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H-VLPL: A three-dimensional relativistic PIC/fluid hybrid code

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ABSTRACT

The novel PIC/fluid hybrid plasma simulation code H-VLPL3D is introduced. In addition to the particle-in-cell algorithm, it uses a new numerical fluid scheme for wake field simulations. Specially designed for the accurate simulation of very long wake fields, this scheme is capable of simulating ~ 1000 plasma oscillations of the wake. A comprehensive description of the discretization schemes is given, and we demonstrate the code's correctness and its order of accuracy. Also, its superior efficiency in the plasma wake field acceleration (PWFA) regime is shown.

1. Introduction

The idea of utilizing wake fields as particle accelerators becomes increasingly promising [1,2]. While conventional accelerators are limited by characteristic breakdown fields, plasma waves do not suffer from such restrictions. They reach field strengths orders of magnitude higher. In this context, TeV proton bunches as drivers for plasma wake fields have recently gained much attention [3]. Due to the high energy of the proton bunches, the need for multiple acceleration stages may be removed.

Recent results [4,5] have shown that even long proton bunches can resonantly drive strong wake fields via self-modulation.

Because of the complexity of such setups as well as the large scale of experiments involving TeV proton beams, reliable simulations are crucial. A commonly preferred method for wake field simulations is the particle-in-cell (PIC) algorithm. It is a kinetic model, statistically populating the phase space with macroparticles. Well-known large-scale three-dimensional PIC codes like OSIRIS [6], VORPAL [7], OOPIC [8], VLPL [9] and others have been an important pillar in plasma wake field research.

However, the self-modulated proton driven plasma wakefield acceleration (SM-PDPWA) process under investigation has special requirements on the numerical algorithms. The proton bunch is about 500 plasma wavelengths long and has to propagate many tens of meters in plasma. PIC methods tend to be very costly in CPU time. They also suffer from numerical diffusion and dispersion, which render them ineffective for this regime.

With H-VLPL3D, we have implemented a PIC/fluid hybrid code, which is very well suited for this problem. It is capable of simulating extremely long wake fields involving hundreds of plasma oscillations without the numerical problems pertinent to PIC. The basic idea is to represent the plasma by two distinct means: First, as a set of PIC macroparticles for parts undergoing kinetic effects. Second, as a fluid through numerical solution of conservation laws. The latter offers a number of advantages over the PIC method: It is far more efficient, with low noise and less numerical dispersion. In the last years,

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hybrid techniques have gained importance in high density plasma simulations, including fast ignition (FI) experiments and solid state density plasma interactions. Most of these codes do not model the propagation of electromagnetic waves as well as electrostatic waves, instead using magnetohydrodynamic (MHD) descriptions. The hybrid PIC code LSP [10] uses a particle-in-cell algorithm along with a fluid model and an implicit electromagnetic field solver. Also, the OSIRIS and the dHybrid [11] code comprise hybrid functionality, treating ions kinetically and electrons as a fluid, under the assumption $\nabla \times \vec{B} = \mu_0 \vec{J}$.

In [7], a cold fluid model is coupled with a kinetic model for the plasma. Using a primitive variable formulation on a collocated mesh, the convective term is solved for with a semi-Lagrange algorithm; the density update is done with a variant of semi-Lagrange advection, which is subdivided into low- and high-order parts. The latter are then combined via the flux-corrected transport (FCT) method [12]. In [13], a cold fluid model is coupled with the vector potential wave equation. Time stepping is done using second order finite differences, while spatial derivatives are computed via Fourier transforms, cutting the highest modes of the spectrum. Recently, the development of the INF&RNO code was reported [14], where a PIC/fluid hybrid model is implemented on a collocated mesh in cylindrical geometry.

There are also other means of reducing the computational cost of PWFA simulations. If the parameters of the driver and the physical structure inside the simulation box change slowly, quasi-static PIC algorithms can be formulated [15]. Here, the particle dynamics are solved for with the approximation of constant EM fields; then, the fields are advanced assuming that the particle trajectories are similar for a long period of time. Furthermore, there is the Boosted Frame approach [16], where the simulation is computed in a Lorentz transformed inertial frame. Since the propagating simulation box contents become stretched, but the plasma is compressed by a relativistic Doppler factor, this approach can provide speed-ups of several orders of magnitude. These methods resemble to taking advantage of the quasi-static nature of the problem. They are complementary to the PIC/fluid hybrid concept and can even be combined with the latter. In this work however, we will focus on how the proper choice of the plasma representation affects the numerical effort.

For the new hybrid system presented here, we choose a different fluid approach. It is specially designed for the simulation of extremely long wakefields. The background plasma is also a cold fluid, covering density modulations and convection. In order to minimize losses, the grid layout for the fluid discretization has been aligned with the Yee grid of the Maxwell solver. To ensure stability and prevent spurious oscillations, we adopt the FCT method. It is combined with a modified quadratic upstream interpolation for convective kinematics (QUICK) [17] scheme. A modified semi-Lagrange scheme is used for the advection of the staggered momenta. Among others, this algorithm can be used for simulations of very long plasma wakefields by modeling the driver with a conventional PIC approach, but the plasma with the fluid scheme. It shows significantly less numerical dispersion, distortions, and damping of the wake than full PIC simulations. This allows for much higher grid steps, greatly increasing the computational performance.

This paper is organized as follows: In Section 2, we give a detailed description of the algorithm. Section 2.1 briefly reviews the particle-in-cell concept and describes the PIC fraction of the scheme. Section 2.2 introduces the fluid equations which are added to the existing PIC model, Section 2.3 explains the spatial scheme used; in Section 2.4, we discuss the various time integrators which can be applied. The H-VLPL implementation is verified first on simple physical examples. Afterwards, more application-oriented setups are tested. Results are depicted in Section 3.

2. Concepts of the hybrid algorithm

2.1. Particle-in-cell model

The hybrid scheme is based on the particle-in-cell (PIC) method, which is widely used in computational plasma physics. The PIC method can solve the six-dimensional relativistic Vlasov equation,

$$\frac{\partial}{\partial t} f_j + \mathbf{v}^T \nabla_x f_j + q_j(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \nabla_p f_j = 0, \tag{1}$$

by populating the phase space with so-called PIC macroparticles. These particles have a pre-defined spatial shape and carry a certain charge, mass, position, and momentum. The standard cycle of a PIC code consists of interpolating the EM fields onto the particles' center of mass, advancing the particles' momenta and positions, computing the currents due to the position change, and advancing the EM fields using these currents.

In the present implementation, the particles have a rectangular spatial density profile, also known as cloud-in-cell. Yet, the hybrid scheme is not restricted to the rectangular shape, and higher-order shapes can also be implemented. The particles' momenta and positions are updated using the leap-frog integrator.

2.2. Fluid model

In the present scheme, a plasma can be modeled by two distinct means: First, using a kinetic description and statistically populating the phasespace with PIC macroparticles. It is capable of simulating effects like wave-breaking while trading speed for a full physics description and suffering from damping effects. Second, it also contains a cold-fluid model. The latter, despite the fact it cannot describe wave-breaking, works far more smoothly and efficiently. The equations related to the fluid part read