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Enabling Lorentz boosted frame particle-in-cell simulations of laser wakefield acceleration in quasi-3D geometry

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A B S T R A C T

When modeling laser wakefield acceleration (LWFA) using the particle-in-cell (PIC) algorithm in a Lorentz boosted frame, the plasma is drifting relativistically at $\beta_b c$ towards the laser, which can lead to a computational speedup of $\sim \gamma_b^2 = (1-\beta_b^2)^{-1}$. Meanwhile, when LWFA is modeled in the quasi-3D geometry in which the electromagnetic fields and current are decomposed into a limited number of azimuthal harmonics, speedups are achieved by modeling three dimensional (3D) problems with the computational loads on the order of two dimensional $r-z$ simulations. Here, we describe a method to combine the speedups from the Lorentz boosted frame and quasi-3D algorithms. The key to the combination is the use of a hybrid Yee–FFT solver in the quasi-3D geometry that significantly mitigates the Numerical Cerenkov Instability (NCI) which inevitably arises in a Lorentz boosted frame due to the unphysical coupling of Langmuir modes and EM modes of the relativistically drifting plasma in these simulations. In addition, based on the space–time distribution of the LWFA data in the lab and boosted frame, we propose to use a moving window to follow the drifting plasma, instead of following the laser driver as is done in the LWFA lab frame simulations, in order to further reduce the computational loads. We describe the details of how the NCI is mitigated for the quasi-3D geometry, the setups for simulations which combine the Lorentz boosted frame, quasi-3D geometry, and the use of a moving window, and compare the results from these simulations against their corresponding lab frame cases. Good agreement is obtained among these sample simulations, particularly when there is no self-trapping, which demonstrates it is possible to combine the Lorentz boosted frame and the quasi-3D algorithms when modeling LWFA. We also discuss the preliminary speedups achieved in these sample simulations.

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1. Introduction

Laser wakefield acceleration (LWFA) [1] offers the potential to construct compact accelerators that have numerous potential applications, including the building blocks for a next generation linear collider and the electron beam source for ultra-compact XFELs. It has thus attracted extensive interest, and the last decade has seen an explosion of experimental results. Fully nonlinear particle-in-cell (PIC) simulations have been instrumental in this progress as an aid in designing new experiments, in interpreting experimental results, and in testing new ideas. Furthermore, developing predictive theoretical models is challenging due to the strong nonlinear effects that are present in the blowout and bubble regimes of LWFA [2]; therefore numerical simulations are also critical in exploring the physics of LWFA. Particle-in-cell simulations have been extensively applied in LWFA research because the PIC algorithm follows the self-consistent interactions of particles through the electromagnetic (EM) fields directly calculated from the full set of Maxwell equations. When modeling LWFA using the PIC algorithm the laser wavelength needs to be resolved which is usually on the scale of 1 μm; meanwhile, the length of the plasma column that the laser propagates through can be on the scale of 10^4 to 10^6 μm. As a result of this disparity in cell size and propagation distance, full three-dimensional (3D) PIC simulations of LWFA can be very CPU-time consuming. To capture the key physics while reducing the computation time, reduced models are continually being proposed. These include models that combine the ponderomotive guiding center with full PIC for the wake [3] or with the quasi-static approach [4,5]. However, these models cannot as yet model full pump depletion lengths, and the quasi-static approach cannot model self-injection.

Recently, two methods have been proposed that can speed up the LWFA simulation without losing key physics in the modeling of LWFA. One method is the Lorentz boosted frame technique [6]. In this method the LWFA simulations are performed in an optimized Lorentz boosted frame with velocity v_b, in which the length of the plasma column is Lorentz contracted, while the laser wavelength is Lorentz expanded. Assuming the reflection of the laser light is not important in the lab frame, then in a properly chosen Lorentz transformed frame the time and space scales to be resolved in a numerical simulation are minimized, and savings of factors that scale as $\gamma_b^2 = (1 - v_b^2/c^2)^{-1}$ can be achieved.

Another speedup method that has been recently proposed is to decompose the EM fields and current density into a Fourier series in the azimuthal angle ϕ,

$$
\begin{aligned}
\vec{F}(r,z,\phi) &= \mathrm{Re}\left\{\sum_{m=0} \vec{F}^m(r,z)e^{im\phi}\right\} \\
&= \vec{F}^0(r,z) + \mathrm{Re}\{\vec{F}^1\}\cos\phi - \mathrm{Im}\{\vec{F}^1\}\sin\phi \\
&\quad + \mathrm{Re}\{\vec{F}^2\}\cos(2\phi) - \mathrm{Im}\{\vec{F}^2\}\sin(2\phi) \\
&\quad + \ldots
\end{aligned}
$$

and truncate the expansion at a low m value [7]. This expansion is substituted into Maxwell's equations to generate a series of equations for the complex amplitudes for each harmonic. The harmonics are then summed to get the total fields. The particles are pushed in 3D Cartesian geometry and are then used to obtain the complex amplitudes for each harmonic of the current. This method can reduce the computational costs of modeling 3D problems with low azimuthal asymmetry to that on the order of 2D $r-z$ simulations. This algorithm, together with a charge conserving current deposition scheme in quasi-3D geometry has been implemented in OSIRIS [8].

It was pointed out in Refs. [9,10] that it would be intriguing to combine these two methods in order to combine the speedups provided by each. Similar to full PIC simulations in the Cartesian geometry, it was found that in the quasi-3D geometry one of the main obstacles to performing Lorentz boosted frame simulations is the multi-dimensional Numerical Cerenkov Instability (NCI) [11–14] that inevitably arises due to the unphysical coupling between Langmuir modes (main and aliasing) and EM modes of the relativistic drifting plasma in the simulations. The coupling arises in the Lorentz boosted frame between modes which are purely longitudinal (Langmuir modes) and purely transverse (EM modes) in the lab frame. The coupling occurs at specific resonances $(\omega - 2\pi\mu/\Delta t) = (k_z - 2\pi\nu_z/\Delta z)v_b$ where μ and ν_z are the time and space aliases and Δt and Δz are the time step and grid size respectively, and ω and k_z are the frequency and wave number in $\hat{z}$ direction.

While the multi-dimensional NCI theory in Cartesian coordinates has been well studied (see e.g. [12–18]), there are currently no analytical expressions for the numerical dispersion relation of a relativistic plasma drift in the quasi-3D geometry. However, OSIRIS [22] simulations have shown that its behavior in the quasi-3D $r-z$ geometry is very similar to that in the Cartesian geometry. It was therefore recently proposed and demonstrated that a hybrid Yee–FFT solver could be used to suppress the NCI in the Cartesian and quasi-3D geometries [18]. In the regular Yee (a finite difference) solver in a quasi-3D geometry [7,21], Maxwell equations are solved in (r,z) space for each azimuthal mode m. In the hybrid Yee–FFT solver, we perform a (discrete) Fourier transform in the drifting direction of the plasma (denote as $\hat{z}$ direction), and solve Maxwell equations in k_z space for each azimuthal mode m; meanwhile, in the $\hat{r}$ direction the derivatives are represented as second order finite difference operators on a Yee grid. The current is corrected to maintain the satisfaction of Gauss' Law. When Maxwell's equations are solved in this way, the corresponding NCI modes can be systematically eliminated by applying similar strategies used for a multi-dimensional spectral Maxwell solver [14,17]. The fastest growing modes of the NCI at $(\mu,\nu_1) = (0,\pm 1)$ can be conveniently suppressed by applying a low-pass filter in the current, the highly localized