A PIC method for solving a paraxial model of highly relativistic beams

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Abstract

Solving the Vlasov–Maxwell problem can lead to very expensive computations. To construct a simpler model, Laval et al. [G. Laval, S. Mas-Gallic, P.A. Raviart, Paraxial approximation of ultrarelativistic intense beams, Numer. Math. 69 (1) (1994) 33–60] proposed to exploit the paraxial property of the charged particle beams, i.e., the property that the particles of the beam remain close to an optical axis. They so constructed a paraxial model and performed its mathematical analysis. In this paper, we investigate how their framework can be adapted to handle the axisymmetric geometry, and its coupling with the Vlasov equation. First, one constructs numerical schemes and error estimates results for this discretization are reported. Then, a Particle In Cell (PIC) method, in the case of highly relativistic beams is proposed. Finally, numerical results are given. In particular, numerical comparisons with the Vlasov–Poisson model illustrate the possibilities of this approach.

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1. Introduction

In recent years, modelling and solving numerically problems which couple charged particle to electromagnetic fields has given rise to challenging mathematical and scientific computing developments. Such simulations require to develop models appropriate for numerical experiments, such as the Vlasov–Maxwell system of equations (cf. [4]). This model, even if it is unavoidable in many situations [1] leads however to very expensive computations.

In these conditions, one easily understands the need for deriving simpler (but accurate) models, by exploiting given physical assumptions. Hence, in some cases, the assumption that the problem is static allows us to replace Maxwell’s equations by a reduced model like Poisson’s equation. Following this idea, one can obtain a hierarchy of reduced models, like Vlasov–Poisson, Vlasov-Darwin, paraxial models, etc… generally obtained by exploiting specific geometries/properties of the problem.

We consider here the transport of a bunch of highly relativistic charged particles in the interior of a perfectly conducting tube. As we are in the same physical assumptions as Laval et al. [7], we start from their approach to investigate a paraxial axisymmetric situation. The aim of the present paper 1 is to develop a Particle In Cell (PIC) method for solving a paraxial model.

In a first section, we recall how one can derive such a paraxial model from the Vlasov–Maxwell one, by focusing on the axisymmetric geometry. Then, we construct numerical schemes and we prove some error estimate results. In a third part, a well-adapted particle approach is used to construct a PIC method. The last section is devoted to numerical illustrations. In particular, we propose comparisons with a Vlasov–Poisson like model, which illustrate in which way the models are different.

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1 A short report appeared in the Proceedings of NumAn’07, see [2].
2. From Vlasov–Maxwell to a paraxial model

Consider a beam of charged particles with a mass \( m \) and a charge \( q \) which moves inside a perfectly conducting cylindrical tube, the \( z \)-axis being the axis of the tube. Suppose that the beam is confined in a neighborhood of the \( z \)-axis, which is chosen as the optical axis of the beam. Each particle can be characterized by its position \( \mathbf{x} = (x, y, z) \) and its velocity \( \mathbf{v} = (v_x, v_y, v_z) \) in the phase space \((\mathbf{x}, \mathbf{v})\). Assuming that the beam is relativistic and noncollisional, the motion of these particles can be described in terms of particle distribution function \( f(\mathbf{x}, \mathbf{p}, t) \) by the relativistic Vlasov equation

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \mathbf{F} \cdot \nabla_p f = 0, \tag{1}
\]

where the momentum \( \mathbf{p} \) verifies \( \mathbf{p} = \gamma m \mathbf{v}, \gamma = (1 - \frac{v^2}{c^2})^{-1/2} \). In Eq. (1), \( \mathbf{F} \) denotes the electromagnetic Lorentz force given by

\[
\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \tag{2}
\]

that describes how an electromagnetic field \( \mathbf{E}(\mathbf{x}, t) \) and \( \mathbf{B}(\mathbf{x}, t) \) acts on a particle with a velocity \( \mathbf{v} \). This electromagnetic field satisfies the Maxwell equations in the vacuum

\[
\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = - \mu_0 j, \quad \nabla \cdot \mathbf{E} = \frac{1}{\varepsilon_0} \rho, \tag{3}
\]

\[
\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \quad \nabla \cdot \mathbf{B} = 0. \tag{4}
\]

The charge and the current densities \( \rho \) and \( \mathbf{J} \) are obtained from the distribution function \( f \)

\[
\rho = q \int_{\mathbb{R}^3} f \, d\mathbf{p}, \quad \mathbf{J} = q \int_{\mathbb{R}^3} \mathbf{v} f \, d\mathbf{p} \tag{5}
\]

and have to satisfy the charge conservation equation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0. \tag{6}
\]

This time-dependent Vlasov–Maxwell model is very complete but also requires an important computational effort, in particular in a three-dimensional domain. Even though this is necessary in several cases, one easily understands the need of deriving simpler (but accurate) models, that approximate the Vlasov–Maxwell system with a known accuracy. For instance, assuming that the problem is static allows us to replaced the time-dependent Maxwell’s equations by the static/quasi-static Poisson equation. Following this idea, one can obtain a hierarchy of approximate models (cf. \cite{10}), like Vlasov–Poisson, Vlasov-Darwin, paraxial models, etc.

In the case of high energy short beams, Laval et al. \cite{7} have derived a simplified model in the following way. The high energy assumption means that \( \gamma \gg 1 \). Consequently, since the particle velocity \( \mathbf{v} \) is close to \( c \) for any particle in the beam, one rewrites the Vlasov–Maxwell equations (1)–(4) in the beam frame, which moves along the \( z \)-axis with the light velocity \( c \). Then, set \( \zeta = ct - \nu_z, \nu_z = \frac{c}{\gamma} \). To derive a paraxial model, one then introduces a scaling of the equations. First one exploits the short beams assumption, i.e. the dimensions of the beam are small compared to the longitudinal length of the device. Moreover, one assumes that the longitudinal particle velocities \( v_z \) are close to the light velocity \( c \), whereas the transverse particle velocities are small compared to \( c \). Hence one introduces the transverse characteristic velocity of the particles \( \overline{\nu} \), and defines a small parameter \( \eta, \eta = \frac{\nu}{\overline{\nu}} \ll 1 \). We thus obtain a Vlasov–Maxwell system of equations expressed in dimensionless variables, where appear powers of the small parameter \( \eta \). The next step consists in developing asymptotic expansions of all these quantities (\( f, \mathbf{E}, \mathbf{B}, \mathbf{F}, \) etc.) in powers of the small parameter \( \eta \). It is proved in \cite{7} that the resulting paraxial model, obtained by retaining the first four terms in the asymptotic expansion, is an approximation exact up to the order 3 in \( \eta \).

In this paper, we examine the axisymmetric case. Using the coordinates \( (r, \theta, \zeta) \) (with obvious notations), the electric field is now denoted \( (E_r, E_\theta, E_z) \), the magnetic one \( (B_r, B_\theta, B_z) \). From \cite{7}, one obtains that the electromagnetic force \( \mathbf{F} \) is entirely determined by the transverse fields, which are zero order fields, the longitudinal ones, that are first order fields, and the so-called pseudo-fields \( \overline{E}_r = E_r - cB_\theta \) and \( \overline{E}_\theta = E_\theta + cB_r \), which are second order corrections. Hence, the paraxial model of ultrarelativistic Maxwell equations is written:

For the zero order fields:

\[
\begin{aligned}
E_r &= cB_\theta = \frac{1}{\varepsilon_0 r} \int_0^r \rho \, s \, ds \\
E_\theta &= B_r = 0.
\end{aligned} \tag{7}
\]
For the first order fields:

\[
\begin{align*}
\frac{\partial E_z}{\partial r} &= \frac{\partial B_\theta}{\partial t} \\
E_z(r = R) &= 0 \quad \text{and} \quad \oint_0 B_z r dr = 0.
\end{align*}
\] (8)

For the second order pseudo-fields \( E_\xi \) and \( E_\phi \):

\[
\begin{align*}
E_\xi &= \frac{1}{r} \int_0^r \left( \mu_0 c J_k - \frac{1}{c} \frac{\partial E_z}{\partial t} \right) \, ds \\
E_\phi &= -\frac{1}{r} \int_0^r \frac{\partial B_x}{\partial t} \, ds,
\end{align*}
\] (9)

where \( J_k \) is defined by \( J_k = \rho c - J_z = q \int v_z f \, dv \).

Remark that, contrary to quasistatic approximations where time derivatives are neglected (like Poisson or “frozen field” approximation [8]) the beam here is not assumed to be steady-state. We refer the reader to [12] for a detailed derivation of this model.

3. Discretization of the fields

As we are working in the beam frame, the particles drift slowly in the direction \( \zeta > 0 \). As a consequence, the computational domain is defined as a simple rectangular domain in variables \((r, \zeta)\), \(0 \leq r \leq R, 0 \leq \zeta \leq Z\). The value of \( R \) is given by the radius of the cylindrical tube, and \( Z \) is chosen in such a way that the particles remain in a fixed geometrical domain \( \Omega \times 10, Z \) (in the beam frame), during the time interval \([0, T]\) of the simulation. Hence a finite difference method is a natural approach to construct the algorithms.

Remark first that the order of the computations of unknown fields is induced by the asymptotic expansion. For example, the zero order fields \( E_r, B_\theta \) have to be first computed, and are necessary to obtain the first order quantities \( E_z, B_z \), etc. Note also that the zero order fields are computed only from the charge density approximation, which is a computed function in the PIC method. In these conditions, it is necessary to analyze the approximation quality of the higher order fields, introduced in the model through the approximation quality of the lower order ones. In other words, despite the simplicity of the paraxial model – numerical schemes will be derived by applying elementary methods of numerical integration and differentiation – these methods will be applied not to exact functions as it is commonly described in the literature, but to numerical approximations. This section describes the way in which the numerical schemes are constructed and analyzed.

3.1. Numerical schemes and error estimates

We introduce a two-dimensional grid in variables \((r, \zeta)\). We denote by \( \Delta r, \Delta \zeta \) the corresponding constant mesh sizes, and we set \( r_i = (i - 1) \Delta r, 1 \leq i \leq I, \zeta_j = (j - 1) \Delta \zeta, 1 \leq j \leq J \). Given a constant time step \( \Delta t \), we set \( t_n = n \Delta t, t_{n+\frac{1}{2}} = (n + \frac{1}{2}) \Delta t \).

3.1.1. Numerical schemes for \( E_r \) and \( B_\theta \)

Using the trapezoidal rule to (7), the numerical schemes for \( E_{r,i,j}, B_{\theta,i,j} \) can be written as follows

\[
E_{r,i,j}^n = cB_{\theta,i,j}^0 = \frac{\Delta t}{2e_0 \epsilon_i} \left[ \sum_{k=2}^{i-1} \rho_{k,i,j}^n - \rho_{i-1,j}^n f_i + \rho_{i,j}^n f_i \right]
\] (10)

that can be reduced to the following iterative relation, which is more efficient from the computational point of view

\[
E_{r,i,j}^{n+1} = E_{r,i-1,j}^{n+1} + \frac{1}{e_0 \epsilon_i} \frac{\Delta r}{2} \left[ \rho_{i-1,j}^{n+1} f_{i-1} + \rho_{i,j}^{n+1} f_i \right].
\] (11)

Concerning error estimate results for the scheme, we assume that \( \rho_{i,j}^n \) is a given discrete approximation of \( \rho(r, \zeta, t) \) up to the order \( ((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s) \), \( r \geq 2 \). Approximating \( rE_r(r, \zeta, t) \) with the trapezoidal rule up the order \( ((\Delta r)^2, (\Delta \zeta)^q, (\Delta t)^s) \), one can find \( k_1, k_2, k_3 > 0 \) such that

\[
|E_{r,i,j}^n - E_r(r, \zeta, t)| \leq \left[ k_1 (\Delta r)^2 + k_2 (\Delta \zeta)^q (\Delta t)^s + k_3 (\Delta r)^{-1} (\Delta \zeta)^q (\Delta t)^s \right],
\] (12)

that can be summarized in the following proposition

**Proposition 3.1.** Let \( \rho_{i,j}^n \) be a discrete function that approximates the function \( \rho(r, \zeta, t) \) up to the order \( ((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s) \), \( p \geq 2 \). Trapezoidal scheme applied to \( \rho_{i,j}^n \), yields \( E_r, cB_\theta \) approximation up to the order \( (\Delta r, (\Delta \zeta)^q, (\Delta t)^s) \).
One can easily improve this result by deriving a scheme based on Simpson-like integration rule. Hence, we obtain the following scheme
\[
E^n_{z,i,j} = \frac{1}{\theta_0} \frac{\Delta r}{6} \left[ \sum_{k=0}^{q-1} 2(\rho^n_{z,k} + \rho^n_{z,k+1}) + \rho^n_{z,k+1} \right],
\]
which shows that the replacement of trapezoidal schemes by their Simpson counterparts is quite straightforward. Using the same elementary arguments, one can prove here

**Proposition 3.2.** Let \( \rho^n_{z,i} \) be a discrete function that approximates the function \( \rho(r, \zeta, t) \) up to the order \( (\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s \), \( p \geq 4 \). Applying Simpson’s scheme to \( \rho^n_{z,i} \), yields \( E_z, cB_0 \) approximation up to the order \( (\Delta r)^3, (\Delta \zeta)^0, (\Delta t)^0 \).

### 3.1.2. Numerical scheme for \( E_z \)

Using the previously computed \( B_0 \), one applies to (8) a first order finite difference scheme, so that the longitudinal electric component \( E_z \) is approximated by
\[
\frac{1}{\Delta r}(E^n_{z,i+1,j} - E^n_{z,i,j}) = -\frac{1}{\Delta t}(B^n_{x,i,j} - B^n_{x,i,j-1}), \quad E^n_{z,i,j} = 0,
\]
or in a more suitable form for practical computations
\[
E^n_{z,i,j} = E^n_{z,i+1,j} + \frac{\Delta r}{\Delta t}(B^n_{x,i,j} - B^n_{x,i,j-1}).
\]

To investigate the error propagation with respect to the radius \( r \) in this case, we first introduce the error
\[
e^n_{z,i,j} = E_z(r, \zeta, t_n) - E^n_{z,i,j},
\]
and prove the following estimation

**Proposition 3.3.** Let \( E^n_{z,i,j} \) be a discrete function that approximates the function \( E_z \) up to the order \( (\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s \), \( p, q, s \geq 2 \). Numerical scheme (15) yields \( E_z \) approximation with an error \( e^n_{z,i,j} \) given by
\[
e^n_{z,i,j} \leq \frac{1}{c} \left[ (\Delta r)^p + (\Delta \zeta)^q + (\Delta t)^s \right]
\]

**Proof.** Using the errors \( e^n_{z,i,j} \) and \( b^n_{x,i,j} = B_0(r, \zeta, t_n) - B^n_{x,i,j} \), Eq. (15) is expressed as
\[
E^n_{z,i,j} = E^n_{z,i+1,j} + \frac{\Delta r}{\Delta t}(B_0(r, \zeta, t_n) + b^n_{x,i,j} - B^n_{x,i,j} - b^{n-1}_{x,i,j}).
\]

Using algebraic manipulations together with Taylor expansion, one can easily verify that there exists a positive constant \( M > 0 \), such that \( M \geq \frac{\partial^2 b_0}{\partial r^2}(r, \zeta, t) \) and
\[
e^n_{z,i,j} \leq \frac{\Delta r}{\Delta t} \left[ (\Delta r)^p + (\Delta \zeta)^q + (\Delta t)^s \right],
\]
\[
e^n_{z,i,j} \leq \frac{\Delta r}{\Delta t} \left[ (\Delta r)^p + (\Delta \zeta)^q + (\Delta t)^s \right] + M((\Delta r)^2 + \Delta r \Delta t).
\]

One solves this recursion equation by taking into account the convergence order for \( cB_0 = E_z \). This yields
\[
|b^n_{x,i,j}| \leq \frac{K}{c} \left[ (\Delta r)^p + (\Delta \zeta)^q + (\Delta t)^s \right] \quad \text{for some } K \geq 0.
\]

Now using that
\[
e^n_{z,i,j} \leq e^n_{z,i+1,j} + \frac{\Delta r}{c\Delta t} K \left[ (\Delta r)^p + (\Delta \zeta)^q + (\Delta t)^s \right] + M((\Delta r)^2 + \Delta r \Delta t), \quad e^n_{z,i,j} = 0,
\]
and converting this recurrent formula into summation, we obtain
\[
e^n_{z,1,j} \leq \sum_{i=1}^{l} \frac{\Delta r}{c\Delta t} K \left[ (\Delta r)^p + (\Delta \zeta)^q + (\Delta t)^s \right] + M((\Delta r)^2 + \Delta r \Delta t),
\]
and finally (with \( l = \frac{1}{\Delta r} \), \( l \) the transverse domain size)
\[
e^n_{z,1,j} \leq \frac{1}{\Delta r} \left[ \frac{\Delta r}{c\Delta t} K \left[ (\Delta r)^p + (\Delta \zeta)^q + (\Delta t)^s \right] + M((\Delta r)^2 + \Delta r \Delta t) \right].
\]

This concludes the proof. □
3.1.3. Numerical scheme for $B_2$

To derive a scheme for computed $B_2$, we first integrate with respect to $r$ the first equation of (8) to get

$$B_2(r, \zeta, t) = \mu_0 \int_0^r J_0(\sigma, \zeta, t) d\sigma + c(\zeta, t).$$

(18)

From the second equation of (8), we have

$$\int_0^R B_2 \sigma d\sigma = \frac{\sigma^2}{2} B_2 \bigg|_0^R - \int_0^R \frac{\sigma^2}{2} \frac{\partial B_2}{\partial r} d\sigma = \frac{R^2}{2} B_2(R, \zeta, t) - \frac{\mu_0}{2} \int_0^R \sigma^2 J_0 d\sigma = 0,$$

that yields

$$B_2(R, \zeta, t) = \frac{\mu_0}{R^2} \int_0^R \sigma^2 J_0(\sigma, \zeta, t) d\sigma.$$  

(20)

Thus we obtain

$$\mu_0 \int_0^R J_0(\sigma, \zeta, t) d\sigma + c(\zeta, t) = \frac{\mu_0}{R^2} \int_0^R \sigma^2 J_0(r, \zeta, t) d\sigma,$$

(21)

and finally

$$c(\zeta, t) = \frac{\mu_0}{R^2} \int_0^R J_0(\sigma, \zeta, t)(\sigma^2 - R^2) d\sigma.$$  

(22)

Introducing now $V^n_j = J^n_{0,i,j}(r^2 - R^2)$, we compute the numerical approximation $C^n_j$ of $c(\zeta, t)$ with

$$C^n_j = \frac{\mu_0}{R^2} \int_0^R J_0(\sigma, \zeta, t)(\sigma^2 - R^2) d\sigma.$$  

(23)

Using still the trapezoidal rule leads to the following scheme

$$B^n_{z,i,j} = -\frac{\mu_0}{2} \Delta r \left[ \sum_{k=2}^{i-1} J^n_{0,k,j} + J^n_{0,i,j} + J^n_{0,i+1,j} \right] + C^n_j, \quad \text{with } B^n_{z,i,j} = 0.$$  

(24)

Let us define now the approximation error $b^n_{z,i,j}$ as $B_2(r, \zeta, t_n) - B^n_{z,i,j}$. The error estimation for $B_2$ is based on the fact that (24) is essentially a numerical integration of $J_0$ and $J_0 r^2$.

Assuming that $J^n_{0,i,j}$ is an approximation of $J_0$ up to the order $((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^r)$, $p \geq 2$. Hence the order of $J^n_{0,i,j} r^2$ is $((\Delta r)^{p+2}, (\Delta \zeta)^q, (\Delta t)^r).$ Applying the trapezoidal rule to $J^n_{0,i,j}$ and to $J^n_{0,i,j} r^2$ respectively gives the following result

**Proposition 3.4.** Let $J^n_{0,i,j}$ be a discrete function that approximates $J_0$, up to the order $((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^r)$, $p \geq 2$. Numerical scheme (24) yields a $((\Delta r)^{p+2}, (\Delta \zeta)^q, (\Delta t)^{r+1})$ order approximation for $B_2$.

3.1.4. The schemes for $\varepsilon_r$ and $\varepsilon_0$

The schemes for $\varepsilon_r$ and $\varepsilon_0$ are derived essentially with the same arguments. The time derivative that appears in (9) is approximated using backward difference scheme. For instance for $\varepsilon_r$

$$\left( \frac{\partial E^n}{\partial t} \right)_{i,j} \simeq \frac{1}{\Delta t} \left( E^n_{z,i,j} - E^{n-1}_{z,i,j} \right).$$  

(25)

Let us define

$$W^n_{z,j} = \mu_0 C^n_{\zeta,i,j} - \frac{1}{C} \left( \frac{\partial E^n}{\partial t} \right)_{i,j},$$  

and apply the trapezoidal rule to $W^n_{z,j}$ gives the final expression

$$\varepsilon^n_{r,i,j} = \frac{\Delta r}{2\Delta t} \left[ 2 \sum_{k=2}^{i-1} W^n_{k,j} r_k + W^n_{i,j} r_1 + W^n_{i,j} r_i \right].$$

(26)

Concerning the approximation error, we also introduce $\varepsilon_r = \mathcal{E}^n_{r,i,j} - \varepsilon_r(r_i, \zeta_i, t_n)$, and assume that $J^n_{z,i,j}$ and $E^n_{z,i,j}$ are given $((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^r)$ order approximations. Hence $\frac{\partial E^n}{\partial t}$ obtained by backward difference scheme is $((\Delta r)^{p+1}, (\Delta \zeta)^q, (\Delta t)^{r+1})$ order approximation and so is $W^n_{z,j}$. This finally gives
Proposition 3.5. Let \( J_{i,j}^n \) and \( E_{z,i,j}^n \) be discrete functions that approximate \( J_z \) and \( E_z \) up to the order \( ((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s) \), \( p, q, s \geq 2 \). Then numerical scheme (26) yields \( ((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s) \) order approximation for \( \varepsilon_r \).

In the same way, we obtain for \( \varepsilon_\theta \)

\[
\varepsilon_{\theta,i,j}^n = -\frac{\Delta r}{2r_i} \left[ 2 \sum_{k=2}^{i-1} \left( \frac{\partial B}{\partial t} \right)_{k,j}^n r_k + \left( \frac{\partial B}{\partial t} \right)_{1,j}^n r_1 + \left( \frac{\partial B}{\partial t} \right)_{i,j}^n r_i \right]
\] (27)

and the error estimate.

Proposition 3.6. Let \( B_{z,i,j}^n \) be a function that approximates \( B_z \) up to the order \( ((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s) \), \( p, q, s \geq 2 \). Then numerical scheme (27) yields \( ((\Delta r)^p, (\Delta \zeta)^q, (\Delta t)^s) \) order approximation for \( \varepsilon_\theta \).

4. Coupling the particles and fields

This section describes the way in which particles are advanced and coupled with the previous field solutions. A detailed introduction to particle-in-cell methods can be found in [4,6].

4.1. Particle integration

The paraxial model of highly relativistic beams couples the above field equations to particle motion at each time step. So we consider the axisymmetric counterpart of the Vlasov equation (1). Let \( \mathbf{x} = (r, z) \) and \( \mathbf{p} = (p_r, p_\theta, p_z) \) denote the position and the momentum in the axisymmetric configuration, and assume that the particle distribution function \( f(\mathbf{x}, \mathbf{p}, t) \) is independent of \( \theta \). According to the particle method (cf. [9]), \( rf(\mathbf{x}, \mathbf{p}, t) \) is approximated in the phase space \( (\mathbf{x}, \mathbf{p}) \) by

\[
rf(\mathbf{x}, \mathbf{p}, t) = \sum_k w_k \delta(\mathbf{x} - \mathbf{x}_k(t)) \delta(\mathbf{p} - \mathbf{p}_k(t)),
\] (28)

where \( w_k \) denotes the weight of the particle \( k \). Now, each particle, represented by its position and momentum, obeys

\[
\begin{align*}
\frac{\partial r}{\partial t} &= \frac{1}{\gamma m} p_r, \\
\frac{\partial \theta}{\partial t} &= \frac{1}{\gamma m} p_\theta, \\
\frac{\partial z}{\partial t} &= \frac{1}{\gamma m} p_z, \\
\frac{\partial p_r}{\partial t} &= \frac{1}{\gamma m} \gamma \mu r p_\theta + F_r, \\
\frac{\partial \theta}{\partial t} &= -\frac{1}{\gamma m} \gamma \mu \gamma p_\theta + F_\theta, \\
\frac{\partial p_z}{\partial t} &= F_z,
\end{align*}
\] (29)

where the paraxial electromagnetic force \( \mathbf{F} = (F_r, F_\theta, F_z) \) satisfies

\[
\begin{align*}
F_r &= q(\varepsilon_r + \nu_v^\theta B_z + \nu_r B_\theta), \\
F_\theta &= q(\varepsilon_\theta + \nu_v B_z), \\
F_z &= q(F_z + \nu_r B_\theta).
\end{align*}
\] (30)

Numerically, these equations of motion are integrated using a leapfrog scheme, which is a second-order centered finite difference scheme. The particle positions are defined at time \( t_n \) and the particle momenta are computed at time \( t_{n+1/2} \).

One of the problems encountered when one considers the relativistic case is the need of \( \gamma^n \) to compute the velocities which appear in the expression of the force (30). Moreover, as we consider the axisymmetric problem, \( \gamma^n \) is also needed to compute the \( p_r \) and \( p_\theta \) components of the momentum, as (29) shows. We therefore use a prediction \( \tilde{\mathbf{p}} \) of \( \mathbf{p} \), that is an adaptation to the paraxial model of the Boris method [5]. More details can be found in [3].

Lastly, remark that the use of regular uniform grids avoid to deal with the problem of locating the particles in an irregular mesh. Indeed, to assign a particle to a particular rectangular element, in order to allocate its charge or current, is trivial.

4.2. Charge and current assignment

In this paragraph, we describe the charge and current assignment, that will give source terms for the paraxial electromagnetic fields. In the continuous case, charge and current densities are linked to the distribution function \( f \) by the relation (5). In PIC simulations, these functions are approximated using the particle method. This gives the following approximations for \( \mathbf{J} \) and \( \rho \)

\[
\begin{align*}
\rho(\mathbf{x}, t) &= q \sum_k w_k \delta(\mathbf{x} - \mathbf{x}_k(t)), \\
\mathbf{J}(\mathbf{x}, t) &= q \sum_k w_k \mathbf{v}_k(t) \delta(\mathbf{x} - \mathbf{x}_k(t)).
\end{align*}
\] (31)
which are defined at the particle locations. Therefore we need to define $\rho(a_i)$ and $\mathbf{J}(a_i)$ at the points $a_i = (r_i, \zeta_i)$ of the grid. We employ here the following inverse bilinear interpolation procedure

$$r_i \rho(a_i) = -e \sum_{k \in \mathcal{K}_{a_i}} w_k c_{ik}, \quad r_i \mathbf{J}(a_i) = -e \sum_{k \in \mathcal{K}_{a_i}} w_k \mathbf{v}_k c_{ik}, \quad \text{(32)}$$

where $\mathcal{K}_{a_i}$ is a set of particles located in the rectangles which have $a_i$ as a vertex, $c_{ik}$ are bilinear interpolation coefficients for the particle $k$, relatively to the grid point $a_i$.

Conversely, the electromagnetic field has to be computed at the particle locations, to get the force acting on the particles. We use bilinear interpolation coefficients (cf. [11]) in the following way. Let $a_1 = (r_1, \zeta_1), a_2 = (r_2, \zeta_2), a_3 = (r_1, \zeta_1), a_4 = (r_1, \zeta_2)$ be the four grid points of the rectangular element surrounding the particle located in $x_k = (r_k, \zeta_k)$. For any field component $A_i$, we define

$$A(x_k) = \sum_{i=1}^{4} c_i A(a_i), \quad \text{(33)}$$

where $c_i$ are bilinear interpolation coefficients,

$$c_1 = \frac{(\zeta - \zeta_2)(r - r_1)}{(r_1 - r_2)(\zeta_1 - \zeta_2)}, \quad c_2 = \frac{(\zeta - \zeta_1)(r - r_1)}{(r_1 - r_2)(\zeta_1 - \zeta_2)},$$

$$c_3 = \frac{(\zeta - \zeta_2)(r - r_2)}{(r_1 - r_2)(\zeta_1 - \zeta_2)}, \quad c_4 = \frac{(\zeta - \zeta_1)(r - r_2)}{(r_1 - r_2)(\zeta_1 - \zeta_2)}. \quad \text{(34)}$$

As expected, such procedures preserve the total charge and current in the following sense.

**Proposition 4.1.** The assignment procedure (32) satisfies

$$\sum_{i \in I} r_i \rho(a_i, t) = -e \sum_{k \in \mathcal{K}} w_k \quad \text{(35)}$$

and

$$\sum_{i \in I} r_i \mathbf{J}(a_i, t) = -e \sum_{k \in \mathcal{K}} w_k \mathbf{v}_k \quad \text{(36)}$$

where $I$ denotes the set of nodes in the domain and $\mathcal{K}$ is the set of particles.

5. Numerical results

We present two test-cases below, to show the validity and the possibilities of the method. The first case is an illustration of the paraxial Maxwell-Vlasov solver. In the second case, we propose a comparison with a Vlasov-Poisson like solver. In both cases, the computational domain is the rectangle $[0, R] \times [0, Z]$ in variables $(r, \zeta)$. The mesh sizes $\Delta r$, $\Delta \zeta$ are chosen such that $R/\Delta r = Z/\Delta \zeta = 0.01$. The time step $\Delta t$ is taken in order to comply with the CFL stability condition (in the first case only). We encoded the problem in Matlab, and numerical experiments were carried out on a usual PC.

5.1. A Vlasov-Paraxial case

As a numerical example, consider a bunch of particles emitted with velocities such that the paraxial assumptions are verified. For accuracy reasons [4], more than 10 particles are placed in each cell, with the same weight and a charge following $w = \frac{1}{N^0}$, $\mathbf{J}$ the total current to be emitted, and $N$ the particle number). Figs. 1 and 2 show respectively the self-consistent electric radial field $E_r$, and the charge density $\rho$ obtained after 50 time steps of simulation with the resulting PIC paraxial code.

5.2. A Vlasov-Poisson like model

Let us assume that we can neglect the time derivative $\partial_t \mathbf{B}$ in Faraday’s law (4), then $\nabla \times \mathbf{E} = 0$ yields $\mathbf{E} = -\nabla \phi$, where $\phi$ denotes the electrostatic potential. From the Coulomb’s law $\nabla \cdot \mathbf{E} = \rho/\varepsilon_0$, we get the classical quasi-static Vlasov-Poisson model

$$\begin{align*}
-\Delta \phi &= \frac{\rho(t)}{\varepsilon_0}, \\
\mathbf{E} &= -\nabla \phi,
\end{align*}$$
coupled with the Vlasov equation (1), in which the Lorentz force is given by
\[ \mathbf{F} = q\mathbf{E} = -q\nabla \phi. \]

The main advantage of this model is that it is not explicitly time-dependent, the charge density \( \rho(t) \) being given at each time step of the Vlasov equation solution.

**Remark 5.1.** This model was also derived in the context of reduced models. In [10], Sonnendrücker et al. assume that the velocity of the particles \( v_p \) is very small compared to the velocity of the electromagnetic waves \( c \), and introduce a small parameter \( \eta = \frac{v_p}{c} \). Then after a scaling and an asymptotic expansion of the solution in power of \( \eta \), they proved that the quasistatic model is a first order approximation of the Maxwell equations.

At first glance, there are interesting similarities between the zero-order terms of the paraxial model and the Vlasov–Poisson equation, both written in the beam frame. This remark motivates the following numerical comparisons. Writing the axisymmetric Poisson equation in the beam frame \((r, \zeta)\), we obtain
\[
\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial \zeta^2} = \frac{1}{\varepsilon_0} \rho, \tag{37}
\]
and the electric field verifies
\[
\mathbf{E} = \left( \frac{\partial \phi}{\partial r}, \frac{\partial \phi}{\partial \zeta} \right). \tag{38}
\]
Then, deriving numerical schemes for Vlasov–Poisson equation by straightforward finite differences approximation leads to

\[
\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta r^2} + \frac{1}{r_i} \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta r} + \frac{\phi_{i,j+1} - 2\phi_{i,j} - \phi_{i,j-1}}{\Delta \zeta^2} = \frac{1}{\varepsilon_0} \rho_{i,j}
\]  

(39)

with the boundary condition

\[
\rho|_{r,j} = \rho|_{r,0} = 0, \quad \text{and} \quad \phi|_{r=0} = 0.
\]  

(40)

The electric field is here approximated with

\[
(E_r, E_\theta, E_z)_{i,j} = \left( \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta r}, 0, -\frac{\phi_{i,j+1} - \phi_{i,j}}{\Delta \zeta} \right).
\]  

(41)

A snapshot of the simulation obtained with this Vlasov–Poisson (VP) solver (in the beam frame) is shown on Figs. 3 and 4.

From a physical point of view, this problem can be partially compared with the previous one. Indeed, in the paraxial model, the particle motion is first governed by the “massive” (zero-order) radial electric field $E_r$, whereas the longitudinal field $E_z$ appears as a first-order correction.
Now, as similar expression can be obtained for the radial electric field \( E_r \) solution to the Vlasov–Poisson model by imposing \( E_z = 0 \). In that case, \( E_r \) can be easily reduced to the zero-order paraxial model

\[
E_r = \frac{1}{\varepsilon_0 r} \int_0^r \rho s \, ds.
\]

Otherwise, \( E_r \) and \( E_z \) solution to Vlasov–Poisson equation will be approximately at the same scale. Indeed, Poisson equation describes electric field that depends only on the distance between particles, without taking into account their velocity. Hence, the cornerstone of the paraxial model, the assumption that particle velocity is close to the speed of light, can not be handled properly in Poisson equation that describes in essence static electric field.

To illustrate this point, we have shown on Figs. 5 and 6 the so-called phase space \( \zeta - p_z \) in both models. Indeed, if the longitudinal electric component \( E_z \) is incorrect (or overestimated), as so is the longitudinal component \( F_z \) (see Eq. (30)). Then with relation (29), \( p_z \) is also incorrect, and so is the position \( z \) (or \( \zeta \)).

Due to its sensitivity to particle velocity, the paraxial model, which appears numerically as simple as a static or quasistatic one, is much more powerful for ultrarelativistic process simulation than a Vlasov–Poisson model.

6. Conclusion

In this paper, a PIC method for solving a paraxial model of highly relativistic beam has been developed. It has been constructed from a paraxial approximation of the Vlasov–Maxwell equations in an axisymmetric geometry. We construct numerical schemes based on finite difference methods for the Maxwell equations, and error estimate results have been proved. Numerical results were presented to illustrate the feasibility and the accuracy of this approach. Numerical
comparisons with a Vlasov–Poisson model written in the beam frame were performed. They help us to illustrate the importance of handling more accurate models than the first order Vlasov–Poisson one.

References