Ultra-fast ionization modeling in laser-plasma interaction

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Abstract. A new ionization model for weighted particle simulation of large density scale plasmas has been developed. It is capable of treating both field and impact ionization. The high-order interpolation scheme we have adopted reduces numerical noises of electromagnetic waves, which ionize the target unphysically. This model has been tested in simulations of high intensity laser interaction with both underdense and overdense targets. With the addition of the treatment of collisions, this new code allows us to perform large-scale simulations of laser matter interaction with atomic physics. This model is a very valuable tool for the design of high-energy density experiments with short pulse lasers.

1. Introduction
Energy densities in excess of $10^{12}$ erg/cc exist in the core of stars. With the current technology of high-power lasers, it is now possible to generate such high energy density plasmas in a laboratory. Such extreme states of matter are of considerable interest for a variety of applications like inertial confinement fusion, compact ion accelerators, pulsed neutron sources and the simulation of astrophysical plasmas in the laboratory. Moreover, they promise to allow the study of equation-of-state and opacity physics in novel ways. It is essential understanding energy transport physics including atomic processes to realize these applications. Because of the nonlinear and non-equilibrium nature of the relativistic plasmas that are typically generated at ultra-high laser intensities of $10^{18}$ W/cm², only a kinetic method can correctly describe laser-plasma interaction. The most prominent model used today is the Particle-in-Cell (PIC) approach. But the physical scale of such simulations has been limited due to computational costs, and most of the studies done with PIC codes have overlooked two important aspects: time-dependent ionization dynamics of initially neutral matter and collisional effects [1].

For a quantitative description of short pulse laser-matter interaction it is important to account for ionization dynamics that occurs on a similar time scale as the laser pulse length itself, modifying the average atomic charge states and thereby the electron density significantly. We have implemented the two dominant ionization mechanisms in the 1D version of the PIC code PICLS: electric field ionization and electron impact ionization based on Ref. [1] in an efficient way. A critical problem of the current ionization model is its computational cost due to requirement of fine resolution to avoid numerical (unphysical) ionization. PICLS optimizations include high order interpolation, directional splitting and weighted particles. We also analyzed the influence of high order interpolation on numerical ionization. Section 2 is dedicated to the presentation and testing of our electric field ionization model. Section 3 is dedicated to the presentation of our electron impact ionization model. In Section 4 we present successful preliminary applications of both types of ionization. Section 5 is dedicated to our conclusions and perspectives.
2. Electric field ionization model for weighted particles

2.1. Model presentation

Our model of field ionization is based on the description of tunnel ionization of complex atoms in alternating electric fields given by Ammosov, Delone and Krainov [2]. The ionization rate of an atom is calculated inline for each ion from a simple formula containing the local electric field strength and the ionization potential at the ion charge state that is tabulated. In order to retain energy conservation throughout the simulation, the ionization energy for a given process is subtracted from the electromagnetic field. This is accomplished by introducing an artificial ionization current that is added to the current in the cell for only one time step; it is called the virtual ionization current. It is directed along the electric field, and its magnitude is determined from the requirement of energy conservation. This virtual ionization current \( j_{\text{ion}}^{(i)} \) is given by equation (1), where \( U_p \) is the ionization potential, \( E \) is the electric field and \( \Delta t \) is the time step.

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j_{\text{ion}}^{(i)} = \frac{U_p e V}{|E_{\text{norm}}|} E^{(i)}, \quad i = x, y, z
\]

We use the ADK formula to calculate the ionization rate \( W(E) \). The ionization probability is \( R = 1 - \exp[-W(E)\Delta t] \), where \( E \) is the electric field. The condition of ionization is that \( R \) has to be larger than a random number between 0 and 1. The new electron has the same weight and position as the ionized ion. It is created with no momentum. The field ionization and ionization current calculation takes place between the fields calculation and particle movement in the PIC cycle. Ionization starts for all charge states from the energetic ground level. Excited electronic states are not considered at present, neither are recombination processes.

2.2. Numerical tests

![Figure 1](image)

**Figure 1.** (a) Charge state of the carbon after irradiating a laser pulse with an intensity of 5.5×10^{18}W/cm^2 during 300 fs with first order interpolation. (b) The same plot with (a) but the simulation was performed with 4 times larger grids. (c) The same plot as (b) but the simulation was performed using third order interpolation.

A critical problem of the current ionization model is its computational cost due to requirement of fine resolution to avoid numerical (unphysical) ionization. To boost the performance of the simulation we need to extend the simulation grid size and also modify the model for the weighted particle modeling to deal the ionization in large density scale target. We first studied field ionization appearing in intense laser (5.5×10^{18}W/cm^2) matter interaction. The target is a carbon foil with low-density gas in front of the target. The simulation was done with 160 grids/m and with 100 particles/cell for the high-resolution case and with 40 grids/m in the low-resolution case. We used first order interpolation in both cases. We see the full ionization in the gas area and the partial ionization inside the solid target. The rear surface is ionized more due to presence of the strong sheath fields. As shown in Figure 1, the numerical ionization is significant in the case, and the ionization level inside the target is higher than that of the fine grids case. Using third order interpolation in the low resolution case described above...
reduces significantly the level of numerical ionization and gives results very similar to the ones of the high resolution case. High order interpolation therefore reduces numerical ionization and allows using larger grids, therefore saving computational time.

3. Electron impact ionization model for weighted particles
At solid target density, electron impact ionization becomes as important as field ionization or even dominant for the high charge states. Ionization probabilities are computed via a Monte-Carlo type algorithm from tabulated cross-sections for each ion charge state present in each individual cell, using the average electron velocity in a cell to save computational time. The ion velocity is not taken into account in the calculation of the average electron velocity in a cell. Energy conservation is achieved by reducing the velocity (but not changing the direction) of the impacting electron. Newborn electrons are initialized at rest relative to the ion. We use tabulated data of impact ionization cross sections from NIFS (1998). The ionization probability is \( R = 1 - \exp\left[-W(<v_e>)\Delta t\right] \), where \( <v_e> \) is the average electron velocity. \( W(v_e) = n_e \sigma(<v_e>)<v_e> \), where \( n_e \) is the electron density and \( \sigma \) is the impact ionization cross section. The condition of ionization is that \( R \) has to be larger than a random number between 0 and 1. The new electron has the same weight and position as the ionized ion. The impact ionization calculation takes place after the currents calculation and collisions calculation in the PIC cycle. Ionization starts for all charge states from the energetic ground level. Excited electronic states are not considered at present, neither are recombination processes.

4. Applications

4.1. Case of an underdense target
We tested the implementation of the field ionization module by simulating in 1D the propagation of a high intensity laser pulse inside a He target. We compared a case with an initially neutral Helium target and a case with an initially fully ionized Helium target. Laser intensity is \( 6 \times 10^{19} \text{ W/cm}^2 \), pulse duration is 36 fs, and target density is 0.2282 \( n_c \), where \( n_c \) is the critical density. The simulations were done with 10 grids/m and with 50 particles/cell. We analyzed wakefield electron acceleration to high energies in both simulations. As shown in Figure 2, the electron phase space is similar in the case with ionization and in the case without ionization. Comparing the longitudinal electric field yields the same result. This was expected as the ionization time scale is small compared to the wakefield electron acceleration timescale, the laser almost instantaneously ionizes the target as it propagates.

![Figure 2](image)

**Figure 2.** Electron phase space 264 fs after the beginning of the simulation in the case of (a) an initially neutral helium target and in the case of (b) an initially fully ionized helium target. The target is composed of Helium ions, laser intensity is \( 6 \times 10^{19} \text{ W/cm}^2 \), pulse duration is 36 fs, and target density is 0.2282 \( n_c \).

4.2. Carbon target with both types of ionization
We also tested the complete ionization implementation with overdense targets. We performed 1D simulations of a high intensity laser pulse interacting with a 100 $n_c$ Carbon target with a 20 microns exponential preplasma located in front of it. $n_c$ corresponds to the critical density. We used third order interpolation and the target was initially composed of only neutral carbons. The simulations were done with 160 grids/m and with 10 particles/cell. For a laser intensity of $5.5 \times 10^{18}$ W/cm$^2$, and a pulse duration of 500 fs, the charge states measured 105 fs after the beginning of the simulation in the case with only field ionization (no collisions) and in the case with both ionizations and collisions are very similar. For a laser intensity of $10^{17}$ W/cm$^2$, and a pulse duration of 1 ps, the charge states measured 168 fs after the beginning of the simulation in the case with only field ionization (no collisions) and in the case with both ionizations and collisions differ more than in the higher intensity cases as shown in Figure 3. These preliminary results show that field ionization is dominant in high intensity cases with preplasma, and collisional ionization becomes important for high density and low intensity cases.

![Figure 3. Charge state of the carbon after irradiating a laser pulse with an intensity of $10^{17}$ W/cm$^2$, and a pulse duration of 1 ps, 168 fs after the beginning of the simulation (a) with only field ionization (no collisions), and (b) with both ionizations and collisions.](image)

5. Conclusions and perspectives
We have developed a new ionization model for weighted particle simulation of large density scale plasmas treating both field and impact ionization. It includes the first model of impact ionization with high order interpolation and weighted particles. The high-order interpolation scheme we have adopted also improves the speed of our PIC algorithm by four orders of magnitude (in 2D runs) and reduces numerical noises of electromagnetic waves, which ionize the target unphysically. With the addition of the treatment of collisions [3], this new code allows us to perform large-scale simulations of laser matter interaction with atomic physics.

This model is a very valuable tool for the design of high-energy density experiments with short pulse lasers and will accelerate the development of efficient inertial fusion confinement designs and compact particle accelerators. Future improvements will include different weight impact ionization, complete comparison with pairing ionization models, extension to 2D and 3D versions and comparisons with other codes and experiments.

References
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