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3D NUMERICAL APPROXIMATION OF RELATIVISTIC PARTICLE BEAMS BY ASYMPTOTIC EXPANSION

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Abstract. We consider the numerical approximation and simulation of a particle beam, usually modeled by the Vlasov-Maxwell system. Our work will deal with a 3D paraxial approximate model, derived from asymptotic expansions. It includes a finite element numerical implementation of the paraxial Maxwell model coupled with a Particle-In-Cell method for the corresponding paraxial Vlasov model. Both methods are implemented with Freefem++ software. Numerical results illustrated the efficiency of the method.

1 INTRODUCTION

Charged particle beams and plasma physics problems are extensively used in Science and Technology. Although we often associate accelerators with the large machines of high-energy physics, charged particle beams have continually expanding applications in many branches of research and technology. Recent active areas include flat-screen cathode-ray tubes, synchrotron light sources, beam lithography for microcircuits, thin-film technology, production of short-lived medical isotopes, radiation processing of food, and free-electron lasers. Clearly, there exists a significant interest in building mathematical models for these beams.

If we consider collisionless plasma or non-collisional beams, one of the most complete mathematical models is the time-dependent Vlasov-Maxwell system of equations. However, the numerical solution of such models requires a large computational effort. Therefore, whenever possible, we have to take into account the particularities of the physical problem to derive asymptotic approximate models leading to cheaper simulations.

In this article, we consider the case of high energy short beams. A typical example is the transport of a bunch of highly relativistic charged particles in the interior of a perfectly conducting hollow tube. Numerical simulations are mostly performed using the particle-in-cell method.

Following [1–5], we introduce a paraxial model that approximate the coupled time-dependent Vlasov-Maxwell equations. This model is derived by introducing a frame which moves along the optical axis at the speed of light. Then, considering a scaling of the equations which reflects the characteristics of the high energy short beam, a small parameter η is introduced, and asymptotic expansion techniques are used to derive a paraxial model, accurate up to fourth order in η.

This model is then approximated by a finite element method, for the paraxial Maxwell model, coupled with a Particle-In-Cell method for the corresponding paraxial Vlasov model. This implementation is based on the Freefem++ software [7]. First numerical results are proposed, and show the efficiency of the method.

2 THE 3D GOVERNING EQUATIONS

2.1 The Vlasov-Maxwell model

We consider the transport of a population of highly relativistic charged particles, with a mass m and a charge q, in the interior of a perfectly conducting hollow tube, whose axis is constituted by the z-axis. We denote by Ω the transverse section of boundary Γ. Let $\mathbf{x}=(x,y,z)$ denote the position of a particle, $\mathbf{p}=(p_x,p_y,p_z)$ its momentum and $\mathbf{v}=(v_x,v_y,v_z)$ its velocity. We assume that the beam is non collisional so that its distribution function $f=f(\mathbf{x},\mathbf{p},t)$ in the phase space $(\mathbf{x},\mathbf{p})$ is a solution to the Vlasov equation

$$\frac{\partial f}{\partial t} + \mathbf{v}.\nabla_{\mathbf{x}} f + \mathbf{F}.\nabla_{\mathbf{p}} f = 0, \qquad \text{where } \mathbf{p} = \gamma m \mathbf{v}, \qquad \gamma = (1 - \frac{|\,\mathbf{v}\,|^2}{c^2})^{-1/2}. \tag{1}$$

Above, $\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ denotes the electromagnetic force acting on the particles. The electric field $\mathbf{E}=\mathbf{E}(\mathbf{x},t)$ and the magnetic field $\mathbf{B}=\mathbf{B}(\mathbf{x},t)$ are solutions to Maxwell's equations

$$\begin{cases} \dfrac{\partial \mathbf{E}}{\partial t} - c^2 \nabla \times \mathbf{B} = -\dfrac{1}{\varepsilon_0}\mathbf{J}, & \dfrac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \\ \nabla.\mathbf{E} = \dfrac{\rho}{\varepsilon_0}, & \nabla.\mathbf{B} = 0, \end{cases} \tag{2}$$

where the charge and the current density ρ and $\mathbf{J}$ are obtained from the distribution function f with

$$\rho = q\int f d\mathbf{p}, \qquad \mathbf{J} = q\int \mathbf{v} f d\mathbf{p}. \tag{3}$$

Assuming the tube being perfectly conducting is equivalent to assuming that $\mathbf{E}$ (respectively $\mathbf{B}$) have a vanishing tangential (respectively normal) trace on the tube boundary.

2.2 The paraxial model

Assuming that the beam is highly relativistic corresponds to assume that $\gamma >> 1$. Since $v_z \simeq c$ for any particle in the beam, the Vlasov-Maxwell equations (1-2) can be written in a frame which moves along z-axis with the light velocity c. For this purpose, we set $\zeta = ct - z$, $v_\zeta = c - v_z$ and we perform the change of variables $(x, y, z, v_x, v_y, v_z, t) \to (x, y, \zeta, v_x, v_y, v_\zeta, t)$. It is also convenient to introduce the transverse quantities

$$\mathbf{x}_\perp = (x, y),\ \mathbf{v}_\perp = (v_x, v_y)$$

and to define the transverse operators

$$\mathbf{grad}_\perp\varphi = (\frac{\partial\varphi}{\partial x}, \frac{\partial\varphi}{\partial y}), \quad \mathbf{curl}_\perp\varphi = (\frac{\partial\varphi}{\partial y}, -\frac{\partial\varphi}{\partial x}), \quad \Delta_\perp\varphi = \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2},$$

for $\varphi = \varphi(x, y)$ a given scalar function. Similarly, for $\mathbf{A}_\perp = (A_x, A_y)$ denoting a transverse vector field, we set

$$div_\perp\mathbf{A}_\perp = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y}, \quad curl_\perp\mathbf{A}_\perp = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}.$$

With these notations, the Vlasov-Maxwell equations (1-2) can be expressed in the new variables. The second step to derive the paraxial model consists in introducing characteristic quantities and rewrite the system of equations in dimensionless variables. Introducing a small parameter, the paraxial model was derived by retaining the terms up to the third order in the asymptotic expansion of the distribution function f. This third order expansion of f is entirely determined from the expansion of the transverse electromagnetic force $\mathbf{F}_\perp$ up to order 2, and from the expansion of the longitudinal electromagnetic force F_z up to order 1 only.

As a consequence, it was proved that the asymptotic paraxial Vlasov- Maxwell model requires the knowledge of the principal parts (zero order) of the transverse electric field $\mathbf{E}_\perp$, the first order part of the longitudinal electromagnetic field (E_z, B_z), and the second order part of the transverse so-called "pseudo-fields" $\mathcal{E}_\perp$, where $\mathcal{E}_\perp = (\mathcal{E}_x, \mathcal{E}_y)$ is defined by $\mathcal{E}_x = E_x - cB_y, \mathcal{E}_y = E_y + cB_x$. Details may be found in [2], [3].

Based on these remarks, we have to approximate by numerical methods the paraxial Vlasov equation, and the electromagnetic components $\mathbf{E}_\perp, E_z, B_z, \mathcal{E}_\perp$, solutions to the following paraxial Maxwell equations:

$$\left\{\begin{array}{l} curl_\perp \mathbf{E}_\perp = 0 \text{ in } \Omega\,, \\ div_\perp \mathbf{E}_\perp = \frac{1}{\varepsilon_0}\rho \text{ in } \Omega\,, \\ \mathbf{E}_\perp \cdot \boldsymbol{\tau} = 0 \text{ on } \Gamma\,, \end{array}\right. \qquad \mathbf{B}_\perp = -\frac{1}{c}\mathbf{E}_\perp \times \mathbf{e}_z\,, \qquad \left\{\begin{array}{l} \mathbf{curl}_\perp E_z = -\frac{\partial \mathbf{B}_\perp}{\partial t} \text{ in } \Omega\,, \\ E_z = 0 \text{ on } \Gamma\,, \end{array}\right.$$

$$\left\{\begin{array}{l} \mathbf{curl}_\perp B_z = \mu_0 \mathbf{J}_\perp + \frac{1}{c^2}\frac{\partial \mathbf{E}_\perp}{\partial t} \text{ in } \Omega\,, \\ \int_\Omega B_z\, d\Omega = 0 \text{ on } \Gamma\,, \end{array}\right. \qquad \left\{\begin{array}{l} curl_\perp \mathcal{E}_\perp = -\frac{\partial B_z}{\partial t} \text{ in } \Omega\,, \\ div_\perp \mathcal{E}_\perp = \mu_0\, c\, J_\zeta - \frac{1}{c}\frac{\partial E_z}{\partial t} \text{ in } \Omega\,, \\ \mathcal{E}_\perp \cdot \boldsymbol{\tau} = 0 \text{ on } \Gamma\,, \end{array}\right. \tag{4}$$

where J_ζ is defined by $J_\zeta = \rho c - J_z = q \int v_\zeta f d\mathbf{V}$. In this model, the expression of the Lorentz force $\mathbf{F} = (\mathbf{F}_\perp, F_z)$ is given by

$$\left\{\begin{array}{l} \mathbf{F}_\perp = q(\mathcal{E}_\perp + (\mathbf{v}_\perp \times \mathbf{e}_z)B_z + v_\zeta(\mathbf{B}_\perp \times \mathbf{e}_z)\,, \\ F_z = q(E_z + \mathbf{v}_\perp \cdot (\mathbf{B}_\perp \times \mathbf{e}_z))\,. \end{array}\right. \tag{5}$$

3 NUMERICAL METHODS

Our aim is now to build numerical methods to solve the problem (4-5). We have chosen to derive a finite element approximation for the electromagnetic fields computations. The Vlasov equation will be solved by a particle method.

3.1 Numerical schemes for the electromagnetic fields

The first step to get the numerical schemes consists in deriving variational formulations of equations (4). Since the model is written in a frame which moves along the optical axis at the speed of light, the bunch of particles is evolving slowly in that frame. As a consequence, the 3D computational domain is defined as the product $\Omega \times]0, Z[$, $0 \leq \zeta \leq Z$.

Let us now introduce the variational formulations which will be the basis of the method. For the sake of simplicity, we will only consider the components $\mathbf{E}_\perp$ and E_z, the other components solving more or less similar equations. Moreover, as the regularity of the fields are not an issue for our study, we will assume that they are smooth enough, for instance belonging to a standard Sobolev space. For the sake of simplicity, we will denote by $\mathbf{V}$ the space of the fields and of the test functions, regardless of the boundary conditions they satisfy.

Let $\mathbf{v}_\perp$ denote a sufficiently smooth vector test function. We first apply the $\mathbf{curl}_\perp$ operator to the first equation of the system. Then, we take the dot product by $\mathbf{v}_\perp$, and integrate over Ω. Applying then Green's formula for the $\mathbf{curl}_\perp$, we obtain the following variational formulation

$$\int_\Omega curl_\perp \mathbf{E}_\perp curl\, \mathbf{v}_\perp d\Omega - \int_\Gamma (\mathbf{v}_\perp \cdot \boldsymbol{\tau}) curl_\perp \mathbf{E}_\perp d\Gamma = 0$$

The divergence equation is handled through an augmented Lagrangian formulation. Multiplying it by $\mathrm{div}_\perp \mathbf{v}_\perp$, integrating over Ω, and adding it to the above equation, we get

$$\int_\Omega \{curl_\perp \mathbf{E}_\perp curl\, \mathbf{v}_\perp + \mathrm{div}_\perp \mathbf{E}_\perp \mathrm{div}_\perp \mathbf{v}_\perp\} d\Omega - \int_\Gamma (\mathbf{v}_\perp \cdot \boldsymbol{\tau}) curl_\perp \mathbf{E}_\perp d\Gamma = \frac{1}{\varepsilon_0} \int_\Omega \rho\, \mathrm{div}_\perp \mathbf{v}_\perp d\Omega$$

To handle the boundary condition on the $curl - div$ system, we will use a Nitsche method, as proposed in [6]. This is performed on the discretization level. Consider a regular finite element mesh T_h (where $T_h = \cup K$) of the domain, and a finite element approximation space $\mathbf{V}_h = \{\mathbf{v}_\perp \in \mathbf{V} \mid \mathbf{v}_{\perp|K} \in \mathbb{P}_k(K)\}$, where $\mathbb{P}_k(K)$ denotes the set of all vector fields which are polynomials componentwise on K with degree $\leqslant k$. Let us denote by $\mathbf{E}_h^\perp$ the approximate solution of $\mathbf{E}_\perp$ in $\mathbf{V}_h$, C_h being the trace mesh induced by T_h on the boundary of the domain. Essentially, Nitsche's method imposes the boundary condition via three boundary terms. Two of them contain the weak form of the tangential trace of the solution and the test functions. These two terms cause the method to be symmetric and consistent. The third term (with a parameter β) depends on the domain tetrahedrization, and causes the method to be stable. In our case, the Nitsche method is written

$$\int_\Omega \{curl_\perp \mathbf{E}_h^\perp curl\, \mathbf{v}^\perp + \mathrm{div}_\perp \mathbf{E}_h^\perp \mathrm{div}_\perp \mathbf{v}_\perp\} d\Omega - \int_\Gamma (\mathbf{v}_\perp \cdot \boldsymbol{\tau}) curl_\perp \mathbf{E}_h^\perp d\Gamma$$
$$- \int_\Gamma (\mathbf{E}_h^\perp \cdot \boldsymbol{\tau}) curl_\perp \mathbf{v}_\perp d\Gamma + \beta \sum_{E \in C_h} \frac{1}{h} \int_E (\mathbf{E}_h^\perp \cdot \boldsymbol{\tau})(\mathbf{v}_\perp \cdot \boldsymbol{\tau}) d\Gamma = \frac{1}{\varepsilon_0} \int_\Omega \rho\, \mathrm{div}_\perp \mathbf{v}_\perp d\Omega\,,$$

where β is some positive sufficiently large constant.

Concerning the computation of E_z, we have first to derive a suitable variational formulation. Basically, we apply the $curl_\perp$ operator to the third equation of (4) and we use the identity $curl_\perp \mathbf{curl}_\perp = -\Delta_\perp$ to get

$$\Delta_\perp E_z = curl_\perp \frac{\partial \mathbf{B}_\perp}{\partial t}$$

As previously, we take the dot product by v_z, a sufficiently smooth scalar test function, and integrate over Ω. We then apply the classical Green's formula for the Laplace operator, and use that E_z vanishes on the boundary Γ. The variational formulation, basis of our finite element method, is finally written

$$\int_\Omega \mathbf{grad}_\perp E_z \cdot \mathbf{grad}_\perp v_z d\Omega = \int_\Omega \partial_t (\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y}) v_z d\Omega\,. \tag{6}$$

Similar formulations are obtained for the components B_z and $\mathcal{E}_\perp$, following the same principles. As a result, one derives the finite element conforming P_1 approximations by using the FreeFem++ package [7]. The time discretization is performed with a classical finite difference scheme. Remark that time discretization is not an issue here, since it only appears in the right-hand sides of the formulations. Hence, there is no necessity to satisfy any stability condition.

3.2 Particle approximation of paraxial Vlasov equation

The paraxial Vlasov equation (1), written in a paraxial form, that is for an electromagnetic force $\mathbf{F}$ deduced from the paraxial model, is numerically solved by means of a particle method [8]. One approximates the function $f(\mathbf{x}, \mathbf{p}, t)$ (where $\mathbf{x} = (\mathbf{x}_\perp, \zeta)$) by a linear combination of delta distributions in the phase space $(\mathbf{x}, \mathbf{p})$, namely:

$$f(\mathbf{x}, \mathbf{p}, t) = \sum_k w_k \, \delta(\mathbf{x} - \mathbf{x}_k(t))\delta(\mathbf{p} - \mathbf{p}_k(t)) \,, \tag{7}$$

where w_k denotes the constant weight of the particle k. Its position in the phase space $\mathbf{x}_k = (x, y, \zeta)$ and $\mathbf{p}_k = (p_x, p_y, p_z)$ is solution to the differential system:

$$\begin{cases} \dfrac{dx}{dt} = \dfrac{p_x}{\gamma m}, & \dfrac{dp_x}{dt} = F_x, \\[2ex] \dfrac{dy}{dt} = \dfrac{p_y}{\gamma m}, & \dfrac{dp_y}{dt} = F_y, \\[2ex] \dfrac{d\zeta}{dt} = c - \dfrac{p_z}{\gamma m}, & \dfrac{dp_z}{dt} = F_z, \end{cases} \tag{8}$$

together with initial conditions.

The corresponding particle charge and current densities ρ and $\mathbf{J}$ are obtained by introducing the particle approximation (7) in equations (3) that yields:

$$\rho(\mathbf{x}, t) = q \sum_k w_k \delta(\mathbf{x} - \mathbf{x}_k(t)) \,, \tag{9}$$

and

$$\mathbf{J}(\mathbf{x}, t) = q \sum_k w_k \mathbf{v}_k(t) \delta(\mathbf{x} - \mathbf{x}_k(t)) \,. \tag{10}$$

Such expressions, built at the particle positions, cannot be used in this form for solving paraxial Maxwell equations. Indeed, a P_1 finite element approximation requires values of ρ and $\mathbf{J}$ at the vertices of the tetrahedral mesh. Following the classical procedure [8, 9], we introduce the assignment and interpolation procedures.

According to the general approach, time discretization of system (8) is built from 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 $t_{n+1/2}$. The equations of momentum $\mathbf{p}_k$ are approximated by

$$\begin{cases} \dfrac{1}{\Delta t}(p_x^{n+\frac{1}{2}} - p_x^{n-\frac{1}{2}}) = F_x^n \,, \\[2ex] \dfrac{1}{\Delta t}(p_y^{n+\frac{1}{2}} - p_y^{n-\frac{1}{2}}) = F_y^n \,, \\[2ex] \dfrac{1}{\Delta t}(p_z^{n+\frac{1}{2}} - p_z^{n-\frac{1}{2}}) = F_z^n \,, \end{cases} \tag{11}$$

where (F_x^n, F_y^n, F_z^n) is a numerical approximation of the Lorentz force (5) at time t_n, the computation of which requiring the knowledge of the paraxial electromagnetic fields. Since they are determined by finite element methods, an interpolation procedure is necessary to recover the values of the fields at the particle locations. For this purpose, we use an interpolation procedure, similar to the one proposed in [3], where the fields are computed by a finite difference method.

The last step consists in computing the particle position solution to (8), that are obtained by solving the following discretized system

$$\begin{cases} \dfrac{x^{n+1} - x^n}{\Delta t} = \dfrac{p_x^{n+\frac{1}{2}}}{\gamma^{n+\frac{1}{2}} m} \,, \\[2ex] \dfrac{y^{n+1} - y^n}{\Delta t} = \dfrac{p_y^{n+\frac{1}{2}}}{\gamma^{n+\frac{1}{2}} m} \,, \\[2ex] \dfrac{\zeta^{n+1} - \zeta^n}{\Delta t} = c - \dfrac{p_z^{n+\frac{1}{2}}}{\gamma^{n+\frac{1}{2}} m} \,, \end{cases} \tag{12}$$

where $\gamma^{n+\frac{1}{2}}$ is computed with $\gamma^{n+\frac{1}{2}} = \left(1 + \dfrac{|\mathbf{p}^{n+\frac{1}{2}}|^2}{(mc)^2}\right)^{\frac{1}{2}}$. The final complete time advance algorithm has the same structure as the one described in [3], where two dimensional paraxial Maxwell equations were approached by a finite-difference method. We refer the interested reader to this reference.

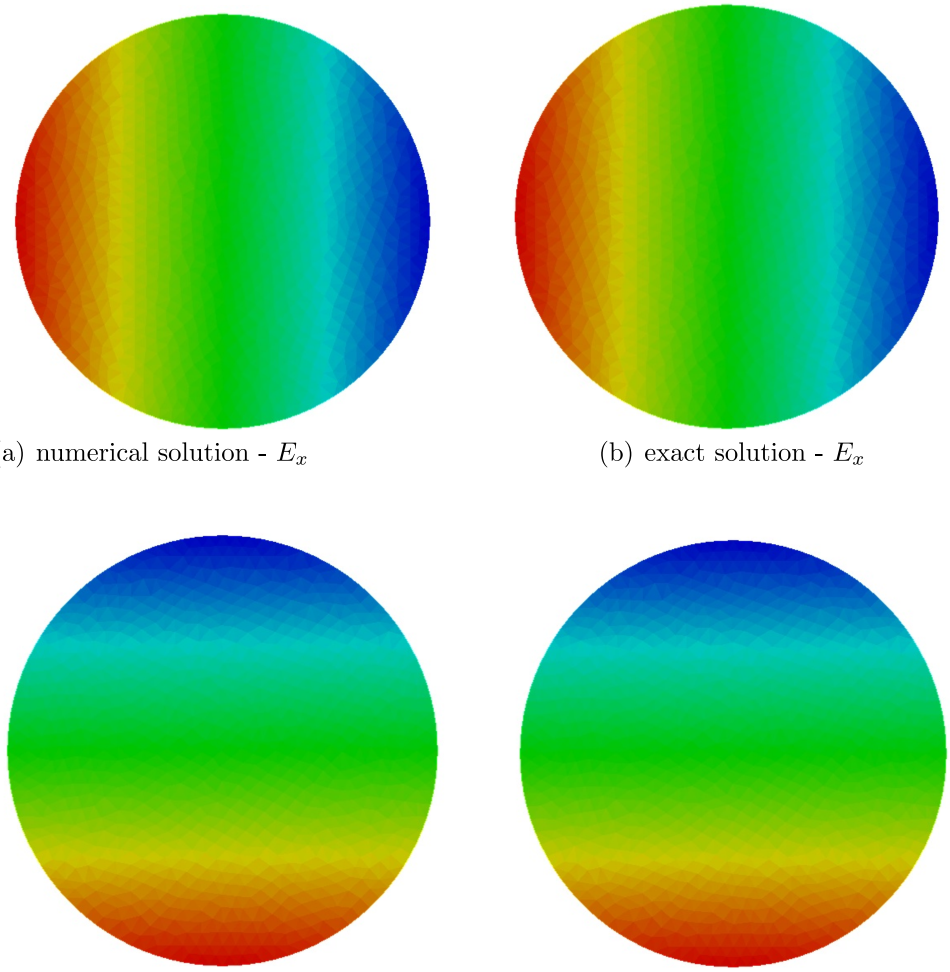
4 NUMERICAL RESULTS

Our aim is to demonstrate the accuracy and the validity of the numerical method, derived from the discrete variational formulations. To this purpose, we consider a 3D computational domain consisting of a cylinder, the axis of which being the ζ axis. The transverse section Ω is made of a disk of radius $R = 0.1$. We choose a mesh made of 100 edges on the base on the cylinder and 30 layers up, for a cylinder of length 0.3. The total number of degrees of freedom is equal to 86862. We also choose a time step $\Delta t = 10^{-4}$s. All runs were performed on a commercial laptop (MacBook Pro, Processor 2.6 GHz Intel Core i5, Memory 8 GB 1600 MHz DDR3).

We first derive an analytic solution $\mathbf{E}_\perp$ for a given charge density $\rho(\mathbf{x}, t)$. Choosing $\rho(\mathbf{x}, t) = 4\varepsilon_0(\cos(x^2 + y^2) - (x^2 + y^2)\sin(x^2 + y^2))\cos t$, one easily finds that the electric field $\mathbf{E}_\perp = (2x\ \cos(x^2+y^2)\cos t, 2y\ \cos(x^2+y^2)\cos t)$ solves the first equation of (4). With these definitions, we can numerically compute the quantities related to the paraxial model and compare the computed solutions to this exact one. Figure 1 shows respectively the x and y components obtained after 100 time steps of simulation. In order to make the visual comparison between the computed and exact solution more convenient, we have chosen to display the solution in a cut plane of the mesh ($\zeta = 0.15$). As one can see there is an good agreement between the computed solution and the exact one, depicted at the same scale. Indeed, there is no way of distinguishing the difference between the two cut plans of the solutions, even if we used a rather coarse mesh.

5 CONCLUSION

In this paper, we proposed a numerical approximation of a paraxial Vlasov-Maxwell model in three dimensions, adapted to highly relativistic beam. The system of equations we got is simpler and easier to solve than the complete 3D Vlasov-Maxwell equations. We have derived a finite element numerical implementation of the Maxwell part of the model, coupled with a Particle-In-Cell method for the Vlasov part. Both methods were implemented by using the Freefem++ software. This approach seems powerful in its ability to get an accurate, but fast and easy to implement algorithm. Numerical results have been presented to illustrate the feasibility of the method. This solver should give an interesting numerical tool for simulating high energy short beams problems, and could be valuable to the computational accelerator physics community.



(a) numerical solution - E_x

(b) exact solution - E_x

(c) numerical solution - E_y

(d) exact solution - E_y

Figure 1: $\mathbf{E}_\perp(\mathbf{x}_\perp, \zeta = -0.15)$ after 100 time steps

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