a fixed ratio of the anode-cathode radii,  $R_a/R_c = 1.5$ , and three different mesh resolutions are shown in Fig. 2. The simulation results show very good agreement with the analytical solution, even for the coarsest mesh resolution. Discrepancy between the analytical and numerical curves is only observed within a few mesh

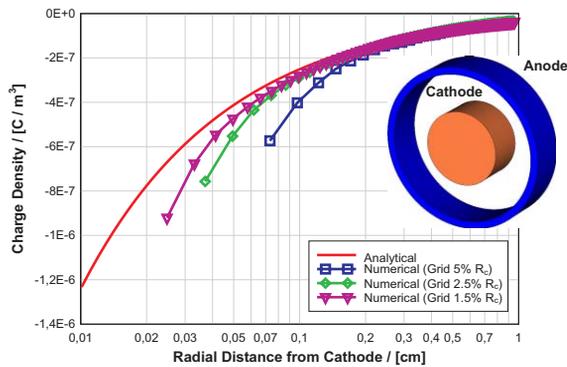


Figure 2: Computed charge density in the diode gap compared to the analytical solution.

lines away from the cathode surface. Note, however, that the analytical solution for the charge density at the cathode surface tends to infinity, which explains the slower numerical convergence in this region. The error in the total emission current, however, remains below 0.1% for all three mesh resolutions.

### 2D-Emission Strip of Finite Width

The second example is that of an emission strip of width  $w$  placed in a planar diode as shown in Fig. 3. If a large focusing magnetic field is applied, the electron motion between the diode plates may be assumed to be one dimensional. However, Luginsland et. al. showed, that for this configuration significant departure of the diode current from the 1D-law may occur [5]. The empirical law for the total current was found to,  $I/I_{CL} = 1 + 0.3145(d/w) + 0.0004(d/w)^2$ , where  $I_{CL}$  denotes the 1D-Child's current for the planar diode. The numerical results of the simulation with different beam widths  $w$ , for a diode gap of  $d = 1$  cm and a diode voltage of  $V = 30$  kV, are shown in Fig. 3. The simulations reveal the predicted current enhancement compared to the planar diode case. As expected, an essentially higher current density is obtained at the beam edges, in particular, for thin beam emission.

### Electron Gun Simulation

A large scale 3D-simulation of an electron gun of Pierce type [6] using the charge conserving algorithm was performed. The gun contains a spherical Dispenser-cathode with Os-coating, anode and focus electrode with an applied voltage of  $V = 90$  kV. Additionally, a focusing magnetic field of strength  $B_0 = 90$  mT on the gun axes was considered in the simulation. Figure 4 shows the geometrical gun arrangement and the simulated electron beam at stationary state. A total of 1.5 mio. computational particles were used in the simulation, corresponding to an average of 3.000 particles injected into the computational domain in every time step. The numerically computed beam current of  $I = 75$  A is in very good agreement with the design data given in [6].

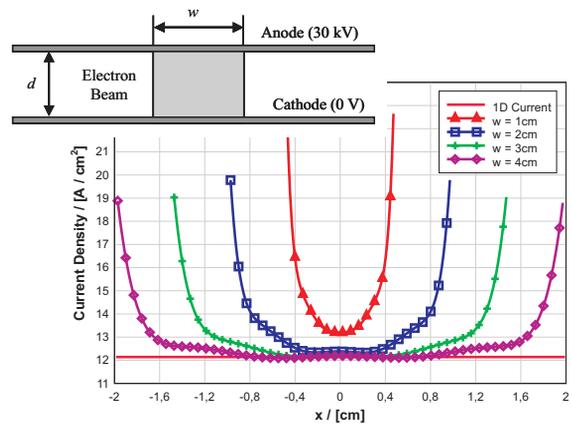


Figure 3: Emission strip geometry and current densities for different beam widths.

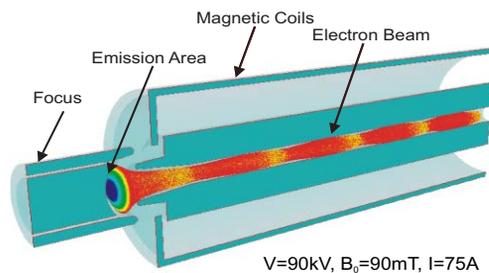


Figure 4: Gun geometry and computed electron paths. Colors scale to the charge carried by computational particles.

## CONCLUSIONS

A 3D-gun code based on a charge conserving algorithm for the simulation of SCL emission was presented. The method shows better accuracy and performance than conventional techniques. Two validation examples were given **i)** the three dimensional simulation of a cylindrical diode and **ii)** the simulation of a planar emission strip of finite width. In both cases, excellent agreement with the corresponding semi-analytical solutions for the limiting current was found. The efficiency of the code was demonstrated in simulation of electron beam emission in a Pierce type gun.

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