Numerical investigation of Maxwell-Vlasov equations.

Part I: basic physics and algorithms

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Abstract

We present a numerical scheme to solve the fully 3D Maxwell-Vlasov equations. The aim is to investigate the interaction of a laser pulse with a plasma and the acceleration of electrons and ions. We choose the approach based on numerical particles to approximate the distribution function interpreted, according to the Klimontovich formalism, as a probability distribution function. The key points are a high order implicit scheme to approximate the space differential operators and a time evolution scheme of adequate accuracy.

Key words: Laser driven acceleration. PIC method. Implicit compact schemes. Symplectic integrators.
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1. Introduction

The acceleration of electrons due to laser-plasma interaction has been intensively investigated during the last decade both theoretically and experimentally [1], [2], [3]. Beams up to 1 GeV with a low energy spread and small emittance have been obtained [4], [5] and proposals to use them to produce hard X-rays in the rage from 10 keV to several hundreds of keV by Compton or Thompson scattering with another laser pulse have been formulated [6]. More recently, ion jets of a few MeV have been produced in the interaction of short pulse with a thin solid target. Rapid progress is expected from the new laser generation with multiterawatt pulses of a few femtoseconds. Many applications are being considered such as new high intensity accelerators, radio-therapy, neutron sources and

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molecular imagining. The basic physical phenomena of the process are understood but an analytical treatment is lacking, except for some simplified models. In addition the similarities with the fast ignition process imply a potential synergy with the inertial nuclear fusion. The possibility of replacing a linac with a multistage laser-plasma accelerator might open a new pathway to a heavy ion driver for the inertial fusion. From the theoretical viewpoint the wave-plasma interaction is a difficult problem requiring a fully 3D self consistent treatment. The solution of the 3D Maxwell-Vlasov equations (MVE) can be obtained only numerically and is affordable since a small number of wave periods is involved in the acceleration process. This justifies the use of a mean field approach since the collisional effects should be irrelevant, unlikely the fast ignition which extends on a much longer time interval involving high plasma densities. The key problems in developing a numerical scheme to solve the MVE concern the wave propagation and the particles evolution. A small error in the dispersion relation and phase velocity of the electromagnetic wave jointly with a reliable approximation to the distribution function characteristics can only be obtained in the fully 3D case by a PIC code. High order discretization methods for the differential operators in configuration space are needed jointly with a sufficiently accurate time integration scheme. A good balance of the computational and communication load among the processors of a parallel architecture is needed in order to use a sufficient number of particles per cell so that the numerical noise on the distribution function does not overcome other discretization errors. A crucial point is the validation of the code which can be achieved at different levels by comparison with the available analytical results. The first step is testing the Maxwell-Liouville version of the code, where the particles move in the field of an assigned plane-wave or wave packet without affecting it. The next step is the comparison of Maxwell-Vlasov version with the known 1D self consistent solutions [7], [8]. To this end a flexible code has been designed in order to choose a 3D, 2D or 1D version. This project was born because some people coming from two different fields (Hamiltonian systems and intense beam dynamics, astrophysical plasmas and large scale gravitationally interacting systems) joined to develop a high quality and high performance code meant to support the new generation experiments and theoretical modelling in some Italian laboratories and universities. The expertise in beam dynamics was achieved in developing 2D/3D electrostatic PIC codes based on spectral Poisson solvers with arbitrary boundary conditions [9] for linacs and storage rings (MICROMAP/HALODYN) [10] and advanced tools based on neoadiabatic, canonical perturbation and spectral theory to analyze the motion of a test particle [11]. Collisional processes and the relaxation towards the Maxwell-Boltzmann equilibrium were investigated by developing a \(N\)-body two-dimensional code [12], validated with the scaling laws of Landau’s kinetic theory and the mean field limit for large \(N\) [13]. The expertise on the numerical treatment of astrophysical plasmas was developed in treating classical and relativistic magnetohydrodynamics containing shocks and other discontinuities [14], [15]. The 3D gravitational interaction for collisionless systems was analyzed by developing \(N\)-body codes [16], [17].

2. Basic physics and numerics

The electric field of a laser pulse may exceed the ionization threshold. Since the period of the wave is large, compared to the atomic transition, the field is quasi-static as long
as the ionization of an electron is concerned. Recalling that the electric potential of an electron in the hydrogen ground state is $V_0 = 25 \, \text{V}$ and the atomic radius is $r_0 = 0.5 \times 10^{-10} \, \text{m}$, the mean electric field is $E = V_0 / r_0 = 50 \times 10^{10} \, \text{V/m}$, namely $0.5 \, \text{TV/m}$. By comparison, the highest fields in a superconducting RFQ cavity may reach $50 \, \text{MV/m}$. Since the ratio between the fields of a laser pulse and a RFQ cavity exceeds $10^4$, very compact devices can be built. The basic mechanism to obtain a beam is self focusing. After ionization an under-dense plasma is formed, the ions are assumed to be at rest and to form the neutralizing background. As the electrons are accelerated, their plasma frequency $\omega_p$ decreases and the refraction index $n$ increases; the medium focuses the pulse and channels it through the plasma. In the case of a circularly polarized wave one has

$$n = \left(1 - \frac{\omega_p^2}{\omega^2}\right)^{1/2} \quad \omega_p^2 = \frac{4\pi ne^2}{\gamma m}. \quad (1)$$

In the present version of the codes we assume the ions at rest and the electrons to be initially free, quasi uniformly space distributed with a Maxwellian velocity distribution and low temperature. In this note we outline the numerical scheme chosen to develop a 3D PIC code for the MVE. An error analysis of the dispersion relations and phase velocity is presented jointly with the first benchmarks on the Maxwell-Liouville version of the code. To this end analytical solutions of a Gaussian wave packet and of trajectory of a particle in a plane wave were computed.

The use of compact finite difference high order schemes for the differential operators in configuration space allows to have a very small error on the dispersion relations and good isotropy. The use of quadratic interpolation for the field values and eventually of filters to kill the unwanted high frequency components appear to be adequate for an accurate propagation of the electromagnetic wave. The use of smooth shape functions allows to obtain the currents with sufficient accuracy provided the number of particles per cell is sufficiently high. One of the main goals of the parallel development is to reach an optimal balance between the number of particles assigned to each processor and the communication of the field values. The full runs on our 56 processors system and comparison with realistic experiments should start within the present year.

3. The Vlasov-Maxwell equations

The system one has to solve is given by Vlasov equations for the electrons and ions density in phase space $f_e$, $f_i$

$$\frac{\partial f_s}{\partial t} + v \frac{\partial f_s}{\partial x} + \left(q_s \frac{\mathbf{E}}{c} + q_s \frac{\mathbf{v} \times \mathbf{B}}{c}\right) \cdot \frac{\partial f_s}{\partial \mathbf{p}} = 0, \quad (2)$$

for $s = e, i$, coupled to Maxwell’s equations for the electromagnetic wave

$$\frac{\partial \mathbf{B}}{\partial t} = -c \, \text{rot} \, \mathbf{E} \quad \frac{\partial \mathbf{E}}{\partial t} = c \, \text{rot} \, \mathbf{B} - 4\pi \mathbf{bfJ}, \quad (3)$$

via the electrons and ions current $bfJ$

$$\mathbf{J}(\mathbf{x}, t) = \sum_{s=e,i} q_s \int v f_s(\mathbf{x}, \mathbf{p}, t) d\mathbf{p}. \quad (4)$$
These equations have to be solved for given initial conditions of the distributions $f_s$ and the fields $E, B$ with the appropriate boundary conditions. Several methods are available to solve Maxwell’s equations on a 3D grid by discretization of the space and time derivatives. For space derivatives, spectral methods, finite elements method, compact (or implicit) finite differences schemes, explicit finite differences schemes have been developed as appropriate for hyperbolic systems, mainly in the fluid dynamical context [18]. For the time evolution the order 2 leap-frog scheme and order 4 schemes Runge-Kutta and symplectic Runge-Kutta are the most commonly referenced methods. To date PIC codes designed to investigated the laser-plasma interaction are based on standard low order Yee schemes (leap-frog in space and time) [19]. However recently a renewed interest arose to extend to the Maxwell equations high order schemes developed for fluid dynamics [20], [21], [18]. The most challenging problem for computational plasma physics remains the proper discretization of the Vlasov equation due the Hamiltonian structure of the flow.

4. Direct integration

A way to handle this problem is to discretize directly on the 6D phase space the Vlasov equation (2), either by approximating the first derivatives of the Eulerian form, [22], [23], [24], or by adopting a semi-Lagrangian approach, where the motion of the Vlasov characteristics is combined with the phase space representation of the distribution function by spline interpolation[25], [26]. Time integration is then performed by a split procedure, giving a second-order approximation in time. For both methods, convergence theorems, at least for the 1D Vlasov-Poisson system, are now available [27],[28]. The direct numerical integration in phase space of equations of this form is a long standing problem, dating back to the investigations of the incompressible two-dimensional Euler equation, which has the same structure properties as the 1D Vlasov-Poisson system. In fact, the Vlasov equation (2) is not a generic hyperbolic scalar equation, but has a richer geometric structure due its Hamiltonian character. In particular, it satisfies an infinite set of conservation laws (Casimirs invariants). Using rigorous mathematical arguments [29] it can be shown that when trying to reduce the Vlasov system to a finite dimensional space by numerical approximation, this Hamiltonian structure gets lost and all Casimirs variables are broken (except for mass conservation). It is still a major challenge in numerical analysis to design discretization schemes for the Vlasov equation, where at least some Casimirs are preserved. In fact, in absence of these conservation properties, numerical results can be heavily distorted by unphysical effects. In a recent numerical investigation of the 1D Vlasov-Poisson system [30] this problem has been carefully addressed, and the failure of the lower order Casimirs conservation has been measured, depending on the adopted finite difference scheme and on the phase space grid resolution. In particular, this investigation shows how different approximations and resolutions may produce different results for the same physical problem and the same initial conditions. To get some insight on this problem, a simple argument based on the truncation error can be used. In fact, after discretization in space and time the truncation error (T.E.) for Vlasov equation, obtained by a straightforward application of Taylor’s expansion, reads

$$T.E. = O \left[ \Delta t^2 + v \left( \frac{\partial^k f}{\partial x^k} \right) (\Delta x)^k + F \left( \frac{\partial^k f}{\partial p^k} \right) (\Delta p)^k \right],$$

(5)
where we have indicated with $k$ the order of the scheme. Even when convergence theorems exist, it is evident that, for finite grid size, the numerical Vlasov equation contains significant dispersive and/or diffusive terms (absent in the original system), which may affect the computed solution. A way to control and to limit these numerical effects, consists in increasing the order of integration and to refine the phase space grid size. However, a systematic investigation of this grid convergence for direct integration of the Vlasov equation to date is feasible for the 2D(1+1) case, it is already extremely time consuming for the 4D(2+2) case and is clearly beyond the present computers capability for the fully 6D(3+3) case.

4.1. The PIC method

Taking into account these difficulties we prefer to implement a particle in cell scheme (PIC) interpreted as an $N$ dimensional sampling of the characteristics of the distribution function $f(x, v, t)$, by adopting the Klimontovich formalism, which relates the $N$ numerical particles system, to an atomic probability measure in phase space. One has then to solve the following relativistic $N$ particles equations of motion

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i = \frac{\mathbf{p}_i}{m} \left(1 + \frac{\mathbf{p}_i \cdot \mathbf{p}_i}{m^2 c^2}\right)^{-1/2}$$

$$\frac{d\mathbf{p}_i}{dt} = q_i \mathbf{E}(\mathbf{x}_i, t) + \frac{q_i}{c} \mathbf{v}_i \times \mathbf{B}(\mathbf{x}_i, t),$$

where $q_i$ is the charge of the numerical particle $i$. The main approximation in this approach is given by the evaluation of the self consistent fields at the particle points (the same procedure applies to the current). This is equivalent to replace the atomic measure with a smooth quadratic spline $S(x - x_i)$. Well experimented and validated, the PIC scheme can be still improved, to face more demanding problems like the laser-plasma interaction, by the use of high order splines and time integration procedures.

Several results are available on the global convergence of the 3D numerical particle method for $N \rightarrow \infty$ and particle size (mollifiers) $h \rightarrow 0$ [31]. It is a main characteristic of the numerical particle method that, at each level of approximation for electromagnetic forces and particle motion, the basic Hamiltonian structure is always exactly preserved by symplectic integrators.

Convergence results, even though relevant, are not sufficient to estimate, for a given 3D problem, what optimal particle number $N$ and grid size $\Delta$ should be chosen, to get significant approximations. In this respect, when benchmarks on analytical models are not available, the only possible criterion is provided by grid convergence ($\Delta \rightarrow 0$, $N \rightarrow \infty$). Long standing numerical experience supports the feasibility of grid convergence analysis [32], [33]. The golden rule for accurate numerical results remains the use of a sufficiently large number of particles per space cell. Typically $n = 50 \sim 100$ is a minimum value for an acceptable error. The choice of $N$ is related to the time interval considered, since the error due to statistical fluctuations is $O(n^{-1/2})$ and causes a diffusive effect. The choice of $N$ large limits the statistical noise and reduces the grid-particles coupling, leading to unwanted high frequency modes. The state of art in the particles shaping by using linear or quadratic splines still provides a solid background. The PIC framework on demanding physical problems like the laser-plasma interaction still requires further development for code validation against analytical models and experimental results. We notice that with a grid of size $128^3$, a good resolution is obtained with $10^5$ numerical particles.
which largely satisfies the previous criterion. Indeed the distribution is concentrated on a smaller volume where $n \gg 100$.

4.2. Acknowledgements

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References