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Tunneling ionization in OSIRIS

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Abstract.: In this work, we describe the ionization module implemented in the PIC code OSIRIS[1]. A benchmark with previously published tunnel ionization results was made. Our ionization module works in 1D, 2D and 3D simulations with barrier suppression ionization or the ADK ionization models, and allows for moving ions. Several illustrative 3D numerical simulations were performed, namely of the propagation of a SLAC 30 GeV electron beam in a Li gas cell, for the parameters of [2]. A systematic study for laser wakefield excitation in a gas target was made, enabling us to determine the laser pulse parameters for optimal acceleration. Detailed comparison with theoretical predictions in a preformed plasma is also provided. Furthermore, we compare the performance of OSIRIS with/without the ionization module. Since the plasma particles are created only after interaction of the laser with the gas particles, the number of simulation particles is strongly reduced, and much less simulation time is usually required when using the ionization module.

1. MOTIVATION

To model accurately the physics of several experiments involving high-intensity lasers, the ionization of neutral gas targets is a crucial feature to be included in particle-in-cell codes. Ionization can play an important role in the dynamics of these systems (see eg. [2]).

2. IONIZATION MODELS

Two ionization models have been implemented in OSIRIS[1]: Barrier Suppression Ionization (BSI) and Ammosov-Delone-Krainov (ADK).

The BSI model is a very simple model that has its physical basis on the superposition of the Coulomb potential of the nucleus with the quasi-static laser field. As the electric field of the laser increases, the electrostatic barrier drops, and, if a threshold is reached, the bounded electron escapes the atom/molecule.

The ADK model [3] is based on a tunneling ionization model, which predicts ionization rates for neutral atoms in the presence of an externally applied electric field. The ionization probability rate is given by [3]:

$$W(s^{-1}) \approx 1.52 \times 10^{15} \frac{4^{n^*} \xi_i}{n^* \Gamma(2n^*)} \left(20.5 \frac{\xi_i^{3/2}}{E_f} \right)^{2n^*-1} \times \exp\left(-6.83 \frac{\xi_i^{3/2}}{E_f} \right) \quad (1)$$

where ξ_i (eV) is the ionization potential of the neutral gas, and E_f (GV/m) is the instantaneous value of the laser electric field. The effective principal quantum number, n^*, is defined has

$$n^* = \frac{Z}{\sqrt{2 * \xi_i / E_a}}$$

with E_a twice the ionization energy for hydrogen ground state, i.e., 1 hartree ~ 27.2 eV and Z the charge number of the ion after ionization.

3. IMPLEMENTATION IN OSIRIS

Both the BSI and ADK models were implemented in OSIRIS with a single ionization level. Implementation of multiple ionization levels is now in progress.

The BSI model has a notable unphysical behavior, due to the threshold of the ionization potential. In fact, one can either have no ionization or total ionization. To overcome this problem, a slight change was made in the BSI model, resulting in BSIRAND. In this modified model, the ionization level n_i increases, for electric fields below the threshold, according to:

$$n_i(t + \delta t) = n_i(t) + \frac{\xi_i^2}{E_{th}^2}$$

where ξ_i is the electric field and E_{th} is the threshold field. This guarantees a smooth increase of the ionization level.

For the ADK model, the ionization level is increased in each time step, according to the ionization rate given by equation (1):

$$\frac{\mathrm{d}n_0(t)}{\mathrm{d}t} = -W(t)n_0(t)$$

where n_0 is the neutral gas density. To simplify the numerical calculations of the ionization rate, equation (1) is implemented as:

$$W(s^{-1}) \approx A \times e^{-B/E_f} \times (E_f)^{-C}$$

where A, B and C are parameters that depend only on the neutral gas, and are tabulated in the code thus reducing the computational cost of computing W. The available neutral gases are, hydrogen, helium, lithium and argon.

Arbitrary density profiles for the neutral gas can be specified and ion injection can be turned on or off, allowing for moving ions originating from the ionization of the neutral gas.

4. LASER WAKEFIELD

Several illustrative 1D, 2D, and 3D numerical simulations were performed.

The propagation of a linearly polarized laser beam, with a wavelength of 800 nm, and with a 30 fs pulse duration was simulated in a hydrogen gas cell. The spot size is 10 μm and $a_0 = 1$, which corresponds to an intensity near 2.1×10^{18} W/cm^2. The laser pulse propagates in the positive x_1 direction. Simulations were performed with a moving window. Ionization levels and the corresponding density profiles are presented in Figs. 1, 2 and 3.

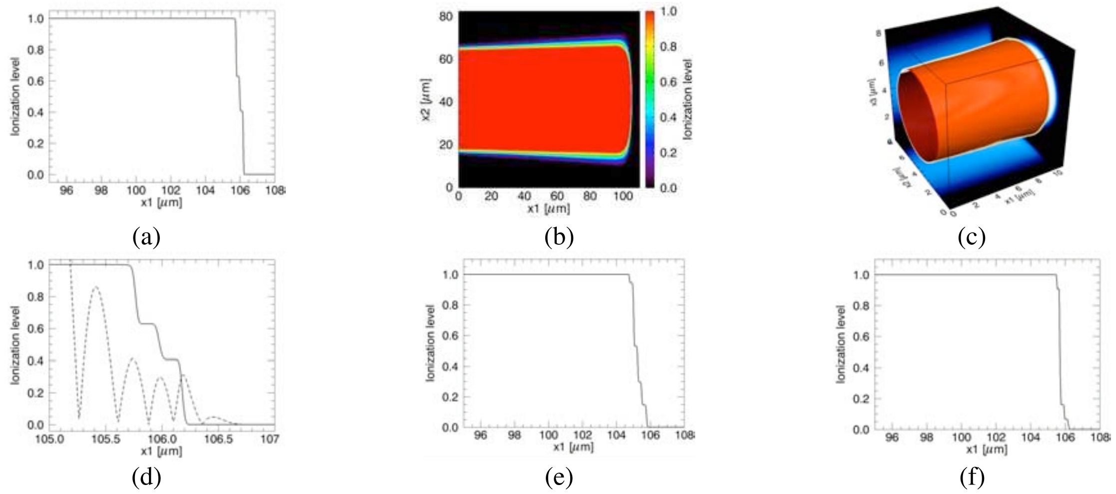

Fig. 1: (a),(b) and (c): Ionization levels for 1D, 2D and 3D simulations of a laser propagating in a hydrogen gas cell after a 220μm propagation distance; (d): zoom of the 1D ionization front. Dashed line shows the variation of the absolute value of electric field;(e),(f): center lineouts of the 2D and 3D ionization levels.

Fig. 1 (d) shows steps in the ionization level at the head of the pulse, due to the oscillations of the electric field. These oscillations can be correctly captured since we have implemented the instantaneous version of the rate *W* [3]. It should be pointed out that the neutral gas is completely ionized in the first oscillation of the field, so that nearly 95% of the pulse is propagating inside the plasma, trailing the ionization front.

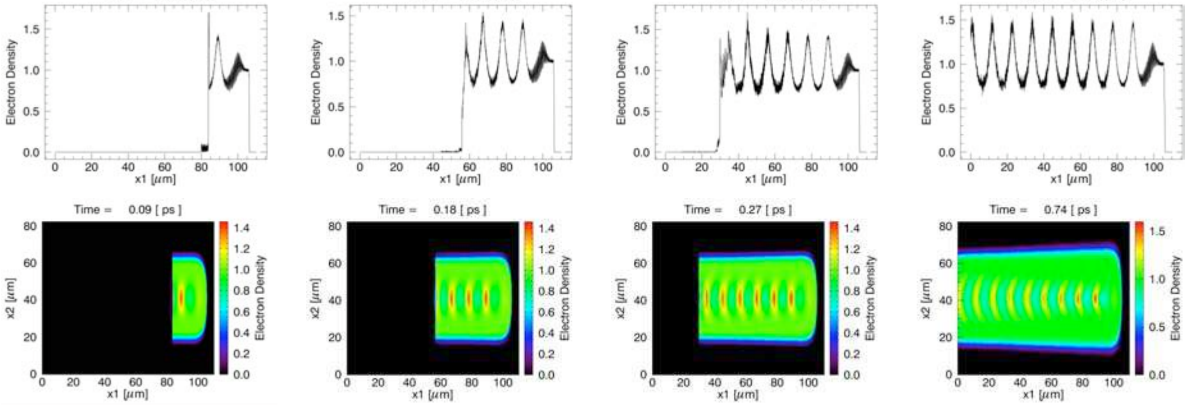

Fig. 2: Time evolution of the electron density for 1D and 2D laser wakefield simulations in a H gas cell.

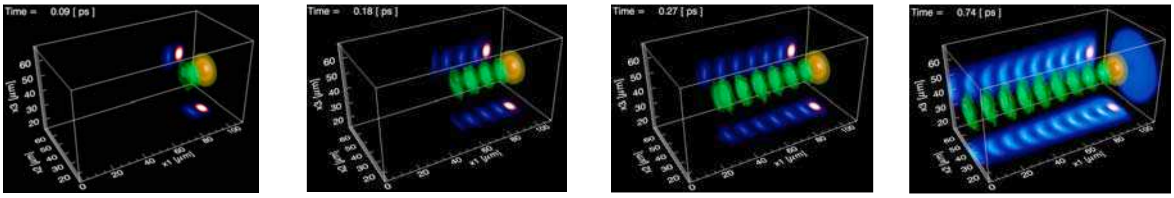

Fig. 3: Time evolution of the electron density for 3D laser wakefield simulations in a H gas cell.

5. 30 GeV ELECTRON BEAM IN A GAS CELL

As a second example, we present the results of the propagation of a 30 GeV electron beam, in a Li gas cell, with the SLAC parameters of [2]. Density profile of the plasma electrons is presented in Fig. 4, clearly demonstrating ionization by the leading edge of the beam, and the blowout of the electrons.

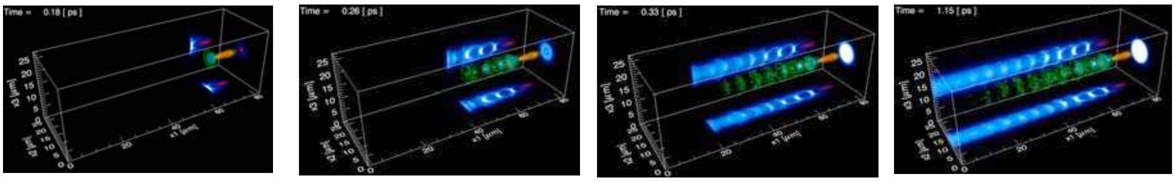

Fig. 4: Time evolution of the electron density generated by a SLAC beam, in a Li cell.

6. CONCLUSIONS

Comparing the ionization runs with those obtained with pre-ionized plasmas, we observe that the generated wakefields are quite similar, but can influence some key parameters. Our 3D simulations confirm the findings of [2].

It is interesting to notice the “C” shape of the laser wakefield and the “D” shape of the electron beam wakefield, thus clearly showing that the wake is generated by two distinct physical mechanisms. These differences will be discussed elsewhere [5].

An important numerical advantage of the ionization module is the lower computational cost. Indeed, the number of particles inside the simulation box is always smaller than in the pre-ionized conditions. Since 3D simulations are dominated by the push time of the particles, less particles lead to reduced computational load, thus leading to runs which are 30% faster varying according to the typical fraction of the neutral gas that is ionized.

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