Numerical modeling of laser tunneling ionization in explicit particle-in-cell codes


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1. Introduction

In numerical studies of ultra-intense laser–plasma interactions, the plasma production via the laser ionization is often omitted due to the fact that the ionization process occurs before the main body of the pulse arrives. For example, a laser–plasma accelerator [1], driven by a short-pulse (tens of fs) laser, typically uses low-Z gas (e.g., H or He) targets that are easily ionized by the ps laser pre-pulse present in the laser temporal profile. For relativistically intense ($I > 10^{18}$ W/cm$^2$) lasers interacting with low-Z gases, ionization effects on plasma wave generation are negligible [2], however pre-pulse effects may still strongly influence the main pulse propagation [3,4]. For laser intensities close to the tunneling ionization threshold, or when a high-Z gas target is used, ionization processes can significantly influence the laser–plasma interaction.

Ionization effects in laser–plasma interactions, including laser frequency blue shifting, harmonic generation, ionization-induced diffraction, and instabilities, have been studied theoretically and experimentally for laser pulses interacting with neutral targets [5–16]. For high-field laser–gas interactions the ionization process is dominated by tunneling ionization. In laser–solid interactions, due to the overdense target, the laser pulse cannot penetrate into the target, and ionization process inside the target is mainly due to impact ionization [17]. Although the impact ionization process is important to correctly describe the laser–solid interaction process, in this work we will focus on the modeling of laser tunneling ionization. Accurate modeling of the ionization process is critical to several recently proposed methods of radiation and particle beam generation. For example, ionization is the key process in ionization-current-based THz radiation generation in laser–gas interactions [18–20] and ionization-induced trapping in laser–plasma accelerators [21–27]. Laser-ionization-based trapping...
in plasma accelerators relies on the use of a high-Z gas target to generate electrons at the appropriate phase of the plasma wakefield. For this application, an accurate description of the ionization process is critical for predicting the laser–plasma accelerated beam properties.

Particle-in-cell (PIC) \([28,29]\) is a common numerical method used to study short-pulse laser–plasma interactions. The PIC numerical method models the Vlasov–Maxwell equations using a particle-grid method, such that the continuous phase-space fluid is sampled by a finite number of (Lagrangian) macro-particles and the Maxwell equations are discretized on a grid. Laser ionization has been implemented and studied in PIC codes, and several types of ionization formulae have been used in the literature (see, for example, Refs. \([30,17]\)). In this paper, we focus on the numerical implementation in a PIC code of optical tunneling ionization based on the Ammosov–Delone–Krainov (ADK) model \([31]\). We compare the alternating current (AC) and direct current (DC) models and show that the DC model must be used to give accurate results in explicit PIC simulations. Multi level ionization in a single simulation step and energy conservation during ionization are considered. The effects of numerical parameters on the modeling of the laser ionization process are presented. We consider the effects of the resolution of the grid and the average number of numerical macro-particles per cell representing the phase-space distribution. A comparison of ionization injection studies using two PIC frameworks (VPL [32] and VORPAL [33]) is also made.

2. Tunneling ionization formulae

Tunneling ionization from the ground state of a Hydrogen atom in an electrostatic (DC) field was first solved schematically by Landau \([34]\) for the dependence of the ionization rate on the applied external field. When the intensity of the external electric field satisfies \(E_{dc} \ll E_0\) (where \(E_0/m_ec^2 = \omega_e^2/r_e\) or \(E_0 \simeq 5.1 \text{ GV/cm}\)), the ionization rate for a Hydrogen-like system is given by the Landau–Lifshitz DC tunneling ionization formula \([34]\):

\[
W_{\text{DC}} = 4\omega_e E_{dc} \left( \frac{U_{\text{ion}}}{U_H} \right)^{5/2} \exp \left[ -\frac{2}{3} \frac{E_a}{E_{dc}} \left( \frac{U_{\text{ion}}}{U_H} \right)^{3/2} \right],
\]

where \(\omega_e = a_0 c/r_e = 4.13 \times 10^{16} \text{ s}^{-1}\) is the atomic unit frequency, \(U_{\text{ion}}\) is the ionization potential, and \(U_H = 13.6 \text{ eV}\) is the ionization potential of Hydrogen at the fundamental state. Here \(m_e\) is the electron mass, \(c\) is the speed of light, \(a_0 = 1/137\) is the fine structure constant, and \(r_e = e^2/m_ec^2\) is the classical electron radius. For complex atoms in a static field \((E_{dc})\) the DC tunneling ionization formula is \([31]\):

\[
W_{\text{DCm}} = \omega_e C_{n^r}^2 \frac{2^{n^r + 1}(l + |m|)!}{2^{n^r}(|m|)!} \left( \frac{U_{\text{ion}}}{2U_H} \right)^2 \exp \left[ -\frac{2}{3} \frac{E_a}{E_{dc}} \left( \frac{U_{\text{ion}}}{U_H} \right)^{3/2} \right],
\]

where \(l, m\) are the electron’s orbital quantum number and its projection, respectively, \(n^r = Z \sqrt{U_H/U_{\text{ion}}}\) is the effective principal quantum number, \(\Gamma = n^r - 1\) is the effective value of the orbital number \((n^r_0\) is the effective principal quantum number of the ground state,\), and \(Z\) is the ion charge number after ionization. The coefficients \(C_{n^r}\) can be found calculated using a semi-classical approximation (see Eq. (20) of Ref. \([31]\)):

\[
C_{n^r}^2 = \frac{2^{2n^r}}{n^r \Gamma(n^r + \Gamma + 1) \Gamma(n^r - \Gamma)} \approx \frac{1}{2\pi n^r} \left( \frac{4e^2}{m^2c^2} \right)^{n^r} \left( \frac{n^r - \Gamma}{n^r + \Gamma} \right)^{\Gamma + 1/2}.
\]

In the limit \(\Gamma \ll n^r\), Eq. (3) reduces to

\[
C_{n^r}^2 = \frac{1}{2\pi n^r} \left( \frac{2e}{n^r} \right)^{2n^r}.
\]

The ionization rate of a hydrogen atom in an alternating (AC) electric field, e.g., a laser field \([E_l \propto \cos(\omega t)]\), where \(\omega\) is the laser frequency, can be treated, in the appropriate limit, as the DC ionization rate averaged over a single period of the electric field oscillation. This model was proposed by Keldysh \([35]\) and then later expanded to hydrogen-like atoms by Ammosov et al. \([31]\) (referred to as the ADK model). The DC ionization rate is related to the AC ionization rate by

\[
W_{\text{AC}} = \left[ \frac{3}{\pi} \frac{E_a}{E_{dc}} \left( \frac{U_H}{U_{\text{ion}}} \right)^{3/2} \right]^{1/2} W_{\text{DC}}.
\]

Combining Eqs. (2), (4), and (5), yields the one cycle averaged ionization rate for a complex atom in an AC field. For a linearly polarized laser pulse \(E_l\), the ionization rate is \([31]\):

\[
W_{\text{ACm}} = \omega_e \left( \frac{3n^r E_l}{\pi Z^2 E_0} \right)^{1/2} \frac{Z^2}{2n^r \pi^{2n^r}} \left( \frac{2e}{n^r} \right)^{2n^r} \exp \left[ -\frac{2}{3} \frac{E_a}{E_l} \frac{Z}{n^r} \right] \frac{(2l + 1)(l + |m|)!}{2\pi n^r 2^{2m(|m|)!} (|m|)!} \left( \frac{2}{E_l} \right)^{2n^r - |m|-1}.
\]
For the fundamental state \( l = m = 0 \), we obtain the ionization rate

\[
W_{AC00} = \omega_0 \sqrt{\frac{3}{\pi}} \left( \frac{e}{m_e} \right)^{3/2} \left( \frac{E_0}{E_l} \right)^{2n^{-3/2}} \exp \left[ -2 \frac{E_0}{3} \left( \frac{Z}{n} \right)^3 \right].
\]

(7)

In the original ADK paper a typographic error gave an ionization rate (see Eq. (13a) of Ref. [31]) of \( \pi/e \) times the correct rate. This and other corrections, including errors in Eq. (20) of Ref. [31], have been pointed out by several authors [36, 37]. However, the original formula with the typographic error has been used in several studies (e.g., Refs. [38, 17]), and is pointed out here to prevent future confusion.

In numerical modeling of laser–plasma interactions via PIC it is essential to use the correct ionization model. If the laser pulse is modeled as an envelope and the time step is much larger than the laser period, an ionization rate based on a cycle-averaged AC model should be used. However, in an explicit PIC simulation, the sub-wavelength scale is well-resolved and the simulation time step is much smaller than the laser period (\( \delta t \ll T_0 \), where \( \delta t \) is the simulation time step and \( T_0 = c/\omega_0 \) is the laser period), and within each simulation time step, the laser field can be viewed as a DC field. In this case the DC ionization rate model should be employed.

To illustrate the differences in the ionization models, Fig. 1 shows numerical calculations comparing the DC model Eq. (2) and the AC model Eq. (6) in a calculation that resolves the laser period. Fig. 1(a) shows the ionization rate from \( \text{N}^{5+} \) to \( \text{N}^{6+} \) versus normalized electric field intensity \( a = eE_l/m_e c \). As shown in Fig. 1(a), the AC ionization model (as used in Ref. [17]) shows the same trend as the DC model; however, it always provides a lower ionization rate, as anticipated from Eq. (5).

The ionization probability may also be considered within a finite time. Fig. 1(b) shows the ionization probability (from \( \text{N}^{5+} \) to \( \text{N}^{6+} \) ) after a single laser cycle (\( a = a_0 \sin(2\pi t) \), with \( 0 \leq t \leq 1 \)) versus laser intensity: The red curve shows the result by using the theoretical calculation of \( 1 - \exp[-W(t_p)T_0] \), where \( t_p \) represents the time at the electric field peak. The black curve (overlapped by the red curve) shows the result from the DC integration model, and the blue curve shows the result from the AC integration model. As shown in Fig. 1(b), use of the AC model in this case has underestimated the ionization probability.

Fig. 1(c) shows the difference of the two models for a temporally Gaussian pulse, with full-width-half-maximum (FWHM) length \( L_{FWHM} = 14.89cT_0 \). Again, the AC model gives a lower ionization probability than the DC model. From this, we expect that, while results of studies using explicit codes with the AC ionization model (or using the uncorrected ADK coefficient) may give qualitatively reasonable results, the use of the corrected DC model in explicit simulations is essential to obtain accurate quantitative results.

![Fig. 1.](image-url)

(a) Ionization rate from \( \text{N}^{5+} \) to \( \text{N}^{6+} \) versus electric field intensity \( a = eE_l/m_e c \). The laser frequency is \( \omega = 2\pi c/a_0 \) with \( a_0 = 0.8 \) \( \mu \)m. The solid black solid curve is based on the DC model and the dashed blue curve is based on the AC averaged model. (b) Ionization probability after one laser cycle calculated using different models: solid black curve integrates over \( W_{DCm} \), the dashed red curve uses the one-cycle-averaged formula \( 1 - \exp[-W(t_p)T_0] \), the blue dashed curve integrates over \( W_{ACm} \). (c) Ionization probability after a Gaussian pulse: solid black curve is integration over \( W_{DCm} \) integration, blue dashed curve integrates over \( W_{ACm} \). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
3. Tunneling ionization model implementation in PIC codes

In an explicit PIC simulation, the ionization process is generally implemented with the following prescription. At each time step, for each un-ionized particle, the local electric field and particle ionization parameters (such as ionization potential and charge state) are used to calculate the ionization rate \( W(t) \). The particle ionization probability is then calculated by

\[
P(t) = 1 - \exp[-W(t)\delta t],
\]

which is approximated as \( P(t) \approx W(t)\delta t \) when \( P(t) \ll 1 \). The code generates a random number \( p \) with a uniform distribution between 0 and 1; once \( p < P(t) \), the particle will be set to be ionized, otherwise the particle will not be ionized and will be evaluated during the next time step. In the PIC code the particles are macro-particles representing the phase space fluid. The ionization probability cannot be accumulated to the next time step if the particle is not ionized; otherwise an over-counted ionization probability results.

Although for most of our simulation cases, the time step of PIC simulations can satisfy \( P(t) \ll 1 \), however, if the ionization potential is too low or a relatively high laser intensity is used, the above approximation can not be satisfied and high level ionization in a single PIC simulation time step may happen. A subroutine will be used to solve this issue. Let us consider an ion particle whose initial state is \( \bar{Z} \) and its highest charge is \( z \). The evolution of the state population \( \langle N^j \rangle \) is as following:

\[
dN^i/dt = -W_i N^i
\]

\[
dN^{i+1}/dt = W_i N^i - W_{i+1}N^{i+1}
\]

\[
\ldots
\]

\[
dN^{z-2}/dt = W_{z-2}N^{z-2} - W_{z-1}N^{z-1}
\]

\[
dN^{z-1}/dt = W_{z-1}N^{z-1}
\]

\[
dN^z/dt = W_{z-1}N^{z-1}
\]

and the initial state is: \( N^j(t = 0) = 1 \) and \( N^j(t = 0) = 0 \) when \( j > i \). Obviously during the whole ionization process \( t \in [0, \delta t] \), the total number of all kinds of ions is constant: \( \sum N^j = 1 \). So only \( z-i \) equations need to be solved. Depends on the specific dependance of \( W_i \) on \( t \) different approximations can be used to simplify these equations. Generally a subroutine can be installed in the PIC code to solve this equation array by using the typical fourth order Runge–Kutta method. Once one knows the state population \( \langle N^j \rangle \) at the end of time step \( t - \delta t \), a random number \( p \) with a uniform distribution between 0 and 1 will be generated to decide the final ionization state. When \( \sum_{j=1}^{z-1} N^j < p < \sum_{j=1}^z N^j \), the particle will be set to be ionized to \( Z^j \) and \( k-i \) electrons will be generated. Here we neglect the different response of the different valence electrons in such a single time step, which is reasonable when the time step \( \delta t \) of the PIC simulation is small enough.

Besides the high level ionization process, ionization induced energy loss \( (E_{\text{loss}}) \) is another issue to be considered. Although in some simulation cases such as laser short–gas interaction, the energy loss due to ionization can be neglected compared with the high laser energy. However, in some special cases such as long distance laser propagation in neutral gas or laser high density high Z neutral matter interaction, energy loss due to ionization should be considered. Currently, to retain the energy conservation, an approach using artificial ionization current \( (\jmath_{\text{ion}}) \) is suggested. Such method has been discussed by Kemp et al. [17] before. The artificial ionization current is directed along the local electric field \( \vec{E} \), and its magnitude is set to satisfy the energy conservation law:

\[
\jmath_{\text{ion}} = E_\Sigma_k \Delta n_k (E_{\text{ion}}^{k\text{net}} + e_k)/\delta t \vec{E}.
\]

Here \( k \) represents the different ionization state, \( \Delta n_k \) represents the number density of the \( k^{\text{th}} \) ionized electrons and \( e_k \) represents their initial energies just after ionization which is usually set to be zero. This current is then added to the physical current in each cell, after charge and current are computed from particle positions and velocities and before the integration of Maxwell’s equations. Such process should be done for every time step and each cell once the ionization process happens.

The above analysis indicates that, to accurately model the ionization process, random number generation, selection of the macro-particle number representing the ionizing atoms, and the choice of time step size are all critical numerical parameters. In the following we examine the effect of these numerical parameters on the ionization modeling using the VULP code [32].

In the VULP code, the ionization rate formula of the DC ionization model Eq. (2) is implemented. A library source random number generator is used to produce random numbers uniformly distributed in the region \( [0, 1] \). To study the effects of time step and macro-particles per cell on the ionization probability calculation, we consider the ionization of a Nitrogen gas by a linearly polarized laser pulse. To exclude other physical effects, the number density of the initial neutral Nitrogen atoms is \( 10^{-7}n_e \), where \( n_e = \pi n_0e^2/e^2 \lambda_0^2 \) is the critical density \( (n_e \approx 1.7 \times 10^{21} \text{ cm}^{-3} \text{ for a laser of wavelength } \lambda_0 = 0.8 \mu \text{m}) \) and the simulation is in a one-dimensional (1D) geometry. The normalized laser intensity is \( E_0 = E_{\text{max}}/n_0e \lambda_0 = 1.8 \) and the pulse length is \( t_0 = 10\pi \lambda_0 \), with the temporal shape of electric field defined as \( \propto \exp(-t^2/t_0^2) \). The highest Nitrogen atoms are initially uniformly distributed within the region of \( 5\lambda_0 - 35\lambda_0 \). No other particle elements are used. For such a laser pulse the highest ionization rate for Nitrogen \( N^5+ \) is \( 4.68 \times 10^{-4} \text{ s}^{-1} \) at the peak of the laser pulse, as shown in Fig. 1(a).

Fig. 2(a) shows the distribution of ionization probability of \( N^5+ \) (fraction of ions in charge states \( N^{5+} \) or \( N^{6+} \)) along the laser propagation direction. The laser propagates from the left to the right and the grey curve shows the laser field (with peak at \( x = 15\lambda_0 \)). The red dashed curve shows the theoretical ionization calculated using Eq. (2) and assuming \( N^{5+} \) is uniformly pre-ionized before the laser arrives. The assumption is reasonable since Nitrogen is easily ionized to the fifth valence
The green dotted curve in Fig. 2 shows the sum density of the N6+ and N7+ normalized by the initial Nitrogen density $N_0$, which represents the total ionization probability of N5+, calculated from the PIC code with a time resolution of $\delta t = 0.1 T_0$ and 40 macro-particles per cell. The ionization probability has been underestimated by $\approx 21.4\%$. At the peak of the laser pulse, $W \delta t \approx 0.125$ and the approximation of $1 - \exp(-W \delta t) \approx W \delta t$ gives a relative error of $+6.38\%$, i.e., the error in the ionization calculation does not come from the small exponent approximation, rather it is largely due to the sampling of the electric fields.

Fig. 2. Ionization probability distribution of N5+ along the laser propagation direction $x/\lambda_0$. (a) The grey curve is the normalized laser electric field with peak field at $x = 15\lambda_0$. The red dashed curve shows the theoretical result, the green dotted curve is calculated from the PIC code with $\delta t = 0.1 T_0$ and 40 macro-particles per cell. (b) The black solid curve uses $\delta t = 0.01 T_0$ and 4 macro-particles per cell, the light blue solid curve used $\delta t = 0.005 T_0$ and 1 macro-particle per cell. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 3. Example of the typical laser–plasma accelerator wake structure and ionization injection scheme: laser electric field (grey curve) along its propagation direction ($x$), the electric field of the wake (red curve), the momentum of the background plasma electron fluid (dashed blue curve), the trapping momentum threshold of the electrons in the wakefield (dotted green curve), and the momentum gap between the trapping threshold and the background electron momentum (black curve). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
Since the ionization mainly happens at the peak of each cycle, if the resolution is too course, the sampling of fields (i.e., the resolution) may not be sufficiently accurate. To study the effect of resolution, we considered increased temporal resolution with the total macro-particle number within a fixed length constant. Increased temporal resolution is equivalent to increased longitudinal spatial resolution, since in the 1D PIC code $\delta x/\lambda_0 = \delta t/T_0$. The black solid curve in Fig. 2(b) shows the ionization probability calculated from the PIC code with $\delta t = 0.01T_0$ and 4 macro-particles per cell. Better agreement with the theoretical curve (dashed red curve) is achieved with the increased resolution. The increase in noise is due to the fewer macro-particles per cell (i.e., larger weight given to each macro-particle). For example, if the resolution is increased to $\delta t = 0.005T_0$ with 1 macro-particle per cell, increased simulation noise is observed (light blue solid curve in Fig. 2(b)).

The ionization probability calculation is sensitive to the resolution, and accurate modeling of the ionization process the time step of each should be sufficiently small. In general, the resolution criterion is more strict than that due to the ionization rate’s sensitivity to the electric field strength $W(t)\delta t \ll 1$. The number of macro-particle per cell affects the simulation noise level. The larger the number per cell, the smaller weight of each macro-particle, and the simulation noise will be less. When modeling ionization with PIC, evaluating the convergence of the resolution is essential for an accurate description of ionization process.

![Graphs showing ionization probability and noisy fluctuations with different resolutions](image-url)
4. Comparison of ionization injection studies

The implementation of the DC ionization model in PIC codes described above has been carried out in two PIC codes VLPL [32] and VORPAL [33]. In this section we compare results obtained in both PIC codes using the same DC ionization model. The case studied is for ionization injection into a laser–plasma accelerator, and the final simulated beam characteristics are compared.

High-Z gas ionization injection has recently been employed experimentally as an effective electron injection method in the laser–plasma accelerator [22–26]. The detailed physics of ionization injection has been described in Ref. [27]. Fig. 3 shows a typical wake structure excited by an intense laser and the injection criterion based on 1D nonlinear cold plasma wake theory at a fixed time. A laser pulse (grey curve) is used to generate a wake in a mixed plasma of pre-ionized electrons and neutral Nitrogen atoms. The red solid curve shows the longitudinal electric field of the wake when only the initial pre-ionized electron plasma is included. Since the concentration of Nitrogen is small (typically <5%), the wake modification due to the newly ionized electrons is negligible. The blue dashed curve shows the spatial distribution of the background electron fluid momenta along the longitudinal (laser propagation) direction. The green dotted curve shows the momentum threshold required for the background electrons to be trapped in the wake. The black solid curve shows the difference of the two curves. Below wavebreaking [39], the momentum of an initially cold plasma electron is always lower than the trapping threshold (the thick black curve is always positive). Trapping in the plasma wake below the wavebreaking amplitude may be accomplished by ionizing electrons at an appropriate phase of the wake. Usually the above-threshold energy of an ionized electron is small compared with the energy of a background electron undergoing fluid motion, and, hence, can be omitted. Ionized electrons enter the plasma wake approximately at rest. Since the injection threshold is negative for some phases, ionized electrons (initially at rest) can be trapped. Ionization injection occurs when the electrons are ionized at the correct phase of the wake (e.g., the red dot in Fig. 3).

Here we use two PIC codes, VLPL and VORPAL, to model the ionization injection process in a laser–plasma accelerator. The two PIC codes are independently written, although both are based on the standard PIC algorithm. In both codes the ionization rate formulae Eq. (2) is implemented. The simulations were carried out in two dimensions (2D). In the simulations a mixed pre-ionized electron and neutral Nitrogen gas was used as the plasma source ($n_N = 9.452 \times 10^{-6} n_c$ and $n_e = 9.4466 \times 10^{-4} n_c$). The concentration of Nitrogen was $n_N/(n_N + n_e) = 1\%$ and it was distributed from $x = 20\lambda_0$ to $x = 50\lambda_0$ with a profile that included an up-ramp (of length $10\lambda_0$), followed by a plateau (of length $10\lambda_0$), followed by a...
down-ramp (of length 10\(\lambda_0\)). The pre-ionized electrons were uniformly distributed after \(x = 30\lambda_0\) with a 10\(\lambda_0\) up-ramp. A single linearly polarized Gaussian pulse with wavelength of \(\lambda_0 = 0.8\ \mu\text{m}\) was used for wake excitation and ionization injection. The peak normalized laser electric field was \(a_0 = 2.0\), with length \(L_0 = 12.6487\lambda_0\), and the transverse width of the laser pulse at the focus plane was \(W_{\text{FWHM}} = 17.66\lambda_0\). The pulse was focused into the plasma 75\(\lambda_0\) from the left simulation box. The simulation box was 80\(\lambda_0\) long and 140\(\lambda_0\) wide. The resolution used was \(\delta x = 0.01\lambda_0\) and \(\delta y = 0.1\lambda_0\), with a time step \(\delta t = 0.009947\tau_0\), 6 macro-particles per cell to represent the Nitrogen atoms, and 1 macro-particle per cell to represent the background electron density.

The simulation results from the two PIC codes are shown in Figs. 4 and 5. As shown in Fig. 4(a) there is good agreement in the evolution of the electron injection number (defined as \(n_\text{p} > 20\ \text{MeV/c}\)) as calculated in the two PIC codes using the DC ionization model. Using the AC model gives a lower injection number, which is approximately half that of the DC model result for these parameters. The calculated injected beam mean energy and root-mean-square (r.m.s.) energy spread are also similar for both codes when the DC ionization model is used (shown in Fig. 4(b)). For ionization-induced injection, the beam transverse momentum spread is mainly due to the residual transverse momentum as a result of the ionization process. In the 1D case, canonical momentum conservation ensures \(\vec{p}_x = \bar{a}(t_i)\), where \(t_i\) is the ionization time. Therefore, the electrons have a transverse momentum equal to the laser vector potential at ionization. After the injection, the transverse momentum evolution depends on the transverse wakefield structure. Fig. 4(c) shows the FWHM transverse momentum distribution as calculated by the two codes, with differences less than 10%. This level of agreement is reasonable, considering the numerical noise generated by the ionization (i.e., the low macro-particles per cell). Increasing the number of macro-particles per cell for the background plasma electrons (from 1 to 4 macro-particles per cell), improves the agreement, indicating the source of errors is numerical noise in the PIC code. It also shows the electrons’ transverse momentum spread not only depends on the correct simulation of ionization process, it depends on the correct wake calculation too.

Typical beam momentum distributions are shown in Fig. 5 (where \(p_x, p_y\) are the longitudinal and transverse beam momenta, respectively). Differences in the beam transverse momenta distribution are the result of differences in the transverse wakefield structure calculated by the two codes. The above comparison provides a benchmark of the ionization algorithms implemented in VLPL and VORPAL for parameters relevant to studies of ionization injection in laser–plasma accelerators.

5. Summary and conclusions

Implementation of laser tunneling ionization rate formulae in explicit PIC codes has been examined. The originally published ionization rate formulae were reviewed, and corrections noted. It was shown, by comparison to theoretical predictions, that the DC form of the ionization rate provides improved accuracy. A subroutine is used to deal with the high level ionization in a single time step and an ionization current is used to consider energy loss due to ionization. The effect of PIC numerical parameters, such as grid resolution and number of macro-particles per cell, on the calculated ionization probability was studied. It was found that the ionization probability is sensitive to the grid resolution, and increased number of macro-particles per cell can reduce the simulation noise. Modeling the ionization injection in a laser–plasma accelerator was used to benchmark the ionization algorithm implemented in two PIC codes.

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