# SELF AND IONIZATION-INJECTION IN LFWA FOR NEAR-TERM LASERS\*

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### Abstract

In plasma based acceleration (PBA), the methods of injecting high quality electron bunches into the accelerating wakefield is of utmost importance for various applications, including next generation light sources and high energy colliders. Numerous simulations are being conducted in order to study various methods of injection and to optimize the beam parameters. Particle-In-Cell simulations using codes such as OSIRIS are used to model PBA. 3D simulations are possible in some cases but are computationally expensive. 2D simulations are computationally less expensive, but 2D simulations in cartesian coordinates only provide qualitative agreement and 2D simulations in cylindrical coordinates cannot model laser wakefield acceleration (LWFA) at all and cannot include important physics such as hosing and low mode azimuthal mode asymmetries for particle beam drivers (PWFA). Here we discuss one method for reducing the computational load of a 3D simulation into those comparable to a 2D simulation that can model LWFA and include hosing. It utilizes a truncated azimuthal mode expansion. We describe how this expansion has been included into the OSIRIS simulation framework and show preliminary results.

#### INTRODUCTION

Simulations have played an essential role in the development of plasma based acceleration from the seminal work of Tajima and Dawson to the very present. Simulations are used to model both laser wakefield acceleration (LWFA) and plasma wakefield acceleration (PWFA). These simulations have evolved from 1D simulations to demonstrate the feasibility of new ideas to full 3D simulations that model current experiments one to one and that model parameters out of reach of current experiments. Although 3D simulations are now possible they are still computational expensive, therefore, when simulating LWFA and PWFA using we often begin with a series of 2D simulations over a range of parameters. The parameters are either for an ongoing experiment, for a future experiment, or for understanding a new theory or concept. We then have to perform a few large-scale 3D simulations to determine in what manner and to what degree the 2D simulations replicate a more realistic result.

# DIFFERENCES IN 2D AND 3D SIMULATIONS

One topic that is receiving much theoretical, computational, and experimental attention is how to best inject electrons into a plasma wave wakefield. One concept is to use field ionization to create electrons inside the wake. An important question is how do the 2D simulation results compare to those from otherwise identical 3D simulations. When using a laser, it is not possible to use 2D azimuthally symmetric simulations as such simulations only allow radially polarized modes. Therefore, 2D cartesian geometry are used and in such simulations both structure of the wakefield and the evolution of the laser can be very different. We provide examples of the differences by showing results from a a series of 2D and 3D simulations that were performed to model experiments conducted using the Callisto laser at LLNL. These simulations highlight some of the differences we see and the importance of the including full 3D physics. In these simulations a linearly polarized, 60 fs laser was focused into an "Injection Section" that is composed of 99.5% He and 0.5% N. After the laser propagates 1.5 mm in the injection section, it enters an "Acceleration Section" composed entirely of He. The total plasma density is  $n_p = 1 \times 10^{18} \text{ cm}^{-3}$  aside from the 0.5 mm up ramp at the beginning. Simulations were conducted with a 100 TW and a 500 TW laser beam. The spot size was 20.0  $\mu$ m for the 100 TW case, and 26.2 $\mu$ m for the 500 TW simulation.

As can be seen from Table 1, the peak energy of the trapped electrons can be significantly different between the 2D and 3D simulations. Another notable difference is that in the two 2D simulations, a comparable number of particles are trapped whereas in the 3D simulations 3.9 times more particles are trapped for the 500TW laser than for the 100TW laser. And in the 2D cartesian simulations only the charge per unit length that is trapped can be obtained. These differences illustrate that if one uses 2D simulations to optimize the process one can be led very far astray.

There is another notable qualitative difference in the 2D and 3D 500 TW simulation. If you look at the particle energy spectrums about 3 mm into the plasma (Figures 1 and 2), you see that there is a large, lower-energy peak exclusively in the 3D simulation. Although this peak eventually falls out, it dynamically affects the shape and the evolution of the wake. The 2D simulation fails to capture this process. Although not shown the evolution of the laser is also very different.

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Table 1: The Peak Energy, Charge, and Normalized Emittance of the Trapped Particles After the Laser Traverses 1.4 cm into the Plasma in the Two-Stage Injection-Acceleration Scheme

Simulation	$E_n$	q	$\epsilon$
	[GeV]		$[\pi \text{ mm-mrad}]$
100TW (2D)	1.49	1.37 a.u.	13
100TW (3D)	1.14	19 pC	34
500TW (2D)	3.37	1.29 a.u.	107
500TW (3D)	3 07	72 nC	86



Figure 1: The spectrum of the trapped particle energies in the 2D, 500 TW simulation 3 mm into the plasma.

## **AZIMUTHAL MODE EXPANSION**

There are various possible ways to reduce the computational requirements for capturing the 3D physics including using boosted frames, the ponderomotive guiding center approximation, and the use of the quasi-static approximation. Another recent idea proposed by Lifshitz et al. [1] is to expand the electromagnetic fields into a truncated Fourier expansion along the poloidal direction in cylindrical coordinates. The idea is to provide key 3D physics for situations where only low mode azimuthal asymmetry exists (a linearly polarized laser can be described by the m=1 mode). Such simulations will have a similar computational load to 2D r-z simulations. Here we describe how this algorithm has been implemented into OSIRIS and present some preliminary results. We can keep an arbitrary number of m modes. As noted in [1] a linearly polarized laser propagating along x, as described in Figure 3, can be expressed in cylindrical coordinates as

$$\mathbf{E}(\mathbf{r}, \mathbf{x}, \theta, t) = E_y(r, x, t)(\cos(\theta)\hat{r} - \sin(\theta)\theta)$$
(1)

$$\mathbf{B}(\mathbf{r}, \mathbf{x}, \theta, t) = B_z(r, x, t)(\sin(\theta)\hat{r} - \cos(\theta)\theta), \quad (2)$$

which are first order terms in the expansion

$$\mathbf{F}(r,x,\theta) = \Re\left(\sum_{m=0} \hat{\mathbf{F}}^m(r,x)e^{-im\theta}\right),\,$$

where  $\mathbf{F}$  is any vector field and the index m is the mode number. The zeroth order mode contains the cylindrically symmetric fields that are already incorporated in the 2D cylindrical coordinate simulation in the OSIRIS framework. Therefore, a linearly polarized laser can be modeled



Figure 2: The spectrum of the trapped particle energies in the 3D, 500 TW simulation 3 mm into the plasma.



Figure 3: Coordinates of the cylindrical mode simulation.

by only keeping the m = 1 mode. PWFA can be modeled in an r-z code, however, while very useful it is limited as it cannot include hosing or spot size asymmetries.

#### Algorithm

Therefore, as suggested above, the vector fields (E, B, and J) are calculated as a series of modes truncated at a number specified at the input. Each mode is stored on a different 2D grid. Due to the linearity of the Maxwells equations they each evolve independently[1], according to Equations 3-8.

$$\frac{\partial \mathbf{B}_{r}^{m}}{\partial t} = \frac{im}{r} \mathbf{E}_{x}^{m} + \frac{\partial \mathbf{E}_{\theta}^{m}}{\partial x}$$
(3)

$$\frac{\partial \mathbf{B}_{\theta}^{m}}{\partial t} = -\frac{\partial \mathbf{E}_{r}^{m}}{\partial \mathbf{x}} + \frac{\partial \mathbf{E}_{x}^{m}}{\partial \mathbf{r}}$$
(4)

$$\frac{\partial \mathbf{E}_{r}^{m}}{\partial t} = -\frac{1}{r} \frac{\partial}{\partial r} (r \mathbf{E}_{\theta}^{m}) - \frac{im}{r} \mathbf{E}_{r}^{m}$$
(5)  

$$\frac{\partial \mathbf{E}_{r}^{m}}{\partial t} = -\frac{im}{r} \mathbf{B}_{x}^{m} + \frac{\partial \mathbf{B}_{\theta}^{m}}{\partial x} \mathbf{J}_{r}^{m}$$
(6)  

$$\frac{\partial \mathbf{E}_{\theta}^{m}}{\partial t} = \frac{\partial \mathbf{B}_{r}^{m}}{\partial \mathbf{x}} + \frac{\partial \mathbf{B}_{\theta}^{m}}{\partial \mathbf{r}} - \mathbf{J}_{\theta}^{m}$$
(7)  

$$\frac{\partial \mathbf{E}_{x}^{m}}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (r \mathbf{B}_{\theta}^{m}) - \frac{im}{r} \mathbf{B}_{r}^{m} - \mathbf{J}_{x}^{m}$$
(8)

$$\frac{\mathbf{E}_{r}^{m}}{\partial t} = -\frac{im}{r}\mathbf{B}_{x}^{m} + \frac{\partial \mathbf{B}_{\theta}^{m}}{\partial x}\mathbf{J}_{r}^{m}$$
(6)

$$\frac{\partial \mathbf{E}_{\theta}^{m}}{\partial t} = \frac{\partial \mathbf{B}_{r}^{m}}{\partial \mathbf{x}} + \frac{\partial \mathbf{B}_{x}^{m}}{\partial \mathbf{r}} - \mathbf{J}_{\theta}^{m}$$
(7)

$$\frac{\partial \mathbf{E}_x^m}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (r \mathbf{B}_\theta^m) - \frac{im}{r} \mathbf{B}_r^m - \mathbf{J}_x^m \tag{8}$$

The mode mixing occurs when there is a presence of macro-particles, which are followed in cartesian space (x, x) $y, z, p_x, p_y, p_z$ ) and pushed according to the Lorentz Force Law (Equation 9). This requires transforming the fields in cylindrical coordinates to cartesian coordinates before pushing the particles.

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$$\dot{\mathbf{P}} = q(\mathbf{E} + 1/cv \times \mathbf{B})$$
  $\dot{\mathbf{x}} = 1/(m\gamma)\mathbf{P}$  (9)

The current density (or charge density) for each cylindrical modes at each r-z grid point i and j is obtained according to the equation

$$\rho_{ij}^m = \frac{1}{\pi} e^{im\theta} S_{ij} q / \Delta V$$

where  $S_{ij}$  is the area-weighing coefficient (subject to the interpolation scheme), and  $\Delta V = 2\pi r \Delta r \Delta x$ . The cylindrical angle  $\theta$  is calculated from the particle's x and y values. Looping over field evolution, particle advance, and charge deposition, we have a complete PIC algorithm.

Laser-Driven Field



Figure 4: A full 3D PIC simulation of a laser propagating through a pre-ionized plasma.  $E_1$  in units of  $[m_e c\omega_o/e]$ .



Figure 5: The 0th mode of the cylindrical mode simulation.

The above algorithm was implemented into the development version of OSIRIS, and tested using the parameters modeled after the LWFA simulation described by Lu et al [2]. Here a linearly polarized 200 TW,30 fs laser pulse is shot into a fully ionized  $n = 1.5 \times 10^{18}$  cm<sup>-3</sup> plasma, with a spot size of 19.5  $\mu$ m. The computational window is of dimension 76.4  $\times$  127 $\mu$ m<sup>3</sup>, with the number of grid points  $3000 \times 256$ . Figures 5 and 6 show the  $E_1$  field formed after the laser propagates 0.1 mm. A clear bubble is formed. In this simulation only the zeroth and first modes of the fields have been included.

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Figure 6:  $\Re[E_1]$  of mode 1 of the cylindrical modes.

The full 3D PIC simulation is shown in Figure 4 for comparison (the plot is sliced in the middle for better comparison with the cylindrical simulations). Since in this simulation the wake is nearly perfectly cylindrical, it appears in the plot of the zeroth order mode of  $E_1$  as shown in Figure 5. The oscillations in the real part of the first mode, however, are directly produced by the laser. You can see in the full 3D simulation that ordinarily these two modes of electric fields are solved together.

Since in this case the full 3D simulation requires another 256 grids along the third dimension, it is necessarily at least 256 times slower then the equivalent 2D simulation. With the cylindrical modes truncated at m = 1, we only need to solve three 2D grids (two for the real and imaginary parts of the 1st nonzero mode). By design this algorithm is magnitudes faster then the 3D simulation while capturing much of the 3-dimensionality of the laser-plasma interaction. It is the ideal tool for wakefield accelerators.

# CONCLUSION

We have illustrated though simulations of a two stage ionization injection LWFA concept that there are both qualitative and quantitative differences between 2D and 3D simulations on injection and acceleration of electrons in LWFA stages. Because 3D simulations are often computationally intensive, it is important to be able to conduct simulations whose computational requirements is comparable to a 2D simulation, and yet includes the physics that makes the 2D simulations unreliable for accurate predictions. We describe how a new algorithm proposed by [1] has been successfully implemented into OSIRIS. This algorithm expands the EM fields into a truncated number of azimuthal mode numbers (often just 2). Preliminary results were also presented that show that using only 2 modes provides good agreement with full 3D simulations.

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