CYBERNETICS AND PHYSICS, VOL. 5, NO. 1, 2016 , 16–20

ON IMPROVING THE PARTICLE-IN-CELL SIMULATIONS ACCURACY FOR SOURCES OF CHARGED PARTICLES

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Abstract
Creation of initial distribution of macroparticles in phase space in the case of electron or ion sources modeling is an important aspect. In this work we will discuss the two main approaches to particles creation random and quiet start. In the case of random distribution, we need less number of macroparticles but it can reduce solution accuracy due to a growth of numerical noises. Numerical noises in solution obtained some particles method manifested primarily in fluctuation the space-charge density distribution. We introduce the criteria for measurement this fluctuation based on a comparison the density distribution with the some “etalon” solution with minimized fluctuations. An approach based on the application of different noise filters is used for suppress the fluctuation. The results of measurements the solution accuracy in the case of planar diode are presented.

Key words
Numerical simulation of planar diode, Particle-In-Cell method, particle tracking method, numerical noise reduction in particle-based methods.

1 Introduction

Numerical simulations today have become one of the most effective tools for studying plasma [Zavadskiy and Kiktenko, 2014; Aminov, Ovsyannikov, 2015] and particle flows dynamics in the emitting devices such as particle accelerators [Andrianov, Edamenko, 2014; Kozynchenko, 2014; Skudnova and Altsybeyev, 2015], electron and ion sources [Altsybeyev *et al.*, 2014a; Altsybeyev *et al.*, 2014b]. The basis of most used algorithms for numerical studies in this field is various particle methods [Hockney, 1988], in which particle flows are simulated as a set of a large number of model particles. A significant drawback of particle-based methods is the occurrence of non-physical numerical noise [Mesyats, 2014], resulting in a distortion of the solution. The origins of noise are various and there is no general approach to solving this problem now. The simplest way to reduce the noise is to increase the number of model particles but it is often impossible due to the limitation of computer resources. To reduce the noise, the scheme of space charge assigning and forces interpolation are modified [Mesyats, 2009], optimal time step and cell size are selected, different noise filters are applied [Jolliet, Bottino and Angelino, 2007]. Creation of initial distribution of macroparticles in phase space is also an important aspect. Two fundamental approaches are common: the random start and the quiet start. The idea of random start is the random initial distribution of macroparticles in phase space. Using this scheme we need less number of macroparticles, but this leads to the growth of numerical noises. The quiet start is an attempt to reduce the noise and indetermination of random starts. But in some cases, application of quiet start is too complicated due to a growth of the required number of model particles, especially during the discretization by the set of phase space dimensions [Lapenta]. Also using of regularly located particles can lead to correlation among the particles that have no equivalence in reality.

In this paper iterative particle tracking and Particle-In-Cell methods are used. We assume that solution obtained by iterative particle tracking method with quiet start is more accurately than the solution obtained using Particle-In-Cell with random start. So, we introduce the criteria for measurement numerical noises based on a comparison the density distribution with solution obtained using iterative particle tracking method. In follow we try to analyze effect of noise reduction methods on solution accuracy using introduced approach.

2 Governing Equations

If we assume that the process at hand is time-independent, we can use the electrostatic approximation. In this case the electric field is irrotational and the space charge distribution is time-independent. Let us consider the computational domain $\overline{\Omega} = \Omega \cup \Gamma$, there

$\Gamma = \Gamma_1 \cup \Gamma_2$ is the computational domain boundary. This assumption allows us to use the Poisson equation to calculate the electric field potential U and electric fields $\mathbf{E}$.

$$\begin{aligned} &\Delta U(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon}, \ \text{ if } \mathbf{r} \in \Omega \\ &\mathbf{E}(\mathbf{r}) = -\text{grad}\, U(\mathbf{r}), \\ &U(\mathbf{r}) = g(\mathbf{r}), \ \text{ if } \mathbf{r} \in \Gamma_1 \\ &\frac{\partial U(\mathbf{r})}{\partial \mathbf{n}} = 0, \ \text{ if } \mathbf{r} \in \Gamma_2. \end{aligned} \tag{1}$$

Here $\mathbf{r}$ is the space phase coordinates vector, $\rho(\mathbf{r})$ is the space charge density distribution, $g(\mathbf{r})$ is some function that describes electrodes potentials, is the electric permittivity of the domain material, $\mathbf{n}$ is a normal vector to the Γ_2 boundary. We will use the following relativistic motion equations for macroparticles in particle-mesh methods:

$$\begin{aligned} &\frac{d\mathbf{p_i}}{d\tau} = \frac{q_i \mathbf{E}(\mathbf{r_i})}{m_0 c^2}, \\ &\frac{d\mathbf{r_i}}{d\tau} = \frac{\mathbf{p_i}}{\gamma_i}, \\ &\mathbf{r_i}(0) \in \Gamma_{em}, \\ &\mathbf{p_i}(0) = \mathbf{p_i^0}. \end{aligned} \tag{2}$$

Here $i = \overline{1...N}$ are the macroparticles labels of the particle flow in which physical particles have rest mass m_0 and charge q_i, γ_i are the macroparticles Lorentz factors, c is the light velocity, $\tau = ct$, $\mathbf{p_i} = \mathbf{v_i}\gamma_i/c$ are the macroparticles momentums ($\mathbf{v_i}$ are the macroparticles velocities), $\mathbf{r_i}$ are the macroparticles positions, Γ_{em} is the emitting surface, $\mathbf{p_i^0}$ is initial macroparticles momentums.

The current density distribution $\mathbf{j}(\mathbf{r})$ satisfy the continuity equation

$$\begin{aligned} &\text{div}\, \mathbf{j}(\mathbf{r}) = 0, \\ &\mathbf{j}(\mathbf{r}) = \mathbf{j_{em}}(\mathbf{r}), \ \text{ if } \mathbf{r} \in \Gamma_{em}. \end{aligned} \tag{3}$$

In the case of the space-charge limited emission current density is determined by Child law for a vacuum planar diode [Child, 1911]

$$\mathbf{j_{em}} = \frac{4}{9}\varepsilon_0 \sqrt{2\frac{e}{m}\frac{U^{3/2}}{d^2}}. \tag{4}$$

Here U is cathode-anode voltage, ε_0 is permittivity, d is the distance between cathode and anode, e and m charge and mass of electron. Also it should be noted that current density can be obtained more precisely using different approaches [Altsybeyev, 2016; Altsybeyev, 2015].

We should determine the stationary solutions of the equations (1)-(3): the self-consistent field and macroparticles traces.

3 Simulations Tools

In this work we will use DAISI (Design of Accelerators, optImizations and SImulations) code for all calculations. DAISI code initially was developed for numerical simulations of electron and ion sources using particle-in-cell method at the Saint-Petersburg State University [Altsybeyev *et al.*, 2014b; Altsybeyev and Ponomarev, 2015; Altsybeyev, 2016].

4 Particle-In-Cell Method

Particle-In-Cell (PIC) simulations are a widely used tool to study plasma and particle flows dynamics in the emitting devices such as particle accelerators, electron and ion sources. In order to numerically solve the Vlasov-Poisson equations particle flows are represented by a set of large number of model particles.In addition to macroparticles data method works with information about the electromagnetic field and current and charge densities specified on a computational Euler grid. The particles do not interact directly but only through the grid values.

Classical scheme of PIC method consists of the four stages:

Particle initialization and emission. To create the initial distribution of macroparticles positions and velocities random and "quiet" start are used [Mudiganti, 2006].

Space charge assigning and force interpolation. To calculate the charge deposited by the macroparticles and force interpolation we use Cloud-In-Cell (CIC) scheme.

Calculate electric field. Poisson equation is solved numerically using the finite-difference method (FDM) with the five-point star stencil [Altsybeyev and Ponomarev, 2015]. The electric field is obtained by numerical differentiation of the electrostatic potential. The forces acting on the particles are computed from the electric fields evaluated at the particle position.

Particle pushing. After calculating the forces acting on each particle we can update the positions and velocities. For the integration of particles motion equations (2) we use the second-order Leap-Frog mover. The Leap-Frog method is economic and good conserves energy on long trajectories.

5 Particle Tracking Method

An iterative particle tracking method can be used to simulate steady-state of the particle flows. The main idea is based on iterative corrections of particle paths inside a problem space. The required number of macroparticles is significantly less, making iterative method attractive to study the steady-states of the beams.

To avoid iteration divergences [Xavier, Motta, 2010], space charge density at the n^{th} iteration is averaged as

$$\rho_h^n = (1-\omega)\rho_h^{n-1} + \omega\rho_h^n \tag{5}$$

where ω represents the under-relaxation factor. Decreasing relaxation factor ω helps to improve method convergence, but at the same time it increases the required time for the simulation.

As a convergence criteria of the iterations we use the following condition

$$\max_{s=1..N} \left| \frac{\rho_s^n - \rho_s^{n-1}}{\rho_s^{n-1}} \right| < \varepsilon \qquad (6)$$

Here ρ_s^n is a space charge density on a n^{th} iteration in the s^{th} computational mesh node, ε is the tolerance.

6 Noise Reducing Methods

In order to improve solution accuracy different charge density smoothing methods were examined.

Linear smoothing filtering. The simplest way to cutoff numerical noise is linear smoothing filters. Linear filters work by a convolution with a moving window called a kernel. In this paper the Gaussian kernel with different sizes is used.

Frequency domain filtering. Numerical noise can be suppressed by frequency domain filtering [Sydora, 1999] in three steps:

1. Transformation of space charge density distribution into frequency domain via FFT.
2. Apply the filter low-pass window function.
3. Transformation back to time domain via inverse FFT.

Smoothing cubic spline. The smoothing spline s is constructed for the specified smoothing parameter p. Parameter p is defined between 0 and 1, $p = 0$ produces a least-squares straight-line fit to the data, while p = 1 produces a cubic spline interpolant.

7 Numerical Experiments

We consider the planar diode in two-dimensional Cartesian coordinates. The geometry and parameters of the diode is presented in Fig. 1 and in Table 1. All simulations were performed on the uniform computational mesh 128 × 128, $h_x = h_y \approx 0.0008$. The number of macroparticles traces is 500, the integration timestep is chosen so that the macroparticles pass no more than half of mesh cell per one step.

Table 1: Planar diode parameters.

Anode-cathode distance, m	$d = 0.1$
Length, m	$L = 0.1$
Emitter length, m	$L_{em} = 0.02$
Anode voltage, V	$U_a = 100\,000$
Current density, A/m^2	$J_{em} = -7368$

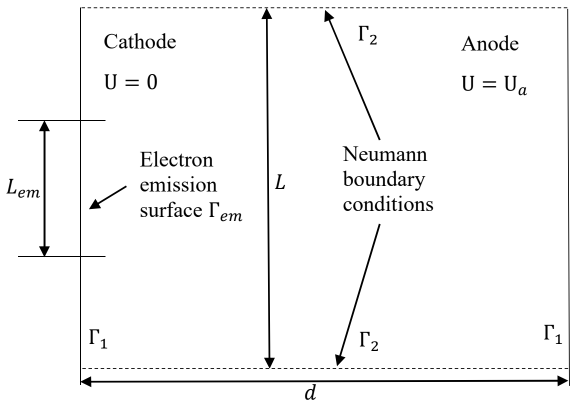

Figure 1: Simulations model of the planar diode.

7.1 Quiet start

The electron traces obtained by iterative particle tracking method presented in Fig. 2. Comparison of the space charge density distributions obtained by the PIC method and the iterative particle tracking method plotted in Fig. 3. We can conclude that results obtained by PIC and iterative solvers with quiet start accurately consistent.

Solution obtained by the iterative particle tracking method with quiet start will be considered as etalon solution. This solution will be used to estimate the efficiency of the discussed noise reducing methods.

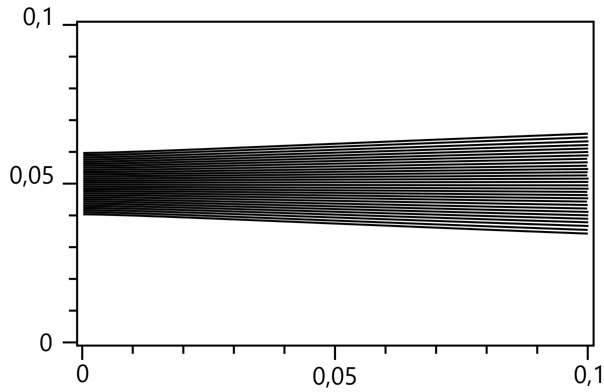

Figure 2: The electron traces obtained by iterative particle tracking method.

7.2 Random start

In the case of iterative solver with random start convergence was not achieved. Smoothing of the space charge density also did not help to achieve convergence. Convergence criterion plotted in Fig. 4.

However, smoothing of the space charge distribution by cubic smoothing splines $s = 0.5$ in the Particle-In-Cell simulation helps to suppress oscillations introduced by random start and increases the accuracy of

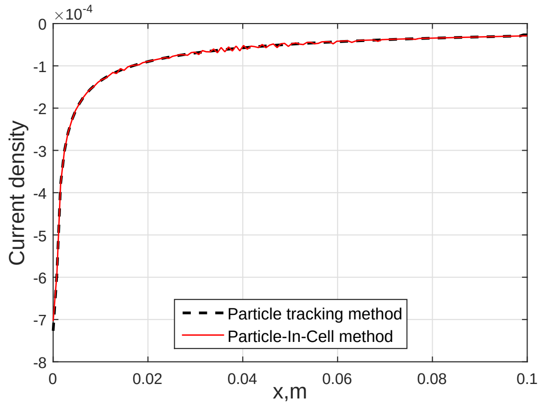

Figure 3: Comparison of the space charge density distributions obtained by the PIC method and the iterative particle tracking method in case of quiet start. Black dashed line is etalon solution.

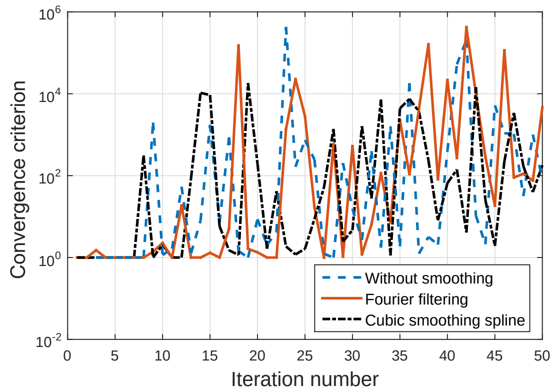

Figure 4: Divergence of the iterative particle tracking method with the random start. Smoothing of the space charge density also did not help to achieve convergence.

simulations. The deviation of the space charge density distribution from etalon solution plotted in Fig. 5.

Three different smoothing methods were considered in this work: linear convolution filter with Gaussian kernel, Fourier filter with Gaussian window and cubic smoothing splines. Comparison of the smoothing methods efficiency presented in Fig. 6.

Influence of smoothing methods on RMS beam emittance was observed. The arithmetic definition of a normalized beam emittance is

$$\epsilon = 4\sqrt{\overline{x^2} \cdot \overline{p_x^2} - (\overline{xp_x})^2} \tag{7}$$

where

$$\overline{x^2} = \frac{1}{N}\sum_{i=1}^{N} x_i^2,$$

$$\overline{p_x^2} = \frac{1}{N}\sum_{i=1}^{N} p_{x_i}^2,$$

$$\overline{xp_x} = \frac{1}{N}\sum_{i=1}^{N} x_i p_{x_i}.$$

Relative normalized RMS beam emittance in case of random start with different smoothing methods is plotted in Fig. 7. Etalon emittance was obtained by iterative particle tracking method with quiet start. It should be noted that smoothing increases value of RMS emittance, despite it improves simulation accuracy.

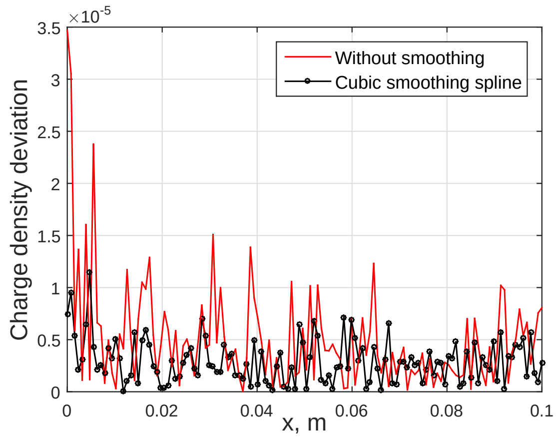

Figure 5: The deviation of the space charge density distribution from etalon solution in the case of the Particle-In-Cell method with cubic smoothing splines $s = 0.5$ and without.

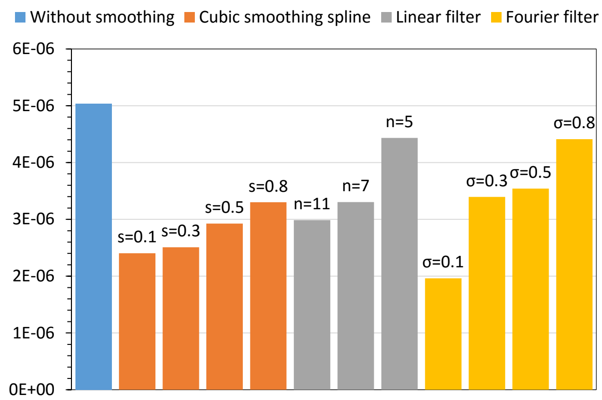

Figure 6: Comparison of the smoothing methods efficiency. Average deviations of the space charge density distribution from etalon solution are presented.
s - smoothing parameter of cubic splines,
n - convolution kernel size,
σ - parameter of Gaussian window function.

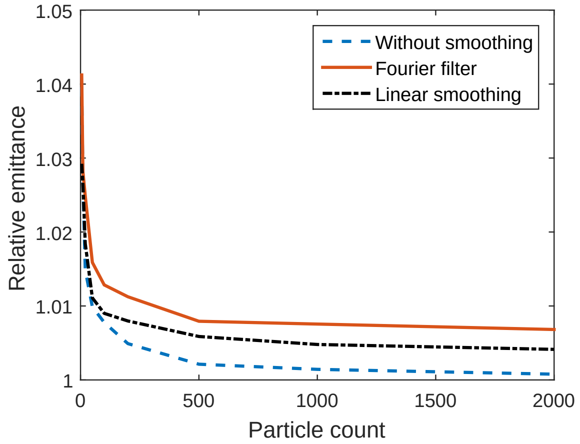

Figure 7: Relative RMS emittance

8 Conclusion

Using a random initial distribution of macroparticles with iterative particle tracking method leads to divergence of the method caused by large oscillations in the space charge distribution. Smoothing methods also did not help to achieve convergence. But in case of Particle-In-Cell simulations with random initial macroparticles distribution smoothing of the space charge distribution helps to suppress oscillations introduced by random start and increases the accuracy of simulations. Different smoothing algorithms were examined and a comparison of their efficiency was produced.

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