Comparison of open boundary conditions realizations for continuous injection of an electron beam into a plasma in the case of the PIC and parabolic form-factors

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Abstract. The paper is devoted to a comparison of methods for realizing open boundary conditions that allow continuous injection of a beam of charged particles into a plasma in the PIC model in the case of different particle form-factors, as well as with two variants of boundary conditions at plasma ends. It is shown that simulation results coincide for the PIC and parabolic form-factors for the problem of injecting an electron beam into a plasma in 1D geometry for all the boundary conditions under consideration. In 2D geometry, we find the discrepancy between these models, as well as the inapplicability of the Mur’s boundary conditions for electromagnetic fields simultaneously with the condition of equality of currents in boundary cells. The number of particles in a cell, which is necessary for convergence of calculations, for each method is determined.

1. Introduction
The problem of creating a powerful and compact source of electromagnetic (EM) radiation in the THz frequency range (0.3-10 THz) is very urgent. Over the past decades, a number of ideas on the basis of accelerator and laser technologies have been proposed. Plasma is one of the most perspective medium for generation of such radiation, since it can sustain electromagnetic oscillations with extremely large amplitudes. However, the output of radiation, whose frequency is close to the plasma one, is limited by the effect of plasma screening, which leads to the necessity of using either magnetic fields or plasma density gradients. In [1] the possibility of effective conversion of counterpropagating plasma waves with different transverse structure into vacuum EM radiation at a doubled plasma frequency is shown. A similar scheme can also be realized for the case of two colliding electron beams into a plasma. The fundamental tool for testing the theory under consideration is numerical simulation by particle-in-cell method, which allows us to describe radiation processes with the self-consistent plasma dynamics. Realization
of open boundary conditions necessary for the continuous beam injection into the system is the most challenging problem in constructing a numerical model for a scheme with colliding beams of particles. Such boundary conditions have been recently used to study the beam-plasma interaction [2] and generation of radiation from the plasma in the case of a single beam [3]. The parabolic form-factor and a special absorbing layer for electromagnetic fields have been used in these works. Further studies will require a significant increase in spatial scales and number of particles, especially for the 3-dimensional case. Therefore, it is important to use faster algorithms, for example, using the PIC form-factor. This paper is devoted to verification of the possibility of using this form-factor for macro particles, as well as the realization of two types of open boundary conditions for solving such problems. The verification is carried out for two problems. The first one is a one-dimensional injection of an electron beam into a plasma [2]. In the second one, the generation of radiation in the plasma by means of colliding electron beams of different widths is considered.

2. Numerical model of continuous injection of an electron beam into a plasma

The dynamics of a plasma-electron beams system can be described by the Vlasov equation for the particle distribution functions and the system of Maxwell’s equations with self-consistent electromagnetic fields:

\[
\frac{\partial f_\alpha}{\partial t} + (\overrightarrow{v} \cdot \nabla) f_\alpha + q_\alpha \left( \overrightarrow{E} + \frac{1}{c} \overrightarrow{v} \times \overrightarrow{B} \right) \frac{\partial f_\alpha}{\partial \overrightarrow{p}} = 0,
\]

\[
\text{rot} \overrightarrow{B} = \frac{4\pi}{c} \overrightarrow{j} + \frac{1}{c} \frac{\partial \overrightarrow{E}}{\partial t}, \quad \text{rot} \overrightarrow{E} = -\frac{1}{c} \frac{\partial \overrightarrow{B}}{\partial t},
\]

\[
\text{div} \overrightarrow{B} = 0,
\]

\[
\text{div} \overrightarrow{E} = 4\pi \rho,
\]

\[
\overrightarrow{j} = \sum_\alpha q_\alpha \int f_\alpha(\overrightarrow{p}, \overrightarrow{r}, t) d\overrightarrow{p}, \quad \rho = \sum_\alpha q_\alpha \int f_\alpha(\overrightarrow{p}, \overrightarrow{r}, t) d\overrightarrow{p},
\]

where \(\alpha\) is a sort of particles (ions and electrons of the plasma, the electrons of the beams), \(\overrightarrow{p} = m\gamma \overrightarrow{v}\) is a relativistic momentum of the particle. Particles in cells (PIC) method [4, 5] is used for solving equation 1.

Equations of particle motion are characteristics of the Vlasov equation:

\[
\frac{d\overrightarrow{p}_\alpha}{dt} = q_\alpha(\overrightarrow{E} + \frac{1}{c} [\overrightarrow{v}_\alpha \times \overrightarrow{B}]), \quad \frac{d\overrightarrow{r}_\alpha}{dt} = \overrightarrow{v}_\alpha.
\]

For solving these equations, the second order leap-frog scheme is used [6]:

\[
\frac{\overrightarrow{p}_i^{m+1/2} - \overrightarrow{p}_i^{m-1/2}}{\tau} = q_i \left( \overrightarrow{E}_i^m + \frac{1}{c} \left[ v_i^{m+1/2} + v_i^{m-1/2} \right] \overrightarrow{v}_i^m, B_i^m \right), \quad \frac{\overrightarrow{r}_i^{m+1} - \overrightarrow{r}_i^m}{\tau} = v_i^{m+1/2}.
\]

Where \(q_i\) is the particle charge with number \(i\), \(v_i\) is the velocity of the particle with number \(i\), \(\overrightarrow{E}_i^m, \overrightarrow{B}_i^m\) are electric and magnetic fields in the point \(\overrightarrow{r}_j\), \(\tau\) is the time step; the superscript indicates the time moment at which the function is calculated. The FDTD scheme [5] is used for solving Maxwell’s equations (2)–(4):

\[
\frac{B_i^{m+1/2} - B_i^{m-1/2}}{\tau} = -c \text{rot}_h E_i^m,
\]
\[
\frac{E^{m+1} - E^m}{\tau} = -4\pi j^{m+1/2} + c \text{rot}_h B^{m+1/2},
\]
\[
div_h E^m = 4\pi \rho^m,
\]
\[
div_h B^{m+1/2} = 0.
\]

The charge densities and current densities are calculated from the velocities and coordinates of the individual particles:
\[
\rho(\vec{r},t) = \sum_i q_i R(\vec{r},\vec{r}_i(t)), \quad \vec{J}(\vec{r},t) = \sum_i q_i \vec{v}_i(t) R(\vec{r},\vec{r}_i(t)).
\]

The form-factor \(R(\vec{r},\vec{r}_i(t))\) characterizes the shape, size of the particle, and the distribution of the charge on it. In this paper, we use the PIC form-factor with the method of current calculation proposed in [7] and parabolic form-factor with the method of current calculation described in [8].

3. Boundary conditions

Let a plasma column have a length \(L_x\) and start at the zero cell of the computational grid. The main difficulty in the problem formulation is the adequate realization of the boundary conditions near the injection and beam extraction points. Let us consider separately the conditions for particles, current densities and electromagnetic fields. The scheme of the calculation area is shown in Fig. 1.

\[
\frac{\partial}{\partial x} j^x(t) = 0.
\]

Figure 1. Scheme of the calculation area.

Obviously, particles crossing the boundaries \(x = 0\) and \(x = L_x\) have to be removed from the simulation area. However, this will lead to the fact that the plasma will constantly flow out of the region and the quasi-neutrality condition will be violated. Thus, it is necessary to simulate the natural reverse current of the plasma through the open boundaries \(x = 0\) and \(x = L_x\). To solve this problem, we consider the following condition on the particle distribution function: \(f(\vec{r},\vec{p},t)|_{x=-1} = f(\vec{r},\vec{p},t)|_{x=0}\).

This is realized in the following way. For a particle that has flown by a time step through the point \(x = h\) from left to right (that is, from the zero cell to the first), we create its copy displaced in the longitudinal direction by the grid spacing \(h\). Other coordinates of the new particle remain the same. The longitudinal \((p_x)\) momentum of particles is also conserved, and the transverse momentum is taken from the initial distribution. The condition on the right boundary \(x = L_x\) is realized similarly.
Beams injection is performed as follows: at each instant of time, the necessary number of beam particles with a given velocity distribution is added to the region beyond the boundary of the plasma column (that is, to the minus first cell for the left beam).

One can calculate the current and electromagnetic fields at the boundary in two ways.

3.1. Boundary condition 1
It is possible to expand the simulation area for electromagnetic fields along the X direction from both sides and to establish in resulting layers the absorption condition SAL [9] - artificial damping of electromagnetic waves by multiplying the electromagnetic field values at each time step by some coefficient \( k < 1 \), depending on the distance to the boundary [10]:

\[
k = \begin{cases} 
\frac{a-1}{l} x^2 - 2 \frac{a-1}{l} x + a, & x < l, \\
1, & x \geq l,
\end{cases}
\](13)

where \( l \) is the absorbing layer width, \( x \) is the distance to the domain boundary, and \( 0 < a < 1 \) characterizes the degree of wave attenuation in the absorbing layer. The current at the boundary \( X = 0 \) (similarly at the other boundary) is calculated as follows. At each time step, virtual copies with the same momentum values and transverse coordinates are created for each particle from the zero and the first cells, but shifted to two cells (-1 and -2 cells). Further, dynamics of these particles are calculated under the action of real fields in order to maintain a contribution to the real currents of the system. Thus, in the zero cell (the extreme cell of a real plasma), the values of the currents reproduce the condition that there is a real plasma behind the left boundary. After calculating the current, the copies of the particles are deleted. On the right boundary, the conditions are the same. These boundary conditions are implemented for the PIC form-factor and parabolic form-factor (PIC-1, Parabolic-1).

3.2. Boundary condition 2
Set the condition \( \mathcal{J}(\mathbf{r},t)|_{x=-1} = \mathcal{J}(\mathbf{r},t)|_{x=0} \), that is, assume that the current in the first cell completely coincides with the current in the second (similarly for the last and the penultimate one). For a parabolic kernel condition

\[
\mathcal{J}(\mathbf{r},t)|_{x=-2} = \mathcal{J}(\mathbf{r},t)|_{x=-1} = \mathcal{J}(\mathbf{r},t)|_{x=0}.
\](14)

In this case, the electromagnetic fields may be calculated using the Mur’s conditions [11]. At first, we consider the one-dimensional 1D3V case, described in detail in [2]. The beam with the velocity \( v_b = 0.9 \), temperature \( T_b = 15 \text{ eV} \), and density \( n_b = 6.25 \times 10^{10} \text{ cm}^{-3} \) is injected into the plasma through the boundary \( x = 0 \). The temperature of the plasma electrons is \( T_e = 50 \text{ eV} \), the plasma density is \( n_p = 10^{15} \text{ cm}^{-3} \). Ions are stationary. The dimensions of the region are \( L_x = 160 c/w_p \). Grid steps \( h_x = 0.04 c/w_p \), \( \tau = 0.021/w_p \), where \( w_p = \sqrt{\frac{4 \pi n_e e^2}{m_e}} \) is the plasma frequency. Figure 2 shows the results of the calculation of the electric field excited by the beam for various form-factors and different number of particles at time \( T = 400/w_p \).

It can be seen from Fig. 2 that the simulation result depends only on the number of particles, and approximately 4 times less particles are required for a comparable noise level in the case of parabolic form-factor. In this calculation, the boundary condition does not have a significant effect on the result.

Table 1 shows the root-mean-square deviation of the value of the X-component of the electric field for each type of boundary conditions, the form-factors and the number of particles in cells.

Since the analytical solution is not known in this case, the comparison is made with a smoothed \( E_x \) field obtained by averaging the numerical solution over 25 points (size \( 1 c/w_p \)). Table 1 shows that in all cases, convergence is observed with respect to the number of particles, and the type of
Figure 2. Results of the calculation of the electric field excited by the beam for different form-factors and different number of particles at time $T = 400/w_p$.

the boundary condition has practically no effect on the result. The error for the PIC form-factor with 1600 particles in a cell coincides with the error for the parabolic core and 400 particles in a cell.

Table 1. Error in comparison with the approximated value of the X-component of the electric field.

| Form-factor/Number of particles in a cell | Boundary condition 1 | Boundary condition 2 |
|-----------------------------------------|----------------------|----------------------|
| PIC / 100                               | 0.00239              | 0.00246              |
| PIC / 400                               | 0.00141              | 0.00146              |
| PIC/ 1024                               | 0.00117              | 0.0012               |
| PIC / 1600                              | 0.00101              | 0.00106              |
| Parabolic / 100                         | 0.00173              | 0.0016               |
| Parabolic / 196                         | 0.00138              | 0.0012               |
| Parabolic / 400                         | 0.00101              | 0.00098              |

Thus, in spite of the fact that the PIC form-factor allows faster computations, it is necessary to take much more particles in a cell than in the case of parabolic form-factor, which negates the advantage of the PIC form-factor. To study the generation of radiation in a plasma, it is necessary to carry out 2D and 3D calculations. We consider the problem of the generation of EM radiation in a plasma under the action of colliding electron beams of different widths [10]. Errors in the boundary conditions can lead to the formation of non-physical fields on the plasma boundaries, which eventually lead to incorrect results of the entire simulation. We shall consider the interaction of two colliding beams with a plasma in the 2D3V formulation, i.e., assuming that the particle density and velocity in the Z direction are homogeneous. Two electron beams move along the X direction and enter a plasma confined by a uniform longitudinal magnetic field $(B_z, 0, 0)$. In the Y direction, the plasma column is separated from the boundaries by vacuum regions.

At the initial time, there are no beams in the area. $n_0 = 3.1 \cdot 10^{13} \text{cm}^{-3}$ is the density of plasma electrons. We consider the ions to be immovable. The plasma electrons have the following momentum distribution:

$$f(p_x, p_y, p_z) = \left( \frac{1}{\sigma_z \sqrt{2\pi}} \right)^3 e^{-\frac{(p_x^2 + p_y^2 + p_z^2)}{2\sigma_z^2}},$$

(15)
where $\sigma^2 = m_e kT_e$.

The electron temperature is given by the average kinetic energy of the electrons

$$K_e = \frac{3}{2} kT_e = 40 \text{ eV}. \quad (16)$$

The beams entering the region have the density $n_{b1} = n_{b2} = 0.002 n_0$ and the momentum distribution

$$f(p_x, p_y, p_z) = \left( \frac{1}{\sigma_b \sqrt{2\pi}} \right)^3 e^{-\frac{(p_x^2 + p_y^2 + p_z^2)}{2\sigma_b^2}}, \quad (17)$$

where $\sigma_b^2 = m_e kT_b$.

The external magnetic field $(B_x, 0, 0)$ is determined by the ratio of the Larmor and plasma frequencies.

The particles that reach the boundaries of the region $(y = 0, y = L_y)$ are removed. Since there is a longitudinal magnetic field in the region, the number of such particles is very small. For the electromagnetic fields of the boundaries $y = 0, y = L_y$, the absorbing layer SAL [9] is used to calculate the radiation power absorbed in these layers.

The radiation power is the energy that has left the system in a unit time, and here it is fairly easy to single out the contribution of individual components of electric and magnetic fields to the total radiation power:

$$P_{rad} = \frac{h_x h_y}{2\pi} \sum_{i,l}(Ex_{i,l}^2(1-k_{i,l}) + Ey_{i,l}^2(1-k_{i,l}) + Ez_{i,l}^2(1-k_{i,l}) +$$

$$Bx_{i,l}^2(1-k_{i,l}) + By_{i,l}^2(1-k_{i,l}) + Bz_{i,l}^2(1-k_{i,l})). \quad (18)$$

The efficiency of the radiation power is calculated as $\Psi = P_{rad}/P_{beam}$, where $P_{rad}$ is the radiation power absorbed at the boundaries of the region, $P_{beam}$ is the power of the incoming beams per time step.

Consider the efficiency of electromagnetic radiation for PIC and parabolic form-factors, depending on the type of boundary conditions and the number of particles.

Figure 3 shows the radiation efficiency graphs for four cases of calculating the current density at the boundaries:

1) Boundary conditions 1 with the PIC form-factor.
2) Boundary conditions 2 with the PIC form-factor.
3) Boundary conditions 1 with the parabolic form-factor.
4) Boundary conditions 2 with the parabolic form-factor.

In all cases, we use the grid steps $h_x = h_y = 0.1 c/w_p$ allowing to resolve plasma oscillations arising in the beam-plasma interaction.

Figure 3 shows that for the PIC form-factor, the use of the method of the calculation of the current on the boundary with using of virtual currents (method 1) gives a lower level of radiation efficiency (almost at 1.5 times) than the method that assumes the equality of currents on the boundary (method 2). Using of the method 1 with the parabolic form-factor leads to more smooth radiation efficiency curve with peak near 7%. Method 2 for the parabolic form-factor yields a similar result as method 1 for the PIC form-factor.

In all cases, the convergence of the solution with the increase of the number of particles in a cell is observed. 1600 particles in a cell for the PIC form-factor and 400 for the parabolic one are used in these simulations. Let us consider the maps of the X and Z-components of the electric field (which represent $E_x$, $E_y$, $B_z$-O-mode and $E_z$, $B_x$, $B_y$-X-mode).
Figure 3. Radiation efficiency for various cases of calculating the current density at the boundaries.

It can be seen from Fig. 4 that in the case of the model with the equality of currents in the boundary cells and the Mur’s boundary condition, the formation of significant nonphysical fields near the injection regions of the beams is observed. On the left border, there are practically no such noises, since the left beam is narrower than the plasma. In this case, for the PIC form-factor, the radiation is sufficiently torn. The use of the parabolic form-factor in both cases makes it possible to obtain smoother radiation.

4. Conclusion
In this paper, we compare the realizations of the PIC model of a plasma with open boundary conditions for the case of the PIC form-factor and the parabolic form-factor of particles with different boundary conditions. In 1D geometry, the results of the simulation of the injection of one beam into the plasma for all the models considered are shown to coincide. It was found that in order to achieve a particle noise factor close to the noise level for a parabolic shape in the PIC model, several times more particles are needed, which leads, finely, to an increase in computation time. Thus, the use of the parabolic form-factor is preferable. For the 2D problem of the generation of radiation by colliding electron beams, a significant difference in the results of calculations of the radiation efficiency in the case of the PIC form-factor from the case of the parabolic form-factor is shown. The Mur’s boundary conditions with the continuity conditions for currents are found to provide the growth of nonphysical fields.
Figure 4. Maps of the X and Z-components of the electric field for various ways of calculating the current at the boundary at time $T = 880/u_p$.

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