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**P. Yu, A. Davidson, X. Xu, et al.**



# Modeling of Laser Wakefield Acceleration In Lorentz Boosted Frame Using a Quasi-3D OSIRIS Algorithm

P. Yu*, A. Davidson†, X. Xu**, A. Tableman†, V. K. Decyk†, F. S. Tsung†, J. Vieira‡, R. A. Fonseca‡,§, W. Lu**, L. O. Silva‡ and W. B. Mori*,†

*Department of Electrical Engineering, University of California Los Angeles, Los Angeles, CA 90095, USA
†Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, CA 90095, USA
**Department of Engineering Physics, Tsinghua University, Beijing 100084, China
‡Instituto Superior Técnico, 1049–001, Lisbon, Portugal
§ISCTE - Instituto Universitário de Lisboa, 1649–026, Lisbon, Portugal

**Abstract.** Recently it was proposed in [A. F. Lifschitz, et. al., J. Comp. Phys. 228, 1803 (2009)] that laser wakefield acceleration could be modeled efficiently using a particle-in-cell code in cylindrical coordinates if the fields and currents were expanded into Fourier modes in the azimuthal angle, $\phi$. We have implemented this algorithm into OSIRIS, including a new rigorous charge conserving deposition routine applicable for it [A. Davidson, et. al., J. Comp. Phys. 281, 1063 (2014)]. This algorithm can be interpreted as a PIC description in $r-z$ and a gridless description in $\phi$ in which the expansion into $\phi$ modes is truncated at a desired level. This new quasi-3D algorithm greatly reduces the computational load by describing important three-dimensional (3D) geometrical effects with nearly two-dimensional calculations. In this paper, we propose to combine this algorithm with the Lorentz boosted frame method for simulations of Laser wakefield acceleration (LWFA). We show preliminary results, including an investigation of the unstable numerical Cerenkov instability modes for this geometry, and discuss directions for future work. These preliminary results indicate that combining the quasi-3D method and the Lorentz boosted frame method together may provide unprecedented speed ups for LWFA simulations.

**Keywords:** Particle-in-cell, laser wakefield acceleration, numerical Cherenkov instability, quasi-3D algorithm, Lorentz boosted frame

## 1. INTRODUCTION

Laser wakefield acceleration (LWFA) [1] has attracted extensive interest due to its potential for developing ultra-compact, high-gradient accelerators that have numerous potential applications, including the building blocks for next generation linear colliders and being the driver for compact light sources. Due to relativistic and nonlinear effects, numerical simulations that follow the trajectories of individual electrons are critical for studying the physics of LWFA. In particular, particle-in-cell (PIC) simulations include the necessary physics and have therefore played an integral role in the development of LWFA. In the nonlinear blowout regime [2, 3, 4], it is important to include 3D geometrical effects in order to accurately model laser propagation, wakefield excitation, and beam loading [5]. Therefore, 3D rather than 2D slab $(x-y)$ simulations are required for quantitative rather than qualitative predictions. Although 2D $r-z$ PIC simulations have proven useful and accurate for modeling beam driven wakefield acceleration (PWFA), they are not amenable to LWFA modeling because the laser fields are not purely azimuthally symmetric (they are radially polarized). Unfortunately, simulating LWFA using a standard PIC code in 3D can be very CPU demanding. For example, 3D PIC simulations of $\sim$10 GeV stages for the nonlinear blowout regime are already reaching the limits of the CPU resources currently available. This makes it difficult to carry out parameter scans in full three dimensions. Therefore, reduced models of LWFA such as the ponderomotive guiding center [6, 7, 8] and the quasi-static approximation have been proposed to find the balance between accuracy of the models and the computational load [8, 9]. In addition, the Lorentz boosted frame has been proposed to significantly reduce the needed CPU time. However, this method is still being tested in the nonlinear blowout regime where self-trapping of electrons is occurring.

Recently, Lifschitz et. al. [10] proposed a method to use $r-z$ 2D PIC simulations to model LWFA. The idea was to expand the electromagnetic fields and the currents into azimuthal modes, $e^{im\phi}$, and to truncate the expansion. This is effective because a linearly polarized laser is represented by only the $m=1$ mode. Therefore, LWFA for nearly azimuthally symmetric cases can be simulated by truncating the expansion after $m=1$. This can reduce modeling a 3D problem with low azimuthal asymmetry into a similar computational cost as using a 2D $r-z$ code. This algorithm was implemented into OSIRIS, which required development of a new rigorous charge conserving scheme valid for the

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azimuthal mode expansion[11]. The new charge conserving scheme makes clear that this algorithm is a hybrid scheme between a PIC description in $r-z$ and a gridless description in $\phi$. It should be noted that the use of such a hybrid scheme was considered many years earlier to study particle beam plasma interactions [12].

As noted earlier, it has been proposed and demonstrated that by performing the simulation in an optimal Lorentz boosted frame with normalized velocity $\beta$, the time and space scales to be resolved in a numerical simulation may be minimized [13]. The basic idea is that in the boosted frame the plasma length is Lorentz contracted while the plasma wake wavelength and laser pulse length are Lorentz expanded. The number of laser cycles is an invariant, so the necessary number of cells needed to resolve the laser is also an invariant while the cell size and hence time step are Lorentz expanded. The increase in time step and cell size, and decrease in the plasma length lead to savings of factors of $\gamma^2 = (1-\beta^2)^{-1}$ as compared to a lab frame simulation using the so-called moving window [14]. Although straightforward in principle, this idea is challenging because the physics on a grid is actually not Lorentz invariant. This is seen by the fact that in a frame where the plasma drifts there is a violent numerical instability, called the Numerical Cerenkov Instability (NCI) [15]. The potential of the Lorentz boosted frame technique has led to a detailed reexamination of the NCI and to techniques to mitigate (effectively eliminate) it [16, 17, 18, 19, 20, 21].

In this paper, we propose to combine together the Lorentz boosted frame technique and the quasi-3D algorithm to achieve unprecedented speed-ups in LWFA simulations. If successful, this will provide the ability to perform rapid parameter scans and real-time steering of experiments. Based on these parameter scans, full 3D (including boosted frame) simulations can be performed for quantitative prediction. We have implemented the quasi-3D algorithm into our finite-difference-time-domain (FDTD) EM-PIC code OSIRIS [22], and have recently begun to explore using it to carry out LWFA simulations in a Lorentz boosted frame.

The rest of the paper is organized as follows. In section 2 we discuss the NCI and explore the unstable modes in the $r-z$ geometry of the quasi-3D code. We show that the optimal time step derived for cartesian geometry [17, 18] still works for the $r-z$ geometry. In section 3, we present preliminary simulation results. We compare simulation results from quasi-3D OSIRIS against UPIC-EMMA (which uses a spectral Maxwell solver) [23, 24] simulations. Good agreement is seen in some cases, illustrating the potential speed-ups that can be possible by combining these two methods. The results are summarized in section 4.

## 2. NUMERICAL CERENKOV INSTABILITY

When modeling LWFA in the Lorentz boosted frame, the plasma is drifting relativistically towards the laser. This inevitably leads to a numerical instability called the Numerical Cerenkov Instability (NCI) that is due to the unphysical coupling between the plasma Langmuir modes and EM modes [17, 18, 21]. This numerical artifact interferes with the physics being studied in the simulation, and therefore it is crucial to reduce the NCI growth rate to enable accurate modeling of physics problem involving relativistically drifting plasmas.

To study behavior of the NCI in the $r-z$ geometry, we performed simulations using the quasi-3D OSIRIS with only a cold relativistic plasma drift, i.e., no laser. Conducting boundary conditions were used in the $r$ direction, while periodic boundary conditions are used in the $z$ direction. The plasma has a drift velocity corresponding to $\gamma = 50$ in the $z$ direction. It has a very small but finite temperature in order to seed the instability. The Yee solver [25] is used in this simulation. For comparison, we likewise performed a 2D Cartesian OSIRIS simulation with the same simulation setups and parameters.

In Fig. 1 (b) and (c) we present snapshots of the NCI spectrum observed in the simulations, for both the quasi-3D and 2D Cartesian algorithms. For the quasi-3D case we use the $m = 0$ fields. In Fig. 1 (a) the corresponding growth rates are plotted for various time steps. When calculating the spectra of the NCI, we performed a Fourier transform to $E_2$ in both $x_1$ and $x_2$ directions (where $x_1$ is the drifting direction) for the 2D cartesian case, and performed a Fourier transform in the $z$ direction and a Hankel transform in the $r$ direction for the quasi-3D case. Interestingly, the two geometries show very similar patterns when the same simulation parameters are used. In addition, the growth rates are also close to each other. More importantly, as is well known for the NCI in Cartesian coordinates, when the momentum conservation field interpolation scheme (others refer to this as the uniform field interpolation) is used (as is the case in this paper), we find an optimal time step [17, 18, 26] at which the maximum NCI growth rate is minimized. It is interesting to see that this same optimal time step is the same value for both the 2D and quasi-3D geometries, and we used this optimal time step in the quasi-3D OSIRIS LWFA simulations in a Lorentz boosted frame. We are currently working on the theory of the NCI for the quasi-3D algorithm in order to explain what we observe in Fig. 1 (a).

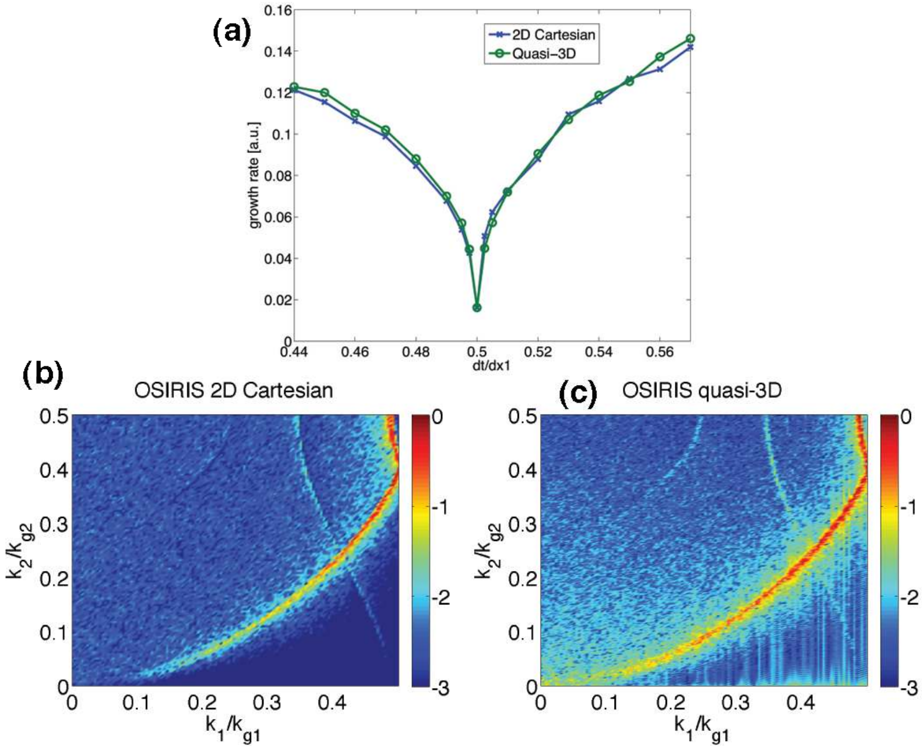


**FIGURE 1.** (a) The dependence of the maximum NCI growth rate on the time step used in the 2D Cartesian and quasi-3D simulations. In both cases an optimal time step at $c\Delta t = \Delta x/2$ can be found, where $\Delta x$ is the grid size along the drift direction. (b) Snapshot of the FFT of $E_2$ field of a 2D Cartesian OSIRIS simulation. (c) Snapshot of the FFT of $E_\phi$ field for the corresponding quasi-3D OSIRIS simulation. In (b) and (c) only the first quadrants are shown due to the symmetry of the pattern.

## 3. PRELIMINARY LWFA SIMULATIONS

The simulation setup used for performing LWFA in the boosted frame using quasi-3D OSIRIS is very similar to that for Cartesian 2D and 3D OSIRIS simulations. The plasma is drifting relativistically in $z$ direction at $\beta_z = -\beta$, where $\gamma = (1-\beta^2)^{-1/2}$ is the Lorentz factor of the boosted frame. The length of the plasma column contracts by $\gamma$, while its density increases by $\gamma$. Due to the Lorentz transform, the laser wavelength and pulse length stretch by $\gamma(1+\beta)$, and its Rayleigh length contracts by $\gamma$. Meanwhile the spot size at the focal point (which is always at the moving plasma edge) does not change. As a result, when $\gamma$ is sufficiently large one needs to use a moving antenna [27] to launch the laser pulse in order to avoid using a simulation box that is too wide in the $r$ direction. In the quasi-3D OSIRIS, each azimuthal mode is independently launched by the moving antenna. We are currently using conducting boundary conditions in the $r$ direction and a moving window in the $z$ direction, and are implementing the perfectly-matched-layers in the $r$ direction in the quasi-3D OSIRIS code.

To investigate the feasibility of combining the quasi-3D OSIRIS and the LWFA boosted frame technique, we conducted 5.8 GeV stage runs [4] using both quasi-3D OSIRIS and UPIC-EMMA. The parameters of the 5.8 GeV stage run in the lab frame is listed in Table 1. We performed quasi-3D OSIRIS simulations at $\gamma = 4$ and $\gamma = 8$, and UPIC-EMMA simulation at $\gamma = 30$. Moving windows are used for the quasi-3D OSIRIS run, and we chose the optimal time step in order to minimize the NCI growth rate. As for the UPIC-EMMA run, we used a low-pass filter to eliminate the fastest growing modes of NCI [18, 21, 24].

In Fig. 2 (a) we present a snapshot of the plasma density in the boosted frame for a $\gamma = 4$ quasi-3D OSIRIS run. As seen in Fig. 2 (a), the NCI is present at the left edge of the simulation box (these are short wavelength perturbations). However, we are mostly interested in the physics of the first bubble where there is much less evidence of the NCI. We likewise compared the corresponding wakefield in the first bubble in the lab frame by transforming the data from the $\gamma = 4, 8$ quasi-3D OSIRIS, and the $\gamma = 30$ UPIC-EMMA simulations back to the lab frame. This is shown in Fig. 2 (b). Good agreement is found within the first bubble. There is significantly more noise in the quasi-3D OSIRIS simulations at the rear of the first bubble. This noise is due to the unphysical numerical Cerenkov radiation from the self-trapped electrons. As noted in [24] there can be differences in the amount of self-trapped particles (and the associated beam loading) in boosted frame simulations with different $\gamma$. This is expected since the macro-particles in each simulation have different charges. For fixed number of particles per cell, the charge represented by a simulation particles increases in proportion to $\sim \gamma^2$ due to length contraction of the plasma and the increase in the cell size. Therefore, the statistics and the resolution of the details of the physics is different in the various frames. A full exploration of how the simulation codes, setups, and parameters influence the modeling of self-injection process in the Lorentz boosted frame are areas of future work.

**TABLE 1.** Parameters of LWFA 5.8 GeV stage simulations using quasi-3D OSIRIS and UPIC-EMMA. $k_0$ is the wavenumber of the driving laser.

| Parameters | Values |
|---|---|
| Plasma | |
| Density $n$ [cm$^{-3}$] | $5\times10^{17}$ |
| Length $L$ [m] | 0.08 |
| Laser | |
| Wavelength $\lambda$ [nm] | 800 |
| Pulse length $\tau$ [fs] | 80 |
| Waist width $W_0$ [$\mu$m] | 35 |
| Normalized vector potential $a_0$ | 5.1 |
| Quasi-3D OSIRIS simulation parameters | |
| Boosted frame Lorentz factor | $\gamma = 4, 8$ |
| Grid size $(\Delta x_z, \Delta x_\phi)$ [$k_0^{-1}$] | $(0.2\gamma(1+\beta), 5.0)$ |
| Time step $c\Delta t$ | $0.5\Delta x_z$ |
| Particle shape | quadratic |
| UPIC-EMMA simulation parameters | |
| Boosted frame Lorentz factor | $\gamma = 30$ |
| Grid size $(\Delta x_1 = \Delta x_2 = \Delta x_3)$ [$k_0^{-1}$] | $0.196\gamma(1+\beta)$ |
| Time step $c\Delta t$ | $0.184\Delta x_1$ |
| Particle shape | quadratic |

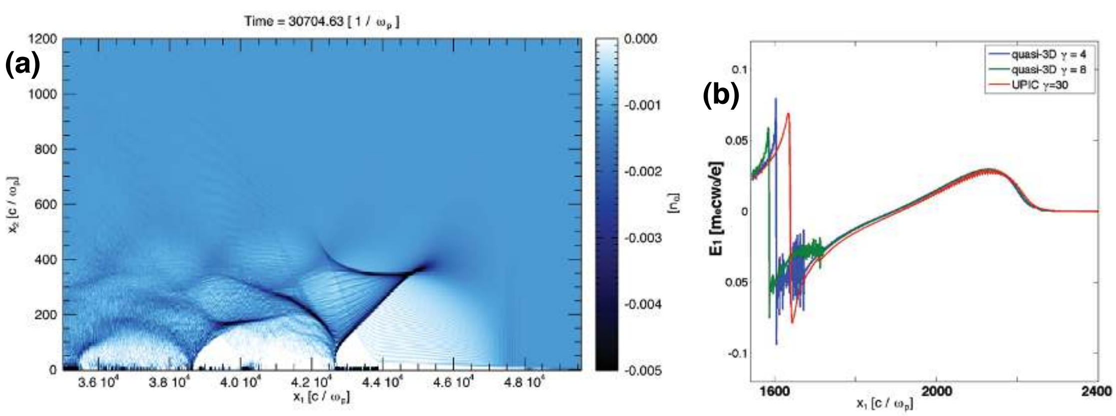


**FIGURE 2.** (a) shows the snapshots of plasma density for a quasi-3D OSIRIS simulation in the Lorentz boosted frame with $\gamma = 4$. (b) shows the on-axis wakefield line outs for the quasi-3D simulations at $\gamma = 4, 8$ and UPIC-EMMA simulations at $\gamma = 30$.

## 4. SUMMARY AND FUTURE WORK

In this paper, we propose combining a new quasi-3D (a hybrid PIC in $r - z$ and gridless in $\phi$) algorithm [10] together with the Lorentz boosted frame technique to obtain unprecedented speed-ups for LWFA simulations. We recently incorporated the quasi-3D algorithm into OSIRIS, including a new rigorous charge conserving scheme [11]. We present preliminary results of performing Lorentz goosed frame LWFA simulations using the quasi-3D algorithm within OSIRIS. We first investigated the NCI in the quasi-3D algorithm and found that both the pattern in $k$ space and growth rates of the NCI are similar to its counterpart in 2D Cartesian coordinates. In particular, the same optimal time step which minimizes the NCI growth rate in cartesian coordinates is found for the quasi-3D algorithm. We present sample LWFA simulations of a 5.8 GeV stage in the nonlinear self-guided regime using both the quasi-3D boosted frame simulations at $\gamma = 4$ and $\gamma = 8$, as well as UPIC-EMMA simulations at $\gamma = 30$. We compared the corresponding on-axis wakefield line outs by transforming them back to the lab frame. Good agreement was found between the three simulations, especially in the $z$ range where the front half of the first bubble and the laser are located. The disagreement appears to be due to numerical Cerenkov radiation as well as due to the different statistics of self-trapped electrons. These results demonstrate the potential of conducting Lorentz boosted frame simulation using the quasi-3D OSIRIS.

In the future, we plan on experimenting with smoothers, and alternative field solvers, to eliminate both the NCI and the numerical Cerenkov radiation of the trapped electrons, which would allow for modeling LWFA in higher $\gamma$ frames. We will also work to incorporate the quasi-3D algorithm onto our GPU and Intel Phi [28] enabled versions of OSIRIS for even greater speed ups. The quasi-3D code runs at the same speed as a 2D simulation. If we take 5.8 GeV case as an example, the combination of using the quasi-3D algorithm, the Lorentz boosted frame, and GPUs or Intel Phis could lead to a speed up of $\sim$500000.

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