CONFORMAL MODELING OF SPACE-CHARGE-LIMITED EMISSION FROM CURVED BOUNDARIES IN PARTICLE SIMULATIONS

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Abstract

The reliability of Particle-In-Cell simulations depends on the accuracy of field and charge characterization at emission boundaries. In this work a novel approach to the modeling of curved emission boundaries in 3D-PIC simulations is presented. The method uses a boundary-conformal discretization for the electrostatic field equations, based on the orthogonal grid formulation of the Finite Integration Technique [1]. It also implements a consistent procedure for injecting particles at arbitrarily curved emission surfaces. The efficiency of the method is shown in 3D-simulations for the space-charge-limited emission in a Pierce gun model.

INTRODUCTION

Motivation

Electromagnetic PIC codes are commonly used for investigating the physics of charged particles in accelerators. A typical PIC simulation consists of a coupled computation of the dynamic particle equations and of the electromagnetic field solution on a computational grid. Among several techniques used for the solution of the field equations, the FD, FDTD and FIT applied on orthogonal, spatially staggered grids are the most popular. This is due to the capability of orthogonal grids of efficiently handling large to huge problems, and to the simplicity of the underlying data structure and implementation. However, the modeling of geometries with curved material boundaries on orthogonal grids, poses principal difficulties in maintaining solution accuracy close to such boundaries. The often used staircase approximation introduces large discretization errors, even when the grid size is very small. The low accuracy of boundary fields at curved emission surfaces strongly affects the overall performance of PIC simulations in two more particular ways. First, the local space-charge-limited emission model will predict inaccurate emission currents at staircase boundaries. Second, the large number of grid nodes needed for resolving geometry details leads to serious restrictions on the time step used in the simulation. This paper introduces a boundary-conformal approach to 3D-PIC simulations which retains the advantages of orthogonal grid modeling while providing accurate solutions for arbitrarily curved emission boundaries.

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Mathematical Model

The model equations considered, consist of the set of equations of motion for N computational particles,

$$\frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t} = \boldsymbol{v}_i\,, \quad \frac{\mathrm{d}m_e\boldsymbol{v}_i}{\mathrm{d}t} = e(\boldsymbol{E} + \boldsymbol{v}_i \times \boldsymbol{B})\,, \qquad (1)$$

with $i = 1 \ldots N$, where e is the electron charge, m_e is the relativistic electron mass; particle positions and velocities are given by $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$, respectively. Assuming only electrostatic particle-particle interactions the space-charge field $\boldsymbol{E}$ is obtained by

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

where ε is the material dielectric constant and q_i the charge carried by the i-th particle.

The set of equations (1,2) is completed by specifying boundary conditions for the electrostatic potential φ, and initial conditions for the particle positions $\boldsymbol{r}_i$ and velocities $\boldsymbol{v}_i$. In the case of space-charge-limited emission particle initial conditions can be derived by locally applying the Child-Langmuir diode equation [2],

$$J_{\mathrm{CL}} = \left(\frac{4\varepsilon_0}{9}\right)\sqrt{\frac{2e}{m_e}}\frac{\delta\varphi_b^{3/2}}{\delta d^2}\,, \qquad (3)$$

where J_{CL} is the current at the emission surface, and $\delta\varphi_b$ denotes the local potential difference at a small distance δd from the emission surface. Thus, the space-charge-limited emission condition is completely determined by the electrostatic potential solution obtained in (2).

CONFORMAL METHOD

Discrete Field Equations

Equations (2) are discretized in space using the Finite Integration Technique (FIT) [1]. This technique uses an orthogonal doublet of staggered grids, with grid potential values Φ_i defined on the primary grid nodes (cf. Fig. 1).

Denoting, $\widehat{\widehat{\mathbf{d}}} = (\widehat{\widehat{\mathbf{d}}}_1, \widehat{\widehat{\mathbf{d}}}_2, \ldots)^{\mathrm{T}}$ the vector of electrostatic fluxes through each of the elementary facets of the dual cells, the discrete equations counterpart to (2) read,

$$\mathbf{S}\widehat{\widehat{\mathbf{d}}} = \mathbf{q}\,, \quad \widehat{\widehat{\mathbf{d}}}_i = \iint_{\Delta A_i}\varepsilon(\nabla\varphi)\mathrm{d}\boldsymbol{A}\,, \qquad (4)$$

where $\mathbf{S}$ is the discrete div-operator, $\mathbf{q}$ is the vector of total charge contained in each of the dual cells and ΔA_i is the area element corresponding to the i-th dual cell facet.

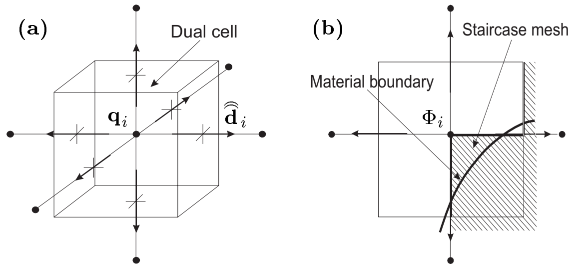

Figure 1: (a) Primary grid and a dual cell in the FIT. (b) Staircase vs. conformal discretization.

Equations (3) are the *exact* representation of (2) in terms of the finite fluxes $\widehat{\widehat{\mathbf{d}}}_i$. A discretization error arises first, when the flux integrals $\widehat{\widehat{\mathbf{d}}}_i$ are approximated using potential grid values Φ_i. The conformal approach used in this paper for evaluating the flux integrals was first proposed for high frequency applications [3]. It minimizes the discretization error by taking into account the geometry of the material boundary within inhomogenously filled cells containing curved material transitions (cf. Fig. 1b). In contrast to the staircase approximation, the conformal method requires no additional mesh refinement at curved boundaries, because subcellular material information is already contained in the formulation.

Particle Injection

Injecting computational particles at emission boundaries involves a) identifying appropriate geometrical samples for the initial particle positions and b) determining charge and velocity values for the emitted particles, which are consistent to the emission current (3).

In this implementation, the first step is realized by means of a triangular mesh of specified size which is generated on the emission surface. Then, static emission samples are located at the triangle barycenters. The algorithm selects all or a random part of these samples, assigning their positions to the emitted particles. In this procedure, uniform as well as locally refined distributions for the particle initial positions (e.g., at sharp emission tips) are obtained.

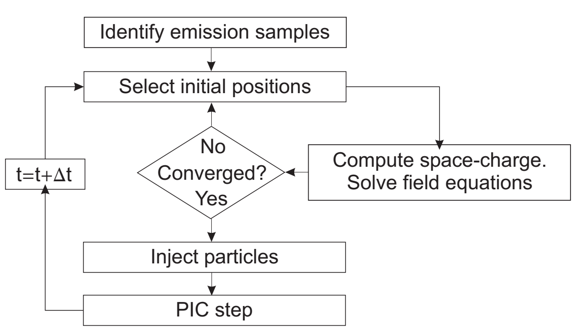

Figure 2: Simulation flow chart with particle injection.

The second task is to compute the charge carried by the emitted particles according to the space-charge-limited emission model. For this purpose, a small constant distance span δd from the emission samples in the direction normal to the source surface is introduced. This allows of determining local currents (3) associated to the emitted particles. The consistency between the computed currents and the field solution is enforced by performing a fixed point iteration as shown in the flow chart of Fig. 2. Here, the particle charges predicted by (3) are assigned to the grid during each iteration using a Cloud-In-Cell (CIC) interpolation scheme [4]. The resulting field equations (4) are repeatedly solved until no additional charge can be extracted from the source surface, i.e., a consistent emission current is established.

RESULTS

In order to demonstrate the performance of the method, test simulations for a Pierce gun model are performed. The fully 3D-model of the gun [5] contains a spherical Dispenser-cathode with Os-coating (M-type), anode and focus electrode with specific parameters listed in Table 1. Additionally, a focusing, static magnetic field of strength $90\mathrm{mT}$ on the gun axes was externally computed with the commercial simulation package CST EM Studio$^{\mathrm{TM}}$ [6] and loaded into the simulations.

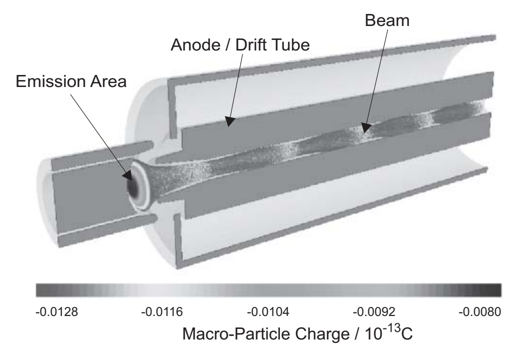

Figure 3: Geometry of the Pierce gun and simulated beam.

Figure 3 shows the geometrical gun arrangement and the simulated electron beam $2.5\,\mathrm{ns}$ after the beginning of the emission process. A total of 1.5 mio. computational particles were used in the simulation, corresponding to an average of 3.000 particles per time step, injected into the emission area according to the above procedure. The beam envelope develops transversal oscillations, which are due to a slight mismatch between accelerating voltage the focusing magnetic field [5]. The computed charge distribution and potential along the gun axes are shown in Fig. 4.

Table 1: Pierce Gun Parameters [7]

Voltage	90kV	Cathode disc radius	$33.1\,\mathrm{mm}$
Convergence angle	$37.15°$	Anode disc radius	$16.8\,\mathrm{mm}$
Anode angle	$47.0°$	Focus angle	$45.0°$
Waist distance	$62.0\,\mathrm{mm}$	Waist radius	$8.0\,\mathrm{mm}$

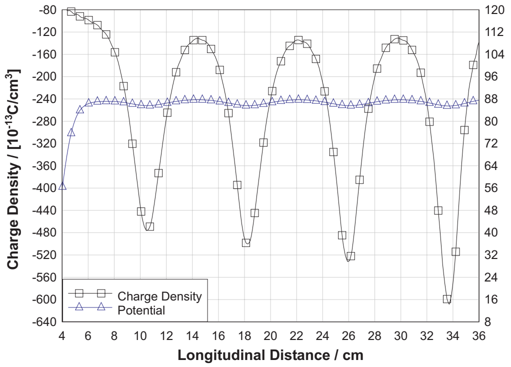

Figure 4: Charge density and potential on the gun axes.

The main result of this investigation is illustrated in Fig. 5–6. The steady state emission current is monitored on the source surface using several discrete models of different mesh resolutions. The numerical convergence of simulations using the staircase approximation is shown in Fig. 5. In this case, the relative error obtained for fine to moderate mesh sizes varies between 10–25%. Only at the very fine discretization of 1.5 mio. mesh nodes, the emission current approaches the correct curve. Despite the slow convergence, the staircase models introduce numerical oscillations in the current curves, resulting from the low order field approximation at the emission surface.

Figure 6 shows the simulation results using the conformal method. The emission current curves do already converge at the lowest mesh resolution For emission dominated problems, the high accuracy of the conformal method implies better numerical performance. Recalling the solution algorithm shown in Fig. 2, a consistent modeling of space-charge-limited emission requires several solutions of the grid-field-equations (4) at every time step; the number of iterations depending on the share of space-charge-fields in the total particle forces. The computational effort for the solution of these equations, typically involving an iterative solver, can therefore be reduced by using the conformal model, since the number of mesh nodes can be decreased without accuracy loss. Note also, that using larger cell sizes in conformal models, improves the stability bounds imposed on the explicit integration of (1). This issue, however, will be discussed in a forthcoming publication.

CONCLUSIONS

The conformal method for the modeling of space-charge-limited emission from curved surfaces is based on a) a boundary conformal discretization of the electrostatic field equations and b) on a boundary conformal technique for particle injection at emission time. The method enforces the field-space-charge consistency implied by Child's law, by iterating the field solution equations until a consistent current is established.

The numerical simulation of a Pierce gun model shows that the conformal method is considerably superior to the staircase approximation. In the presented simulation, the fast numerical convergence of the method allows of reducing the number of mesh nodes by at least 10 times compared to the staircase simulation.

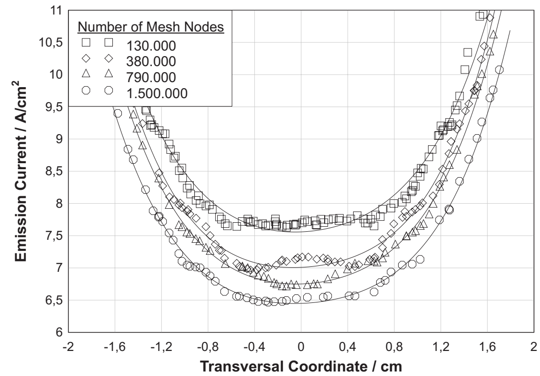

Figure 5: Emission currents on the source surface using staircase modeling.

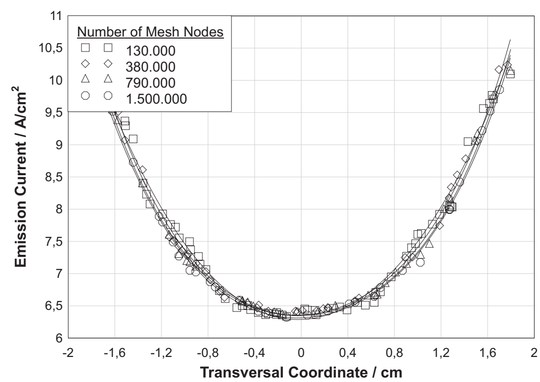

Figure 6: Emission currents on the source surface using the conformal method.

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