Reduced models for solving particle beams and plasma physics problems

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Abstract: 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. In the industry, a variety of examples can be thought of, such as the ion or electron injectors for particle accelerators, the free electron lasers, the hyperfrequency devices, the vulnerability of spatial devices to particle flows, etc. In this paper, we are concerned with the construction of numerical methods required for solving particle beams and plasma physics applications. The main lines of this paper will treat about the analysis and the development of the reduced models. We present two situations in which this strategy can be applied. Numerical results illustrate the possibilities of the approach.

Key–Words: Vlasov-Maxwell, Vlasov-Poisson, paraxial approximation, reduced models, PIC code

1 Introduction

Charged particles appear essentially in two kinds of physics problems: charged particle beams, like in hyperfrequency devices or vacuum diode technology, and plasma physics, a plasma being roughly speaking a gas of quasi neutral charged particles. Plasmas are involved in a lot of real-life applications. They are commonly used in Science and Technology and play an important role in the energy production (for instance in the magnetic confinement fusion). They are also ingredients of instruments and others devices (see the Introduction of [9] for a survey of the applications). Moreover, all fusion applications involve non linear interaction of charge particle beams.

Quite complete mathematical models to solve these problems are based on the time-dependent Vlasov-Maxwell system of equations, sometimes under the relativistic assumption. However, the numerical solution of the Vlasov-Maxwell system requires an important computational effort, and can be very expensive in terms of computational cost. This point is particularly important if the code has to be intensively used to analyse a lot of experimental results. In such a situation, one have to take into account the particularities of the physical problem (geometries, physical properties, etc.) to derive reduced models leading to cheaper computations.

Deriving such realistic but rigorous mathematical models is challenging. Moreover, efficient algorithms are needed for instance in order to be able to select between several issues in the design of devices, especially to take into account the three-dimensional effects.

In this paper, we propose two examples of such problems, for which reduced models have been derived leading to easier computations than the original model. The outline of the paper is as follows. In the next Section, we recall the Vlasov-Maxwell system of equations, and the methods generally used to solve it. In Section 3, we introduce two examples of reduced models. The first is based on a low frequency assumption, whereas the second is derived from a paraxial hypothesis. Numerical applications illustrate the possibilities of this approach. Concluding remarks follow.

2 The Vlasov-Maxwell model

In this section, we recall the Vlasov-Maxwell system of equations and briefly review the most popular methods to solve it.

2.1 The Vlasov equation

Let us consider a population of charged particles, with a mass $m$ and a charge $q$, submitted to the electromag-
electric Lorentz force
\[ \mathbf{F} = q (\mathbf{E}(\mathbf{x}, t) + \mathbf{v}(t) \times \mathbf{B}(\mathbf{x}, t)) , \] (1)

that describes how the electromagnetic field \( \mathbf{E}(\mathbf{x}, t) \) and \( \mathbf{B}(\mathbf{x}, t) \) acts on a particle with a velocity \( \mathbf{v}(t) \). Each particle is characterized by its position \( \mathbf{x} \) and its velocity \( \mathbf{v} \) in the so-called phase space \((\mathbf{x}, \mathbf{v})\). We introduce the distribution function \( f(\mathbf{x}, \mathbf{v}, t) \), which can be defined as the average number of particles in a volume \( dx \, dv \) of the phase space. Assuming that collisions between particles can be neglected, the distribution function \( f(\mathbf{x}, \mathbf{v}, t) \) is solution to the following transport equation, named the Vlasov equation
\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \frac{q}{m} (\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t)) \cdot \nabla_v f = 0. \] (2)

For the relativistic case, denote by \( \mathbf{p} \) the momentum and \( c \) the speed of the light, we introduce the distribution function \( f(\mathbf{x}, \mathbf{p}, t) \) such that
\[ \mathbf{p} = \gamma m \mathbf{v}, \quad \text{with} \quad \gamma = \frac{\sqrt{\mathbf{p}^2 + m^2 c^2}}{c} , \]
then the relativistic Vlasov equation is obtained by substituting the term \( \frac{1}{m} \nabla_v f \) in Equation (2) by the term \( \nabla_p f \).

Solving the time-dependent Vlasov equation in the six-dimensional phase space \((\mathbf{x}, \mathbf{p})\) (or \((\mathbf{x}, \mathbf{v})\) in a non-relativistic case) with a grid method (finite difference, finite volume or finite element method) is almost impossible, since we rapidly reach the limit in memory available on a computer, leading then to an intractable cpu time. For this reason, a well suited method is the widely used particle method (see [5] or [13] for a theoretical description). However, due to the increase of the computer memory, especially when using supercomputer or multiple processors (parallel computers), grid methods are considered again for one or two-dimensional Vlasov problems coupled with the static Poisson equation.

Solving the Vlasov equation by means of a particle method consists in approximating the distribution function \( f(\mathbf{x}, \mathbf{v}, t) \) at any time \( t \), by a linear combination of delta distributions in the phase space:
\[ f(\mathbf{x}, \mathbf{v}, t) \simeq \sum_k w_k \delta(\mathbf{x} - \mathbf{x}_k(t))\delta(\mathbf{v} - \mathbf{v}_k(t)) \] (3)

where each term of the sum can be identified with a macro-particle, characterized by its weight \( w_k \), its position \( \mathbf{x}_k \) and its velocity \( \mathbf{v}_k \). This distribution function is a solution of the Vlasov equation (2) if and only if \((\mathbf{x}_k, \mathbf{v}_k)\) is a solution to the differential system:
\[ \frac{d\mathbf{x}_k}{dt} = \mathbf{v}_k , \] (4)
\[ \frac{d\mathbf{p}_k}{dt} = \mathbf{F}(\mathbf{x}_k, \mathbf{p}_k) , \] (5)

which describes the time evolution of a particle \( k \), submitted to the electromagnetic Lorentz force \( \mathbf{F} \) (see (1)). This system is generally solved by an explicit time discretization scheme. A leapfrog scheme is well-adapted in this case (see [3] for more details).

2.2 The Maxwell equations

The expressions of the charge and the current density induced by the motion of these particles are given by
\[ \rho(\mathbf{x}, t) = q \int_{\mathbb{R}^3} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{p}, \] (6)
\[ \mathcal{J}(\mathbf{x}, t) = q \int_{\mathbb{R}^3} \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) \, d\mathbf{p}, \] (7)

that express the coupling of the Maxwell and Vlasov equations. Indeed \( \rho(\mathbf{x}, t) \) and \( \mathcal{J}(\mathbf{x}, t) \) appear as the right-hand sides of the Maxwell equations (in the vacuum)
\[ \frac{1}{c^2} \frac{\partial \mathcal{E}}{\partial t} - \nabla \times \mathcal{B} = -\mu_0 \mathcal{J} , \] (8)
\[ \frac{\partial \mathcal{B}}{\partial t} + \nabla \times \mathcal{E} = 0 , \] (9)
\[ \nabla \cdot \mathcal{E} = \frac{\rho}{\varepsilon_0} , \] (10)
\[ \nabla \cdot \mathcal{B} = 0 , \] (11)

where the constants \( \varepsilon_0, \mu_0 \) are respectively the dielectric permittivity and the magnetic permeability in the vacuum, that satisfies \( \varepsilon_0 \mu_0 c^2 = 1 \).

The Vlasov and Maxwell equations separately are linear hyperbolic systems, but the expression of the Lorentz force \( \mathbf{F} \) in a way and those of the charge and current density \( \rho \) and \( \mathcal{J} \) in another way leads to a strong coupling, that makes the whole problem quadratic. Indeed, the term
\[ \mathbf{F} \cdot \nabla_p f = q(\mathcal{E}(\mathbf{x}, t) + \mathbf{v} \times \mathcal{B}(\mathbf{x}, t)) \cdot \nabla_p f \]
is a quadratic term since \( \mathcal{E} \) and \( \mathcal{B} \) depend on the distribution function \( f \) in an affine way, through \( \rho \) and \( \mathcal{J} \).

For computing the solution of Maxwell’s equations, some of the numerical codes which are developed are based on finite difference approximations of Maxwell’s equations on structured meshes. These
are completely explicit, at least when the charge conservation equation \( \partial_t \rho + \nabla \cdot J = 0 \) is numerically verified. The first and probably most popular method was introduced by Yee [16] in 1966, and is straightforward to implement in simple cases. However, despite its simplicity and its efficiency, as soon as the domain geometry becomes too complex, or when local refinements are necessary, the structured mesh strategy is not well adapted, and suffers from the inaccurate representation of the solution on curved boundaries.

An alternative is to use the flexibility of unstructured meshes to approximate complex geometries and to achieve local refinements. For the finite element discretization, different formulations are available. Examples are the edge elements [12], the vector finite element method [15], or the Cartesian elements eventually in a constrained form [2]. Other nodal finite element techniques based on a least-squares approach were also proposed. Concerning finite volumes solvers, several kind have been developed: Delaunay-Voronoi finite volume methods [10], or other types of methods include traditional vertex centered or cell centered [11] finite volume methods, regarding the Maxwell equations as a first-order strictly hyperbolic system.

From a mathematical point of view, the Cauchy problem for the Vlasov-Maxwell system is quite well understood. The existence of a weak solution was proved by DiPerna-Lions [6]. From a numerical point of view, this model is very complete but also not easy to solve numerically, in particular in a three-dimensional domain. Even though this is necessary in several cases, one easy understands the need of deriving simpler (but accurate) models, by exploiting given physical assumptions. Hence, in some cases, assuming that the problem is static allows to replaced 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, gyrokinetic models, laser-plasma interaction models, etc... generally obtained by exploiting specific geometries/properties of the problem.

In what follows, taking into account the particularities of the physical problems, we derive such reduced models leading to cheaper computations.

### 3 A low frequency reduced model

As a first example of reduced model, we consider the modelling and the simulation of the multipaction effect. This is an unwanted breakdown phenomenon, which can occur in high power space components. This can be schematized as follows: consider for instance in a step waveguide (see Fig. 1) a free electron accelerated by an applied electromagnetic field. A secondary emission and the electron reflection result from the electron impact on the waveguide wall. These two electrons may now be accelerated across the waveguide if the applied field reverses at the proper time, and strike an opposite waveguide wall leading to new secondary and reflected electrons. This process repeated many times can lead to an exponential growth of the charge density. In this case the component can no more fulfill its function and may even be destroyed. Obviously, this multipaction process can occur under some conditions on the cycles of the applied field (to accelerate the electrons) and on the energy of the incident electrons (to induce the number of particles to increase). The aim of the modelling is to determine, for a given waveguide and an applied field, a threshold voltage above which multipaction can occur. Therefore simulations of this phenomenon require a priori a Maxwell-Vlasov solver.

![Figure 1: step waveguide.](image)

#### 3.1 From Vlasov-Maxwell to Vlasov-Poisson

By using first the linearity of the Maxwell equations, one can decompose the electric field \( \mathcal{E} \) into two parts, \( \mathcal{E} = \mathcal{E}_{\text{ext}} + \mathcal{E}_s \), where \( \mathcal{E}_{\text{ext}} \) is the applied field which is external, and \( \mathcal{E}_s \) denotes the self-consistent field, created by the electrons displacement. Remark then that the external field is solution to the time-dependent Maxwell equations, without any coupling with the Vlasov equation. For the self-consistent field \( \mathcal{E}_s \), using that the velocity of the extracted electrons \( \frac{\mathcal{V}_{\text{ele}}}{} \) is very small compared to the light velocity of the electromagnetic waves, one introduces a small parameter \( \varepsilon = \frac{\mathcal{V}_{\text{ele}}}{c} \). Following [14], reduced models of
Maxwell’s equations can be derived after a scaling and an asymptotic expansion of the solution in power of this parameter $\varepsilon$. There, it is proved that the quasi-static Vlasov-Poisson model is a first order approximation of the Vlasov-Maxwell equations. Hence, one assume that $E_S$ can be accurately computed by solving the Poisson problem

$$-\Delta \phi = \frac{\rho(t)}{\varepsilon_0} \text{ with } E_S = -\nabla \phi,$$

(12)
coupled with the Vlasov equation, and supplemented with suitable boundary and initial conditions. The main advantage of this model is that Equation (12) is not explicitly time dependent, the density $\rho(t)$ being given at each timestep of the Vlasov equation solution. This avoids to use a time stepping method for the self-consistent field, that is generally expensive in terms of computing time.

Based on the above remarks, the methodology for the numerical study of the multipaction effect can be divided into three steps.

1. **Computation of the overvoltage coefficient:**
   the propagation of an incoming plane wave of amplitude $E_0$ is computed with a time dependent Maxwell solver to obtain the amplitude $E_c$ of the wave in the gap (see Fig. 1). Then, the overvoltage coefficient $\eta$ is determined with
   $$\eta = \frac{|E_c|}{|E_0|}.$$ (12)
   Since the coefficient $\eta$ depends only on the geometry of the waveguide and on the frequency of the incoming wave, the computations are carried out only once for each applied frequency.

2. **Solving Vlasov-Poisson in a reduced domain:**
   Consider a given exterior field of the form
   $$E(t) = E \sum_{i=1}^{i=n} \cos(2\pi f_i t).$$ (13)
   As $n = 1$ (resp $n > 1$), it is a single carrier (resp. multicarrier) simulation. In the computational domain restricted to the gap area, solve the Vlasov-Poisson equations augmented with secondary emission laws to model the behaviour of the extracted electrons (cf. [1]). From these results, one deduces the multipaction threshold voltage.

3. **Determination of the multipaction threshold:**
   from the amplitude $E$ used in the step 2 and the values $\eta$ of the step 1, on can easily deduce the amplitude $E_0$ at the input of the component corresponding to the multipaction threshold.

### 3.2 Numerical illustration

Let us consider the two-dimensional domain depicted in Fig. 1. The ingoing signal is a sum of three given frequencies: $f_1 = 10.911$ GHz, $f_2 = 11.075$ GHz and $f_3 = 11.158$ GHz. The corresponding overvoltage coefficients we obtain are $\eta_1 = 9$, $\eta_2 = 9.1$ and $\eta_3 = 9.2$. In such a multicarrier multipaction, the envelope of the applied voltage is obtained by combining all the carriers in phase. In this case, the multipaction effect is characterized by a periodic series of charge density peaks corresponding to the voltage of the envelope. In the numerical simulations, the charge grows exponentially as a multipaction occurs during an envelope peak, but decays again when the voltage falls below the threshold. Examples are shown on Fig. 2 and 3.

### 4 A highly relativistic reduced model

This second example is devoted to the case of high energy short beams. The aim is to study the transport of a bunch of highly relativistic charged particles in the interior of a perfectly conducting tube. Following [8], one can derive a reduced model which exploits the property that the particles of the beam remain close to an optical axis.

#### 4.1 From Vlasov-Maxwell to a paraxial model

Consider a beam of charged particles which moves in the interior of a perfectly conducting hollow tube. We choose the axis of the tube as the $z-$axis. Assuming that the beam is a high energy short beam, Laval et al. [8] have derived a reduced model in the
following way. The high energy assumption means that relativistic factor \( \gamma >> 1 \). Consequently, since the particle velocity \( v \) is close to \( c \) for any particle in the beam, one rewrites the Vlasov-Maxwell equations in the beam frame, which moves along the \( z \)-axis with the light velocity \( c \). Then, set \( \zeta = ct - v_z, \quad v_\zeta = c - v_z \). To derive a paraxial model, one then introduces a scaling of the equations. First exploiting 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 \( \tau \), and define a small parameter \( \eta \), \( \eta = \frac{c}{\tau} \ll 1 \). 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 \( (f, E, B, F, \) etc.) in powers of the small parameter \( \eta \). It is proved in [8] 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 can consider the axisymmetric counterpart. Using the coordinates \( (r, \theta, \zeta) \) (with obvious notations), the electric field is now denoted \( (E_r, E_\theta, E_z) \), the magnetic one \( (B_r, B_\theta, B_z) \). One thus obtains that the electromagnetic force \( F \) 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 \( E_r = E_r - cB_\theta \) and \( E_\theta = E_\theta + cB_r \), which are second order corrections. Hence, the paraxial model of ultra-relativistic Maxwell equations is written:

For the zero order fields:

\[
\begin{align*}
E_r &= cB_\theta = \frac{1}{\varepsilon_0 v} \int_0^r \rho s \, ds \\
E_\theta &= B_r = 0
\end{align*}
\]  \hspace{1cm} (13)

For the first order fields:

\[
\begin{align*}
\frac{\partial E_z}{\partial r} &= \frac{\partial B_\theta}{\partial t} \quad \text{and} \quad \frac{\partial B_z}{\partial r} = \mu_0 J_\theta \\
E_z(r = R) &= 0 \quad \text{and} \quad \int_0^R B_z r \, dr = 0
\end{align*}
\]  \hspace{1cm} (14)

For the second order pseudo-fields \( E_r \) and \( E_\theta \):

\[
\begin{align*}
E_r &= \frac{1}{r} \int_0^r \left( \mu_0 c J_\zeta - \frac{1}{c} \frac{\partial E_z}{\partial t} \right) s \, ds \\
E_\theta &= -\frac{1}{r} \int_0^r \frac{\partial B_z}{\partial t} s \, ds,
\end{align*}
\]  \hspace{1cm} (15)

where \( J_\zeta \) is defined by \( J_\zeta = \rho c - J_z = q \int v_\zeta f \, dv \). We approximate these equations with specific numerical schemes based on a finite-difference approach. The order of the computations is induced by the asymptotic expansion. Hence, the zero order fields have to be first computed, and are necessary to obtain the first order quantities etc. More details can be found in [4].

4.2 A numerical example

As we are working in the beam frame, the computational domain is the rectangle \([-R, R] \times [0, Z] \) 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. As a numerical example, consider a bunch of particles emitted with velocities such that the paraxial assumptions are verified. According to stability condition, more than 10 particles are placed in each cell, with the same weight and a charge following \( w = Jt / Ne \), (\( J \) the total current to be emitted, and \( N \) the particle number). Fig. 4 and 5 show respectively the self-consistent electric radial and longitudinal field \( E_r \) and \( E_z \) obtained after 50 time steps of simulation with the resulting PIC paraxial code.

5 Conclusion

In this paper, we are concerned with the development of numerical methods required for solving particle
beams and plasma physics problems. Exploiting the particularities of the physical problem, we proposed to develop reduced models. We hope this approach to be very powerful in its ability to get accurate, but fast and easy to implement algorithms. As a first example we proposed a numerical methodology to study the multipaction effect, that significantly improved the computational time of the simulations. In the second example, a PIC method for solving a paraxial model of highly relativistic beam has been developed. Numerical results were presented to illustrate the possibilities these models.

References:


