

2D electrostatic PIC algorithm for studying laser induced plasma in vacuum

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Abstract. Particle-In-Cell(PIC) method is widely used for simulating plasma kinetic models. A 2D-PIC electrostatic algorithm is implemented for simulating the expansion of a laser-induced plasma plume. For potential and Electric Field calculation, Dirichlet and periodic boundary conditions are used in the X (perpendicular to the ablated material) and Y directions, respectively. Poisson-solver employs FFTW3 library and the five-point Laplacian to compute the electric potential. Electric field calculation is made by central finite differences method. Leap-frog scheme updates particle positions and velocities at each iteration. Plume expansion analysis is done for the Emission and Post-Emission stages. In the Emission phase (while the laser is turned on), fast electron expansion is observed and ion particles remain near the surface of the ablated material. In the post-emission stage (with the laser turned off) the charge separation produces an electric field that accelerates the ions leading to the formation of a KeV per particle Ion-Front. At the end of the expansion, fastest electrons escape from the simulation space; an almost homogeneous ion-electron distribution is observed, decreasing the electric field value and the Coulomb interactions.

1. Introduction

In the process known as PLD, a pulsed laser is focused onto a target of the material to be deposited. For sufficiently high laser energy density, each laser pulse vaporizes or ablates a small amount of the material creating a plasma plume [1]. The ablated material is ejected and a plasma cloud forms in front of the surface which expands into the vacuum above it [2]. Laser ablation cloud consist of excited or ground-state neutrals, electrons and ions [3].

Collective interaction between the species in the plume represents a complicated theoretical problem which can be studied through computational models. Particle-In-Cell method [4–6] is used for simulating plasma from a kinetic approach. It consists on solving the differential equations involved in plasma evolution (Electric Potential, Electric Field and kinetic equations are solved on every step). Computational space is taken as a grid point collection where finite size particles phase-space change in discrete time-steps. Preliminary results for a 2D PIC model for Silver (Ag) laser-induced plasma expanding in vacuum are presented in this paper with emphasis on the ion front behaviour.

2. Model

We will consider an isothermal initial expansion for the species at temperature T_0 , with a constant evaporation flux $J_{e,0} = n_{e,0}v_{e,0} = J_{i,0} = n_{i,0}v_{i,0}$. $n_{i,0}$ and $n_{e,0}$ are the densities outside



of the surface for ions and electrons respectively, and the flow velocities are given by:

$$v_{i,0} = \left(\frac{2k_b T_0}{\pi m_i} \right)^{1/2}, \quad v_{e,0} = \left(\frac{2k_b T_0}{\pi m_e} \right)^{1/2} \quad (1)$$

When particles are ejected from the surface ($x = 0$), we assume a half Maxwellian distribution ($v_x > 0$ in front of the surface, obviating the negative velocities) and a full Maxwellian distribution for velocities in X (perpendicular to the surface) and Y (parallel to the surface) directions, respectively [2, 7, 8]:

$$f_0^\alpha(v_x) = n_0 \sqrt{\frac{2m_\alpha}{\pi k_b T_0}} \exp\left(\frac{-m_\alpha v_x^2}{2k_b T_0}\right), \quad f_0^\alpha(v_y) = n_0 \sqrt{\frac{m_\alpha}{2\pi k_b T_0}} \exp\left(\frac{-m_\alpha v_y^2}{2k_b T_0}\right) \quad (2)$$

α represents plasma species and k_b is the Boltzmann constant.

In PIC method, the plasma is represented by a finite number of “computational particles”, whose dynamics are followed by self-consistent fields. N_k real particles are represented by a computational particle. The expansion space is divided in a spatial grid where each grid point has size Δx ; computational steps advance time on Δt , solving field equations on each iteration. To compute the charge densities on the grid and for projecting forces that are found on the grid back to the particles, we use the weighting scheme known as Cloud in Cell [9]. Charge distribution on grid cells is given by:

$$\rho_{jk} = e N_k (n_{i,jk} - n_{e,jk}) W(x - x_{jk}) \quad (3)$$

The electric potential and field equations are solved by five-point discrete version of the Poisson equation using Fast Fourier Transform and central finite difference scheme respectively (see equations 4 and 5).

$$\frac{\phi_{j+1,k} + \phi_{j-1,k} + \phi_{j,k+1} + \phi_{j,k-1} - 4\phi_{j,k}}{\Delta x^2} = -\frac{\rho_{j,k}}{\epsilon_0} \quad (4)$$

$$E_{x,i} = -\frac{(\phi_{x,i+1} - \phi_{x,i-1})}{\Delta x} \quad (5)$$

The particle trajectories are advanced with the “leap-frog” method, where the position and velocity values are staggered in time. The leap-frog method for k-th particle yields:

$$\vec{r}^{k+1} = \vec{r}^k + \vec{v}^{k+0.5} \Delta t, \quad \vec{v}^{k+0.5} = \vec{v}^{k-0.5} + \frac{q_\alpha}{m_\alpha} \vec{E}_p \Delta t \quad (6)$$

where $\vec{r}^k$, $\vec{v}^k$, m_α are the position, velocity and mass of k-th particle respectively, $\vec{E}_p$ is the electric field acting on the particle, and Δt is the computational time step.

3. Parameters

Laser and solid surface parameters used in this work are the same employed in [10]. Laser pulse $t_0 = 100 \text{ fs}$, fluence 1.0 J/cm^2 and Ag solid surface (ion-electron mass relationship $m_i/m_e = 1.98 \times 10^5$). Under these conditions we have a particle flux $J_0 = 4.5 \times 10^{33} \text{ particles/m}^2 \text{ s}$ with $v_{i,0} = 10^3 \text{ m/s}$. Initial temperature for both species is $T_0 = 1.77 \text{ eV}$.

We choose $\Delta t = 10^{-5} t_0 = 10^{-18} \text{ s}$ and $\Delta x = \lambda_D \approx 10^{-11} \text{ m}$ in order to satisfy Courant stability criterion ($\Delta t \leq \Delta x/v_{max}$) which avoids that the particles go through more than a cell per iteration [2, 11].

In our model, 10000 superparticles are used with a weight $N_k = 10$. Simulation space will be $L_x = 4097 \Delta x$, $L_y = 8 \Delta x$. Since the same number of ions and electrons are ejected on emission

time, the boundary conditions are: at $x = 0$ electric potential is zero $\phi(x = 0) = 0$, at $x = L_x$ $\phi = 0$ and in Y-direction we assume periodical conditions due to L_y small size.

In order to achieve a higher computational efficiency, dimensionless parameters are used, taking for normalization the initial values $v_0 = v_{i,0}$, t_0 , $x_0 = v_0 t_0$, the mass m_i , $n_0 = 10000/x_0^3$ and $E_0 = k_b T_0 / \pi e x_0$ [12]. The algorithm is implemented in a C++ code and the electric potential is computed using the modern FFTW3 Fast Fourier Transform library.

4. Results

At the beginning of the expansion, the electrons velocity is higher than the ions velocity; this leads to a charge separation on the simulation space, which generates an electric field that accelerates ions. Figure 1 shows ion velocity distribution for different times of the expansion. At $t/t_0 = 1$ most ion superparticles have $v = 0$; the number of superparticles decrease quickly up to $v = 5v_0$. At $t/t_0 = 2$ superparticle number with $v = 0$ is smaller than at $t = t_0$. However, the most superparticles have high velocities with the highest values around $15v_0$; this suggests that these superparticles are the ion front [4]. At $t/t_0 = 4.5$ the superparticles have an almost homogeneous velocity distribution. Fastest ions present $T > 1 \text{ keV}$. Figure 2 shows ion phase-space at $t = 2t_0$; the superparticles with velocities near $v = 16v_0$ and $x = 12x_0$ are the ion front of plasma [13].

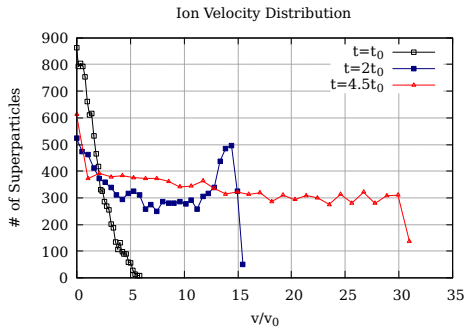


Figure 1. Ion velocity distribution for different times.

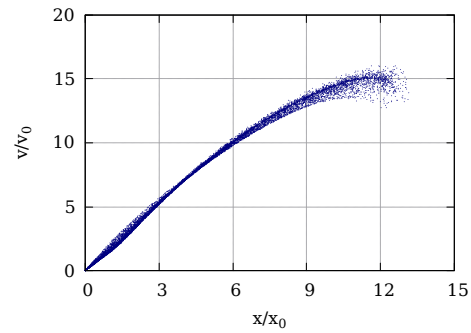


Figure 2. Ion Phase-space, $t = 2t_0$.

Figures 3 and 4 show ion and electron number density at $t = 5t_0$. An almost uniform distribution is observed for both species; therefore, electric field becomes zero, but in $x \approx 90x_0$ it is maximum as it is shown in (Figure 5).

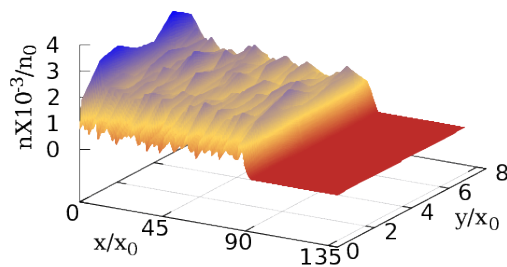


Figure 3. Ion Number Density at $t=5t_0$.

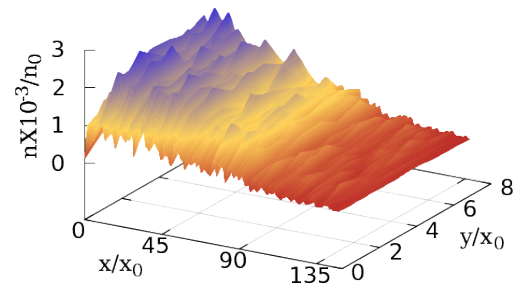


Figure 4. Electron Number Density at $t=5t_0$.

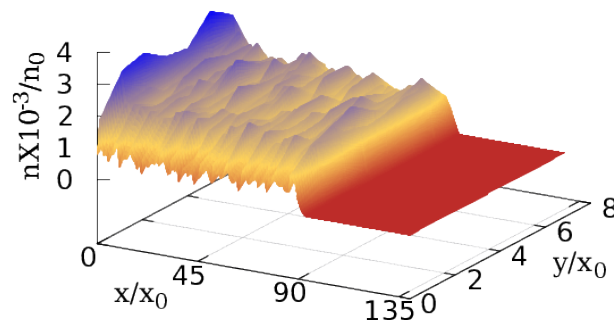


Figure 5. Electric field on X direction at $t=5t_0$.

5. Conclusions

Electrostatic expansion of the laser-induced plasma plume is generally studied as a one-dimensional problem, due to the symmetry of the Coulomb forces in the directions that are parallel to the ablated surface. Results from 1D electrostatic studies were corroborated, allowing us to continue with the full 2D electromagnetic case.

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The authors would like to correct the title of this work. The correct title for the paper ‘2D electrostatic PIC algorithm for laser induced studying plasma in vacuum’ is:

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