Overview of Codes Simulating Plasma Acceleration

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Abstract

The main physical parameters, and the equations to be solved, for numerical simulation of Laser Wake Field Acceleration (LWFA) are presented. Two different regimes are considered. In the highly non-linear regime the full Maxwell-Vlasov equations in three dimensions have to be solved. Recent works have demonstrated than 3D PIC simulations are now enable to be quantitatively compared with experimental results. These simulations however required a large amount of computer resources and are not well adapted to describe the acceleration of injected electron bunches over long distances. To deal with these latter case efficient methods have been developed that reduce dramatically the required computer time. Using these methods, a full 3D simulation of multi-stage acceleration by LWFA seems feasible in a near future.

Introduction

The laser wake-field acceleration (LWFA) of electrons in under-dense plasmas [1] has been the subject of intense study for many years. As the performances of the laser installations are being improved in term of intensity, shortening of pulse duration, and control of the pulse shape, various acceleration schemes [2-3] are being experimentally checked and new ones are proposed for one or multi-stage acceleration of electrons by LWFA, and we assist to a continually growing number of published works devoted to this subject. Numerical simulations (NS) play a central role in the development of this field mainly because the processes involved in the experiments are in general too complex to be analysed, in a quantitative way, with analytical methods, but the physics is simple enough to be tractable by full ab initio NS. In particular, it has been demonstrated that NS can be in quantitative good agreement with experimental results of LWFA, even in the strong non-linear regime, for the energy distribution function of the accelerated electrons [4-5] and also for the emittance of the beam [6].

The various proposed acceleration schemes pertain to quite different regimes, ranging from the semi-linear LWFA at intensities about 10^{17} W.cm^{-2}, where the injected electron bunch is expected to be accelerated over several cm, up to the ultra-relativistic regime above 10^{20} W.cm^{-2}, for which a caviton, named a bubble by A. Pukhov [7], is created inside the plasma and accelerates electrons up to GeV energy within 1 mm. There is not a unique numerical method that is well adapted to describe efficiently the acceleration mechanism in all the regimes. In the following the main physical parameters of the interaction process, and the equation to be solved, will be briefly given. Then we will present a short overview of the numerical codes that are developed in the strongly and weakly non-linear regimes.

Basic physical parameters

Here we present the main physical parameters entering the LWFA. It will allow to retain only processes that have a significant contribution for LWFA and also to determine the boundary between highly and weakly non-linear regimes.

Let us consider a laser beam with frequency ω_L, wavelength $\lambda = 2\pi c/\omega_L$ and duration $\tau_L \approx (5\text{-}50)\ 2\pi/\omega_L$, which is focused at the entrance of an hydrogen or an helium gas. The radius r_0 of the focal spot is in the range of 10-100 µm, while a typical value for λ is 0.8µm. We thus have $r_0/\lambda >> 1$, which indicates that the paraxial approximation can be applied in the vacuum. In the vacuum, the characteristic length for the intensity variation along the propagation axis is the Rayleigh length $z_R = \pi r_0^2 / \lambda$ that has a mm range. Guiding is thus necessary when considering acceleration lengths of several cm.

The energy of one photon is 1.24 eV, which is much too low to have a direct binary interaction with the electron. The beam-plasma interaction can thus be described mainly on the macroscopic level. At a sufficiently high value of the laser intensity, the bound electrons are ionised by tunnelling. For a linearly polarised field, ionisation occurs at the intensity given by

$$I(\mathrm{W.cm^{-2}}) = 4 \times 10^9 \frac{I_p^4}{Z^2}(\mathrm{eV}), \qquad (1)$$

with I_p the ionisation potential and Z the atomic number of the target atoms. For H and He, Eq. (1) yields I=1.4 and 3.6 respectively, in units of 10^{14} W.cm^{-2}. These values are well below

the considered intensity for LWFA. Thus the light pulse interacts mainly with a fully ionised plasma. Ionisation occurs only at the front of the pulse, and is very fast.

The dynamic of the plasma particles interacting with the laser can be separated into two time scales: The high frequency oscillation at ω_L, and the time related to the electron displacement induced by the ponderomotive force. The latter is proportional to the square of the gradient of the field, and tends to push the electrons outside the region of highest intensity. For sub-picosecond pulse, one can suppose that the nucleus remains fix, the ions can then be described as a uniform neutralising background.

If the displacement induced by the laser is small, the electron begins to oscillate, with a frequency given by the plasma frequency $\omega_p = \sqrt{n_p e^2 / \varepsilon_0}$, with n_p the density of the plasma electrons. For describing the dynamic of the electron fluid, we are in a density regime where the collisionless classical approximation can be safely used. The e-e and e-i collision frequencies are much smaller than ω_p. It means that the associated damping plays a role only far from the laser-plasma interaction domain, and also plasma heating through inverse-bremsstrahlung is inefficient. Moreover the fermionic nature of the electrons can be neglected.

For a specific value of the density, named the critical density n_{cr}, we have $\omega_p = \omega_L$. At densities higher than n_{cr}, the electrons can efficiently screen the laser field and the beam cannot propagate inside the plasma. At lower densities, the plasma is qualified as under-dense, it can be considered as a dielectric medium with a relative dielectric constant given by

$$\varepsilon = 1 - n_p / (\gamma n_{cr}), \qquad (2)$$

γ being the relativistic factor. In our case n_{cr}=1.75x10^{21} cm^{-3}, while n_p is about 10^{17} to 10^{19} cm^{-3}. We are thus in the case of an under-dense plasma. ε as given by Eq. (2) being close to one. The phase and group velocity of the laser pulse are thus close to c and the γ factor related to the group velocity of the pulse is $\gamma_G = \left(n_{cr} / n_p\right)^{1/2} \approx 10 - 100$. The propagating pulse generates a plasma wake with a wavelength of λ_p ; $c / \omega_p = \lambda \left(n_{cr} / n_p\right)^{1/2} \approx$ (10-100)λ. In the linear regime, the laser beam is only slightly affected by the plasma. The characteristic length for variation of the pulse shape along the beam axis is then still given by z_R. The duration of the interaction between the electron and the pulse $\approx \tau_L$, which is much shorter than z_R/c. Therefore we can assume, as in the quasi-static approximation, that the electron interacts with a pulse of constant shape.

There are two parameters to determine whether we are in the highly or in the weakly non-linear regimes. The first one is $a_0 = eE / m\omega_L c = 0.85\lambda[\mu\text{m}] I^{1/2} \left[10^{18}\,\text{W.cm}^{-2}\right]$, the amplitude in reduced units, such that for $a_0 \geq 1$ the dynamics of the electron is in the relativistic domain. Moreover $a_0 \geq 1$ corresponds also to the limit at which the plasma electrons can be trapped by the wake, whereas for $a_0 \geq \sqrt{2\gamma_G}$ we are above the cold wave-breaking limit at which the plasma density exhibits a singularity within a cold fluid description. The second parameter is the critical power P_{cr} =17(n_{cr} /n_p) GW. At higher power, due to the γ factor in Eq. (2), the beam is self-focusing inside the plasma. So even starting with a small value of a_0, the intensity increases during propagation until the point where a_0>1.

In the case of acceleration of an injected bunch, the bunch generates its own plasma-wake, the influence of which is called the beam loading effect. For relativistic electrons, the interaction with the plasma is weak. In particular, the range of the electrons in the ionised gas is much larger than the size of the target. Therefore beam loading can have significant effects only when the density of the bunch electron is comparable to the perturbation of density induced by the laser pulse. An important parameter for bunch acceleration is the dephasing

length $L_D = \lambda_p \gamma_G^2$; $\left(10^3 - 10^6\right)\lambda$ that gives the maximum length of the target for which the acceleration is efficient.

The equations to be solved in LWFA

When considering a gas interacting with a high intensity laser pulse, the basic equations to be solved are the Maxwell-Boltzmann equations that connect the electromagnetic fields with the electron and ion distribution functions. The electric **E** and magnetic **B** fields are derived from the charge ρ and current **j** densities, through the Maxwell equations

$$\nabla \cdot \mathbf{B} = 0, \nabla \cdot \mathbf{E} = 0$$
$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \frac{\partial \mathbf{E}}{\partial t} + \frac{\mathbf{j}}{\varepsilon_0} - c^2 \nabla \times \mathbf{E} = \mathbf{0}. \tag{3}$$

The charge and current densities are determined from the distribution functions $f_i(\mathbf{x},\mathbf{p},t)$ for the ions of charge $q_i=Z_i e$, **x** and **p** being the position and momentum of the particles, and $f_e(\mathbf{x},\mathbf{p},t)$ for the electrons of charge $q_e=-e$:

$$\rho(\mathbf{x},t) = q_i \int f_i(\mathbf{x},\mathbf{p},t)d\mathbf{p} + q_e \int f_e(\mathbf{x},\mathbf{p},t)d\mathbf{p}$$
$$\mathbf{j}(\mathbf{x},t) = q_i \int \mathbf{v}_i f_i(\mathbf{x},\mathbf{p},t)d\mathbf{p} + q_e \int \mathbf{v}_e f_e(\mathbf{x},\mathbf{p},t)d\mathbf{p} + \mathbf{j}_{\mathbf{ion}}(\mathbf{x},t). \tag{4}$$

The term $\mathbf{j}_{\mathbf{ion}}(\mathbf{x},t)$ is introduced in the last equation to take into account the ionisation process [8]. It has a significant contribution for channelling in a capillary tube. In this case, close to the inner-wall of the tube, the intensity of the field can be below the value given by Eq. (1), and therefore the structure of the field in this region can depend on the ionisation process, particularly when considering helium gas.

As stated above, for the considered densities, we can safely make use of classical statistics. The distribution functions are thus given by the Boltzmann equations

$$\frac{\partial f_{e,i}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_{e,i} + q_{e,i}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \nabla_{\mathbf{p}} f_{e,i} = S + \left(\frac{\partial f_{e,i}}{\partial t}\right)_{\text{col.}} \tag{5}$$

In the right hand side (RHS) of this equation S is the source term, coming form the ionisation process already mentioned and the second term is a correction coming from close collisions.

Equations (1-3) have to be solved with the boundary conditions relevant to the considered experiment. Let us suppose that the target is situated between z=0 and z=L and that the laser-target interaction process begins at t=0, the boundary conditions are then:

- The electromagnetic field at z=0, has to be written as a linear combination of propagating modes that satisfy the Maxwell equation in the vacuum, to fix **E, B** at $z=0^-$ and $t>0$. In most calculations it is supposed that the incoming beam is linearly polarized and in the fundamental gaussian mode, the focal plane being the surface entrance of the target. In many laser installations however; the incoming laser beam is far from the diffraction limit. A precise comparison with experiment thus requires to take into account the actual structure of the laser field at z=0. This point was recently stressed out when considering channelling in capillary tube [9]
- $f_e(z=0^-,t>0)$ is non-zero in case of an incoming electron bunch
- When considering the guiding by an external structure, for a plasma channel one has to know the initial profile: $f_e(z>0^-,t=0)= Z_i f_i(z>0^-,t>0)$, whereas for a capillary tube, the E.M. fields have to satisfy boundary conditions at the inner-wall. If the transverse flux at the wall, is lower than the threshold damage, then these boundaries do not depend on time,

otherwise one has to include the influence of plasma formation on the boundary conditions [10].

To solve Eqs (1-3) with the above boundary conditions is in general a formidable task. When considering a sub-picosecond laser pulse at high intensity, which interacts with a gas, the problem can be simplified as stated in Sec. 2: the dynamic of the ions as well as e-e and e-i collisions are neglected. Moreover in many situations, the influence of the front of ionisation can be disregarded. The problem to be solved is then the Maxwell-Vlasov system of equations for the electrons, which is by no mean a simple task.

3D PIC simulation in the highly non-linear regime

In the strong non-linear regime, a clear distinction between well separated time scales is in general not possible. For example if the ponderomotive force is strong enough, it will expel all the electrons, and behind the front of the pulse a caviton appears, in which the electron density is zero. The group velocity of the field will then be different in the front and rear side of the pulse leading to a strong compression of the pulse [5]. In this case, no simplification can be made, and one has to solve the full relativistic Maxwell-Valsov equations.

The Particle In Cell method is now a well-established powerful technique to determine the dynamic of plasmas [11]. It is a full ab initio method, with no approximation other than the ones used to derive the classical Maxwell-Vlasov equations. The basic advantage of PIC simulation over direct molecular dynamics calculations is that the computer time increases only linearly with the number of pseudo-particles. It enables to treat much larger systems, presently of the order of 100^3 μm^3. The main difficulty still resides on its practical implementation, because it requires large computer resources and the implementation of efficient numerical procedures, which in general are machine dependent. A typical example is given by the VLPL PIC code of A. Pukhov [12], who was the first to publish results obtained in 3D geometry. In the VLPL code up to 10^9 particles and 10^8 cells are considered, the code is parallelized and run on a cluster of 784 nodes. Similar values are used in the Osiris [13] and Calder [4,6] codes. An important point concerning the PIC codes is that they can be developed for many applications other than the LWFA. In particular the Calder code has been constructed for the French-CEA inertial fusion program LMJ.

Recently [4,6] is was demonstrated that 3D-PIC codes are now enable to reproduce, with a good accuracy, the experimental results of LWFA in the highly non-linear regime. It concerns not only the energy distribution, but also the angular distribution of the accelerated electrons. In [4,6] it was also stressed out, that the obtained results cannot be reproduced within a 2D approach.

Simulation of the acceleration of an injected bunch

When considering the acceleration of an injected beam, for applications such that multi-stage acceleration, one needs to have a precise control on the electron beam dynamics. The non-linear effects have thus to be kept at a relatively low level. The pressure of the gas and the intensity of the field have thus the lowest values among those given in Sec. 2. However the distance to be considered is much larger than in the previous case being of the order of 10^6 λ. A direct 3D-PIC simulation of this process is thus not tractable even with the next generation of computers. In this regime however one can reduce significantly the computer time by averaging the high frequency components of the E.M. fields and of the particle dynamics, and also by using the static approximation. The Maxwell and Vlasov equations are modified, such that the terms that depend on the small parameter $\delta = \omega_p / \omega_L$ are identified. Then only the zero and first order terms in δ are retained. This

procedure was first applied in the Wake code of Mora and Antonsen [15], in which a PIC-type simulation is used but with characteristic time and length given by the plasma wake and not by the laser field.

When the field is well below the wave-breaking limit, the electrons from the bunch can be distinguished from the plasma electrons. For the latter, the Vlasov equations can be solved by considering only its first moments, within the cold fluid approximation [3,8], while for the electrons of the bunch a particle method is still used. For the standard scheme, where the bunch is placed behind the laser pulse, the beam dynamics is only connected to the frequency plasma wake. In this case A. Reitsma [3] has shown that the main characteristics of the acceleration process can already be performed through analytical analysis. Numerical procedures are however still needed to investigate large beam-loading and 2 or 3D effects connected, for example to imperfect guiding over large distances.

Situations that require further investigation are mainly the case where the bunch is interacting with the laser pulse. It has been recently proposed that by injection of the bunch in front of the laser pulse, it is possible to consider bunches with initial sizes much longer than λ_p [8,15]. In this case however, the bunch will interact with the laser pulse over a large distances, and the quasi-static approximation does not seem to hold.

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