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# Improved modelisation of laser-particle interaction in PIC simulations

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A new method named B-TIS (Bourgeois & Davoine 2020) has recently been proposed to suppress the influence of numerical Cherenkov radiation (NCR) that appears in Particle-In-Cell (PIC) simulation of Laser WakeField Acceleration (LWFA). However, while this method provides good results when applied to the already accelerated electrons, we show here that it cannot model correctly most of the plasma electron bulk interacting with the laser field. We thus investigate in this paper the origins of this limitation and propose an improved method for which this limitation is removed. This new method, named B-TIS3, can now be applied to a much broader variety of problems and improve the performance in comparison to the standard PIC algorithm. We show that, for an electron interacting directly with a laser pulse, this new technique offers greater accuracy in term of momentum and motion than the conventional scheme used in many PIC codes. These improvements translate into more faithful energy spectrum and electric charge for the accelerated beam in simulations of Vacuum Laser Acceleration (VLA) or LWFA involving Direct Laser Acceleration (DLA) at low plasma density. This new method, easy to implement and not computationally demanding, should then prove useful to study in depth and help develop novel VLA, DLA and LWFA techniques.

## 1. Introduction

Particle-in-cell (PIC) codes are known for their versatility and relative speed, they are used to simulate a wide range of phenomena in kinetic and collisionless (or weakly collisional) plasma physics. To solve Maxwell equations, many of them use the finite-difference time-domain (FDTD) method first proposed by K. Yee (Yee 1966), a simple second-order method easily parallelisable but suffering from some numerical dispersion error which gives rise to what is known as numerical Cherenkov radiation (NCR) (Godfrey 1974). There has been lots of work in recent years proposing different ways to limit the impact of NCR (Xu *et al.* 2013; Lehe *et al.* 2013, 2016; Godfrey & Vay 2014; Yu *et al.* 2015; Li *et al.* 2017, 2021). We recently proposed a novel approach to mitigate the effects of this numerical artefact through the modification of the fields interpolation (Bourgeois & Davoine 2020).

This new technique, that we called B-TIS for B-translated interpolation scheme, is easy to implement in most PIC codes using the Yee scheme, has negligible impact on performance or communications and showed good results to reduce the impact of NCR in Laser WakeField Acceleration (LWFA) simulations but we believe it could also help to improve the modelisation of laser-particle interaction in a number of cases.

One domain where this interaction is particularly important, and thus could benefit

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greatly from such improvements, is the simulation of Vacuum Laser Acceleration (VLA); where a laser beam directly interact with electrons propagating in vacuum to accelerate them (Esarey *et al.* 1995; Quesnel & Mora 1998; Yu *et al.* 2000; Cline *et al.* 2013; Varin *et al.* 2013). Though it is a difficult technique to set up experimentally, it benefits from the extremely strong fields of the laser pulse (a few TV m<sup>-1</sup>) which make it a good candidate to produce MeV electrons at high repetition rate (Marceau *et al.* 2015; Carbajo *et al.* 2016).

B-TIS allows for a better modelisation of laser-electron interaction by reducing the error on the computed magnetic field which in turn lead to more accurate Lorentz force and particle motion. The improvement is especially significant for electromagnetic fields propagating at  $c$  along the electron acceleration axis. The study of VLA thus appears as a logical next step as it fits well within the limitations of B-TIS and provides a good benchmark to investigate the reproduction of the physical phenomena at play in laser-electron interaction. This should also help to improve the modelisation of the Direct Laser Acceleration (DLA) regime appearing in LWFA which presents great similarities to VLA (Pukhov *et al.* 1999; Shaw *et al.* 2014, 2017; Zhang *et al.* 2015).

In this article, we will start in section 2 with the study of a single electron interacting with a plane wave so as to compare and validate the simulation results against a simple analytical model. This simple study highlights the limitations of the different simulation techniques available and prompted us to develop an improved version of B-TIS that should be even more robust and accurate than the previous one. In section 3 we will see how the gaussian shape of a laser pulse impact those results before, in section 4, looking into the acceleration of a bunch of electrons by a laser beam and finally the application of our results to a case of DLA in a LWFA simulation.

## 2. Electron dynamic in an electromagnetic plane wave

We first study the case of a single electron interacting with a propagating plane wave. This simple situation can be analytically modelled which gives us a useful benchmark to evaluate the accuracy of our numerical simulations.

### 2.1. Analytical model

Considering one electron in vacuum, we can write its motion equation in terms of the electromagnetic vector potential  $\mathbf{A}$  as:

$$\frac{d\mathbf{p}}{dt} = -e \left[ -\frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \times (\nabla \times \mathbf{A}) \right] \quad (2.1)$$

where  $\mathbf{p}$  is the electron momentum,  $\mathbf{v}$  its velocity,  $e$  the elementary charge and the scalar potential  $\phi = 0$ .

For a plane wave propagating along the  $x$  axis, the vector potential depends only on  $x$  and is polarised in the  $yz$  plane. Assuming an electron initially at rest, we thus get to:

$$\frac{dp_x}{dt} = -\frac{e^2}{m_e \gamma} \mathbf{A} \cdot \frac{\partial \mathbf{A}}{\partial x} = -\frac{e^2}{2m_e \gamma} \frac{\partial A^2}{\partial x} \quad (2.2)$$

$$\mathbf{p}_\perp = e\mathbf{A} \quad (2.3)$$

with  $\mathbf{p}_\perp = p_y \mathbf{e}_y + p_z \mathbf{e}_z$ ,  $m_e$  being the electron mass and  $\gamma$  its Lorentz factor. We can recognise in eq. 2.2 the expression for the relativist ponderomotive force in the 1D case.

From the conservation of energy equation for the electron and using the fact that for a plane wave propagating at  $c$  along the  $x$  axis,  $(\frac{\partial}{\partial t} + c \frac{\partial}{\partial x}) A = 0$ , we can then show that

the quantity  $\gamma - p_x/m_e c$  is conserved. With the electron being initially at rest, we have  $\gamma(t=0) = \gamma_0 = 1$  and  $p_x(t=0) = p_{x,0} = 0$  which leads to:

$$\gamma = 1 + \frac{p_x}{m_e c} \quad (2.4)$$

We thus have three equations describing the dynamic of an initially at rest electron in a propagating plane wave.

$$\frac{p_x}{m_e c} = \frac{1}{2} \left( \frac{e\mathbf{A}}{m_e c} \right)^2 \quad (2.5)$$

$$\frac{\mathbf{p}_\perp}{m_e c} = \frac{e\mathbf{A}}{m_e c} \quad (2.6)$$

$$\gamma = 1 + \frac{1}{2} \left( \frac{e\mathbf{A}}{m_e c} \right)^2 \quad (2.7)$$

## 2.2. Numerical simulations

All numerical simulations presented in this article were performed using the code CALDER (Lefebvre *et al.* 2003). Before we delve into the results of those simulations though, we will first discuss the computation of electromagnetic fields and their resulting actions in PIC codes in order to introduce and summarise the B-TIS method proposed in (Bourgeois & Davoine 2020).

### 2.2.1. Temporal interpolation of the magnetic field $B$ in PIC codes

#### Standard Temporal Interpolation

Although there have been interesting new developments to create dispersionless Maxwell solvers in recent years, notably most recently (Pukhov 2020), CALDER, as many other PIC codes, still uses the simple and robust FDTD Yee scheme (Yee 1966) to solve the Maxwell equations. Electric ( $E$ ) and magnetic ( $B$ ) fields are thus calculated using a leap-frog method: they are defined on different grids which are offset spatially by half a cell but also temporally by  $\Delta t/2$ .

Let us consider the computation of the transverse Lorentz force applied to a moving particle in our simulation. The particle can move freely in the whole simulated space while the fields are computed only on specific grid points, it is thus necessary to interpolate the electromagnetic fields onto the charged particle position to calculate its motion.

This simple situation, with the fields amplitude values known on the different points of the grid and an electron moving freely between those points, is shown in Fig. 1 for a simple 1D grid. Considering only the longitudinal dimension  $x$  to simplify the notations,  $A_i^n$  then denotes the value of the field  $A$  at the  $n^{\text{th}}$  time step and the  $i^{\text{th}}$  point of the spatial grid or in other terms  $A_i^n = A(t = n\Delta t, x = i\Delta x)$ . Due to the leap-frog nature of the Yee scheme, values of the  $E_y$  fields are known at integer time-steps and grid points while values for  $B_z$  are known at half-integer time-steps and grid points. In the remainder of this section, we will only consider  $E_y$  and  $B_z$  - which are required to compute the transverse force  $F_y$  - and then omit the  $y$  and  $z$  indices when it is not absolutely necessary so as not to clutter the notation.

As the fields are initially not known at the same time step, a temporal interpolation is necessary to get  $\tilde{B}^n$  before the spatial interpolation and the computation of the force which is done at the integer time step  $n$ . The simplest and most common method is the linear time interpolation (LTI)  $\tilde{B}^n = \frac{1}{2}(B^{n-\frac{1}{2}} + B^{n+\frac{1}{2}})$  as is shown in the Fig. 1.a but a quadratic time interpolation (QTI) - with  $\tilde{B}_{i+\frac{1}{2}}^n = \frac{3}{8}B_{i+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{3}{4}B_{i+\frac{1}{2}}^{n-\frac{1}{2}} - \frac{1}{8}B_{i+\frac{1}{2}}^{n-\frac{3}{2}}$  - can

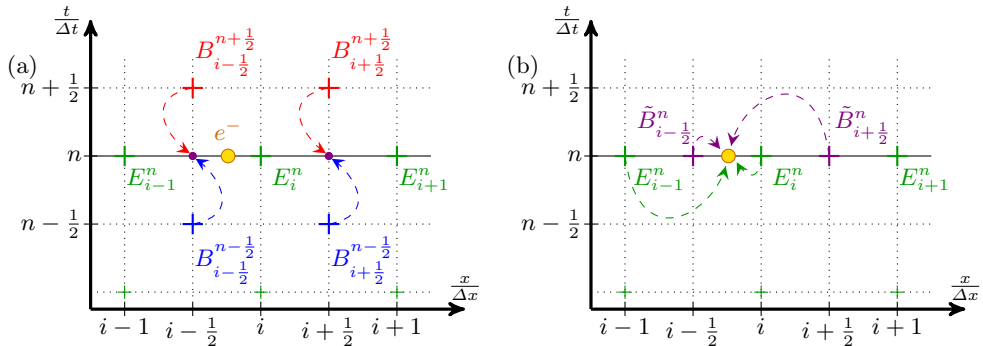


FIGURE 1. Usual interpolation process of EM fields on a 1D spatial grid at the  $n^{\text{th}}$  time step in order to get the transverse force  $F_y^n$  applied on the particle represented by the yellow dot. (a) shows the initial configuration where the fields values are known at different times and spatial points. The temporal interpolation to get  $\tilde{B}^n$  is shown with dashed lined arrows. Then (b) shows the subsequent spatial interpolation of  $E^n$  and  $\tilde{B}^n$  on the particle (again with dashed lined arrows and first order).

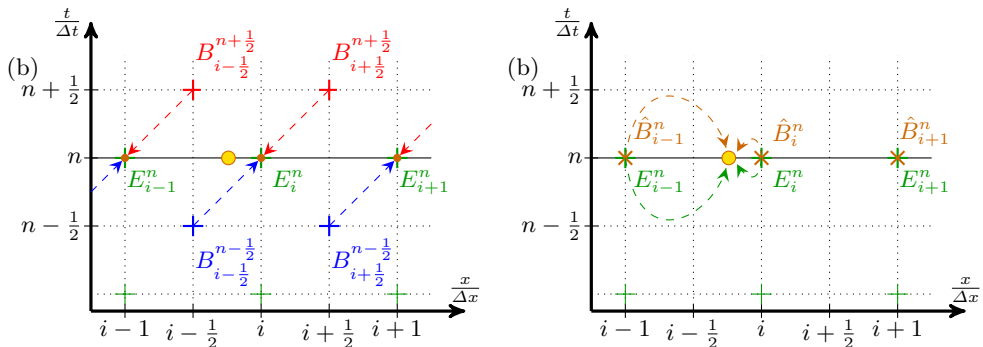


FIGURE 2. Modified interpolation process of EM fields: B-TIS on a 1D grid at the  $n^{\text{th}}$  time step. (a) shows the same initial configuration as Fig. 1 (a) but instead of the temporal interpolation of  $B$ , the relation  $\hat{B}_i^n = B_{i+\frac{1}{2}}^{n+\frac{1}{2}}$  is used. (b) shows the result of this translation and the subsequent spatial interpolation of  $E^n$  and  $\hat{B}_i^n$  on a particle.

sometimes be used instead for higher accuracy (Lehe *et al.* 2014). Once both fields  $E$  and  $B$  are known at the same time step, they are interpolated spatially onto the particles. This step is shown in Fig. 1.b. Once again different kinds of spatial interpolation can be used with varying orders of interpolation. The one depicted here is, for simplicity's sake, a 1<sup>st</sup> order method (linear interpolation).

#### Bypassing the need for a temporal interpolation: B-TIS

The idea behind our new scheme proposed in (Bourgeois & Davoine 2020) is to simply use the available value of the magnetic field as the value we need. That is, interpolating the fields at the particle position using  $(E_i^n, \hat{B}_i^n = B_{i+\frac{1}{2}}^{n+\frac{1}{2}})$  instead of  $(E_i^n, \tilde{B}_{i+\frac{1}{2}}^n)$  as previously shown. Of course, doing so is only physically sound if  $B_i^n \approx B_{i+\frac{1}{2}}^{n+\frac{1}{2}}$ . Thankfully this condition means for a wave propagating at  $c$  that  $B(x, t) \approx B(x + \Delta x/2, t + \Delta t/2)$  which is true as long as  $\Delta x \approx c\Delta t$ . Although this last condition can be limited in

the simulation by the Courant-Friedrichs-Lewy condition, it is usually verified in PIC simulations as having a ratio  $\Delta x/\Delta t$  close to  $c$  improves the quality of the results.

This new method effectively results in a translation of the calculated  $B$  field before the spatial interpolation, hence its name: *B-Translated Interpolation Scheme* (B-TIS). This process is described in Fig. 2.

### Computational error introduced

Both approaches introduces an error on the computed values of the magnetic field compared to an ideal situation where the magnetic field can be computed at integer time steps.

Let us consider a given magnetic field  $B(\varphi) = B_0 \cos(\varphi)$ . The computation of the numerical value of that field in the simulation introduces an error  $\varepsilon$  which depends on the method used:

$$\varepsilon_{\text{LTI}} = -B_0 \cos(\varphi) (1 - \cos(\delta\varphi)) \quad (2.8)$$

$$\varepsilon_{\text{QTI}} = -B_0 \cos(\varphi) \left( 1 - \cos(\delta\varphi) \left( 1 + \frac{1}{2} \sin^2(\delta\varphi) \right) \right) - \frac{1}{2} B_0 \sin(\varphi) \sin^3(\delta\varphi) \quad (2.9)$$

$$\varepsilon_{\text{B-TIS}} = -B_0 \cos(\varphi) \left( 1 - \cos(\widehat{\delta\varphi}) \right) - B_0 \sin(\varphi) \sin(\widehat{\delta\varphi}) \quad (2.10)$$

with  $\varphi = k_x x + k_y y + k_z z - \omega t$ ,  $\delta\varphi = \frac{\omega\Delta t}{2}$  and  $\widehat{\delta\varphi} = \frac{1}{2}(k_x \Delta x - \omega\Delta t)$ .  $\omega$  is the field's angular frequency and  $k_x, k_y, k_z$  its wavevector components.

For longitudinally propagating waves with  $\omega/k_x \approx c$  and  $c\Delta t \approx \Delta x$ ,  $\widehat{\delta\varphi}$  can become very small and the gain in accuracy should then be significant. This improvement of the computation of the magnetic field is what enables B-TIS to effectively suppress the effects of NCR. Indeed, the more accurate computation result in the induced Lorentz force, from the interaction of the NCR with particles, being negligible. In effect, the spurious radiation is still generated and present in the simulation but has no impact on the simulated particles.

### 2.2.2. Comparison of the different temporal interpolation methods

Three simulations were originally performed, each with a different temporal interpolation method introduced earlier: LTI, QTI and B-TIS. To reproduce in a 2D simulation the situation presented above, we use a plane wave propagating along the  $x$  axis, infinite in width along the  $y$  axis. Periodical boundaries conditions are used on the longitudinal edges of the simulation box to recreate the infinite transverse property of the wave.

We chose the polarisation direction in the simulation plane (along the  $y$  axis). The laser wavelength is  $\lambda_0 = 2\pi c/\omega_0$ , with  $\omega_0$  the laser angular frequency, and the wave amplitude is characterised by  $a_0 = eA_0/m_e c = 5$ . Simulations were performed in a moving window following the wave propagation of  $960 \times 200$  cells with  $\Delta x = 0.15 c/\omega_0$ ,  $\Delta y = 10 c/\omega_0$  and a time step  $\Delta t = 0.149 1/\omega_0$ .

The propagating wave's temporal profile has a finite extension with a trapezoidal envelop as shown in figure 3.a. Each ramp and the plateau of the trapezoidal profile are  $4\lambda_0$  long. We take care that  $\int E_y(t)dt = 0$ , otherwise,  $A_y$ , and thus  $p_y$ , is non zero even once the laser has passed. To make the analysis easier we also chose the temporal profile so that  $\int_{t_1}^{t_2} E_y(t)dt = 0$ , with  $t_1$  and  $t_2$  being the time boundaries of the profile ramps or plateau. This ensures that the transverse impulsion  $p_y$  is zero on average during the whole passing of the laser intensity plateau by the electron.

Only one particle is considered here. It is initially at rest at the centre of the simulation box. This single particle is given a very small statistical weight in the simulation so that

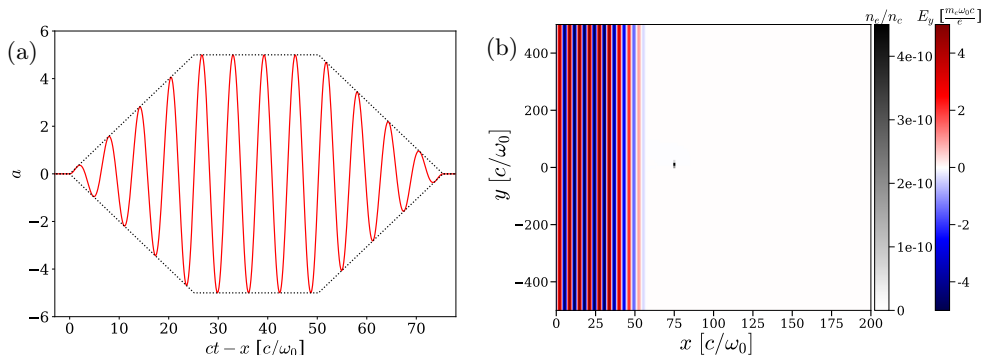


FIGURE 3. (a) Temporal profile (normalised vector potential  $a$ ) of the incident wave. The dashed line describes the trapezoidal envelop. (b) Initial situation of the simulation. The incident wave is propagating to the right.

the charge density (computed within each cell of the simulation) around the particle is negligible and doesn't affect the particle dynamic. The figure 3.b shows the initial state of the simulation. It is an electron density map (normalised to the plasma critical density  $n_c = \epsilon_0 m_e \omega_0^2 / e^2$ ) showing the initial position of the particle superimposed on a map of the wave transverse electric field  $E_y$ .

Considering a propagating plane wave along  $x$ , polarised along the  $y$  axis and with a temporal envelop  $f$  such as  $\mathbf{A} = A_0 f(t - x/c) \sin(\omega_0(t - x/c)) \mathbf{e}_y$ , then equations (2.5), (2.6) and (2.7) may be rewritten as:

$$\frac{p_x}{m_e c} = \frac{1}{2} a_0^2 f^2(t - x/c) \sin^2(\omega_0(t - x/c)) \quad (2.11)$$

$$\frac{p_y}{m_e c} = a_0 f(t - x/c) \sin(\omega_0(t - x/c)) \quad (2.12)$$

$$\gamma = 1 + \frac{1}{2} a_0^2 f^2(t - x/c) \sin^2(\omega_0(t - x/c)) \quad (2.13)$$

The figure 4 shows results for each simulation by comparing the particle momenta  $p_x$  and  $p_y$  to those expected according to theoretical computations based on equations (2.11) and (2.12). These figures uses normalised values, meaning  $t$  is expressed as multiples of  $1/\omega_0$ ,  $x$  as multiples of  $c/\omega_0$  and the momentum  $p$  as multiples of  $m_e c$ .

The QTI and B-TIS methods give values of  $p_y$  closer to the theoretical value than LTI but overall, all three simulations reproduce fairly well the transverse behaviour of the particle with small differences.

Still, notable differences between analytical and simulation results though are present at the beginning and end of the trapezoid ramps ( $t - x \approx 20$  and  $t - x \approx 90$ ) in figure 4.b. Those are due to a small difference in how the laser temporal profile is defined: in the theoretical case we considered a trapezoidal envelop for the vector potential  $A$ , whereas we considered a trapezoidal envelop for the electric and magnetic fields  $E$  and  $B$  in the simulation, as it is easier to initialise the value of those fields. This definition gives rise to vector potential  $A$  with a slightly different shape when  $A$  varies significantly within a single wavelength, as is the case at the boundaries of the temporal profile of the wave.

The longitudinal momentum is more problematic and only the LTI method reproduces qualitatively the expected behaviour of the particle, with a notable error on the maximal value of  $p_x$  which is underestimated. Both QTI and B-TIS lead to an overestimation of

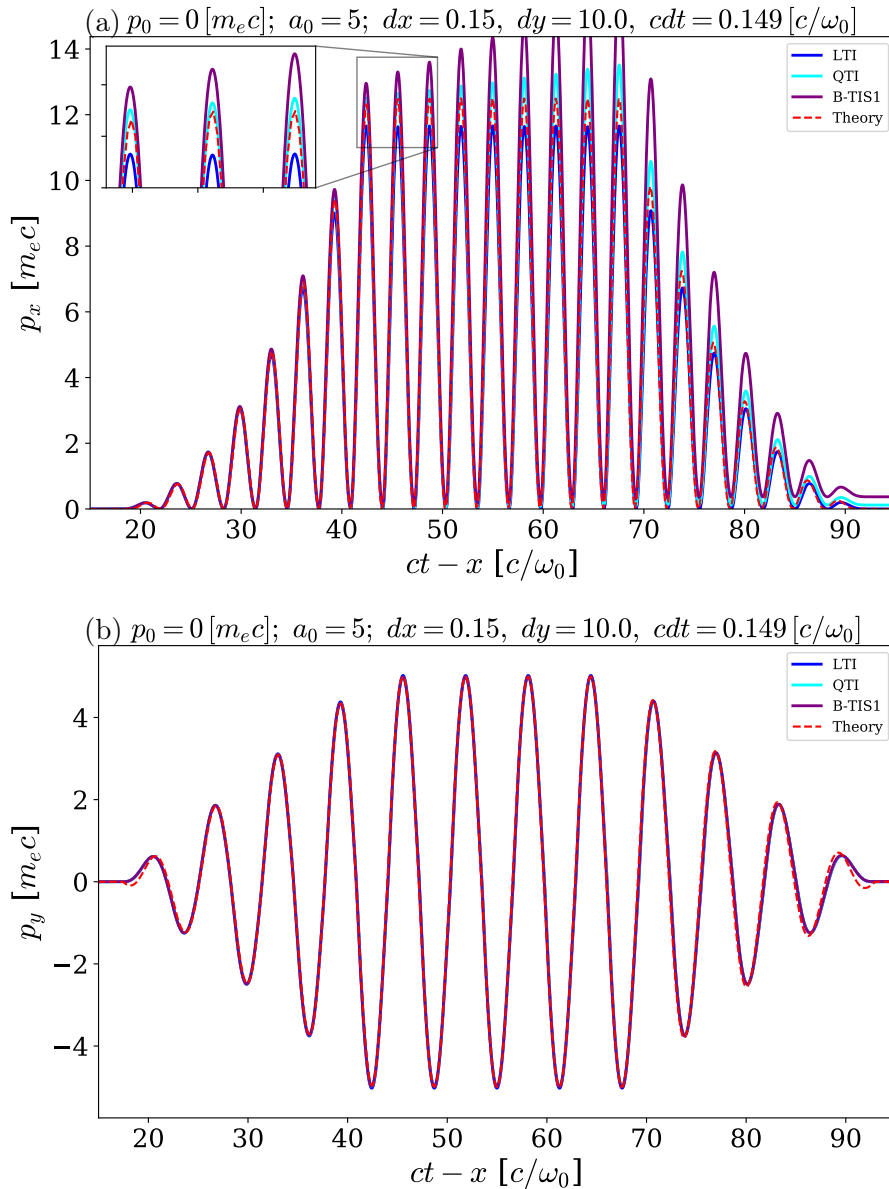


FIGURE 4. Evolution of the electron normalised momenta  $p_x$  (a) and  $p_y$  (b) with respect to the normalised coordinate  $ct - x$  for the considered different methods. The red dashed line shows the theoretical  $p_x$  (respectively  $p_y$ ) given by equation (2.11) (respectively equation (2.12)).

$p_x$  with an error increasing over time (artificial increase in the energy of the particle). This error leads to a nonphysical residual momentum after the wave went by.

The next section investigate the source of this error and present a possible solution for the B-TIS method.



### 2.3. Inaccurate longitudinal momentum with QTI and B-TIS

The laser wave propagation in CALDER is computed using the fields  $E$  and  $B$  not the vector potential  $A$  so we will use here expressions with respect to the electromagnetic fields. The electron motion equation, for the longitudinal momentum is thus:

$$\frac{dp_x}{dt} = -e(E_x + v_y B_z - v_z B_y) \quad (2.14)$$

Considering a plane wave propagating along  $x$  and polarised along the  $y$  axis such that  $E_y = E_0 \cos(\varphi)$  with  $\varphi = \omega_0(t - x/c)$ , then  $B_z = (E_0/c) \cos(\varphi)$  and  $E_x = 0$ ,  $B_y = 0$ . The previous equation thus becomes:

$$\frac{dp_x}{dt} = -\frac{eE_0}{c} v_y \cos(\varphi) \quad (2.15)$$

From equation (2.6), we get that  $v_y \propto A(\varphi) \propto \sin(\varphi)$ , which leads to:

$$p_x(t) = \int_0^t \frac{dp_x}{dt} dt \propto \int_0^t \sin(\varphi) \cos(\varphi) d\varphi \quad (2.16)$$

This means that for an electron initially at rest, after an integer number of wave period, the momentum  $p_x$  should be 0 again as  $\int_0^{2\pi} \sin(\varphi) \cos(\varphi) d\varphi = 0$ . This is indeed what is observed in figure 4 for the theoretical curve and LTI but not for QTI and B-TIS. This error comes from the computational error introduced during the magnetic field interpolation step.

Looking at equations (2.8,2.9,2.10), for all three methods, we can see that the error depends on a term that is proportional to  $\cos(\varphi)$  but in the case of QTI and B-TIS there is a second term proportional to  $\sin(\varphi)$ . That is this last part which is problematic here. Taking a look at the numerically computed momentum  $p_x^{num}$  in our simulation, we can express it as:

$$p_x^{num}(t) = p_x(t) + \int_0^t -\frac{eE_0}{c} v_y \varepsilon dt = p_x(t) + \varepsilon_p \quad (2.17)$$

Where  $\varepsilon_p$  is the numerical error on the momentum  $p_x$ . Thus, with LTI, we get that:

$$\varepsilon_p^{LTI} = K (1 - \cos(\delta\varphi)) \int_0^t \sin(\varphi) \cos(\varphi) d\varphi \quad (2.18)$$

With  $K$  a constant depending on the wave amplitude. This error will fluctuate with time but it will periodically cancel out whereas with QTI and B-TIS we get:

$$\varepsilon_p^{QTI} = K' \int_0^t \sin(\varphi) \cos(\varphi) d\varphi + \frac{1}{2} K \sin^3(\delta\varphi) \int_0^t \sin^2(\varphi) d\varphi \quad (2.19)$$

$$\varepsilon_p^{B-TIS} = K'' \int_0^t \sin(\varphi) \cos(\varphi) d\varphi + K \sin(\widehat{\delta\varphi}) \int_0^t \sin^2(\varphi) d\varphi \quad (2.20)$$

With  $K' = K (1 - \cos(\delta\varphi) (1 + \frac{1}{2} \sin^2(\delta\varphi)))$  and  $K'' = K (1 - \cos(\widehat{\delta\varphi}))$ . The second term in these expressions leads to an error that grows continuously and monotonically with time instead of periodically cancelling out. This explain the divergence of results observed in figure 4 though the initial error is really small. Note also that, with our values for the parameters  $\Delta x$  and  $\Delta t$ ,  $\frac{1}{2} \sin^3(\delta\varphi) \approx 2.10^{-4}$  where as  $\sin(\widehat{\delta\varphi}) \approx 5.10^{-4}$ . This explains the difference in growth rate for the error with QTI and B-TIS.

The obvious solution would be to use a finer grid so as to minimise  $\Delta t$  and  $\Delta x - c\Delta t$  - thus minimising  $\delta\varphi$ ,  $\widehat{\delta\varphi}$  and the induced error - but this is highly detrimental to

computation performance. Restricting oneself to using only small values of  $a_0$  is another way to circumvent this problem - as the error is proportional to  $a_0^2$  - but it is problematic in the case of the study of VLA or DLA. In any case, both of those approaches only mitigate the problem as the error will still be present and, though small initially, it will compound and increase with time.

It is however possible to slightly modify B-TIS in a way that drastically reduces this source of error while still benefiting from all of the advantages of this method.

#### 2.4. B-TIS modification

As we saw earlier, B-TIS replaces the following temporal interpolation of the magnetic field:

$$\tilde{B}_{i+\frac{1}{2}}^n = \frac{1}{2} \left( B_{i+\frac{1}{2}}^{n+\frac{1}{2}} + B_{i+\frac{1}{2}}^{n-\frac{1}{2}} \right) \quad (2.21)$$

with the following translation (as shown in figure 2.a):

$$\hat{B}_i^n = B_{i+\frac{1}{2}}^{n+\frac{1}{2}} \quad (2.22)$$

This is based on the assumption that the wave propagates at  $c$  along the  $x$  axis and that  $c\Delta t \approx \Delta x$ .

However, if the value of the magnetic field is conserved going forward in time and space, it is also conserved when going backward, and within those assumptions, that translation is completely equivalent to this one:

$$\hat{B}_i^n = B_{i-\frac{1}{2}}^{n-\frac{1}{2}} \quad (2.23)$$

Both possible translations are shown in figure 2.b where the assumption that the magnetic field  $B$  propagates at  $c$  and that  $c\Delta t \approx \Delta x$  means that  $B$  is constant along the diagonals of the grid, hence the equivalence of the two translations.

Let us call r-BTIS the 'reversed' version of B-TIS using  $\hat{B}_i^n = B_{i-\frac{1}{2}}^{n-\frac{1}{2}}$ . This method then introduces the following error on the magnetic field:

$$\varepsilon_{\text{r-B-TIS}} = -B_0 \cos(\varphi) \left( 1 - \cos(-\widehat{\delta\varphi}) \right) - B_0 \sin(\varphi) \sin(-\widehat{\delta\varphi}) \quad (2.24)$$

$$= -B_0 \cos(\varphi) \left( 1 - \cos(\widehat{\delta\varphi}) \right) + B_0 \sin(\varphi) \sin(\widehat{\delta\varphi}) \quad (2.25)$$

With the exception of the second term sign, this is the same expression as the error for the 'classical' B-TIS. As such, we should be able to eliminate that second term by combining both B-TIS and rB-TIS. We can indeed choose to use both translations in conjunction at each time step through a simple average such as:

$$\hat{B}_i^n = \frac{1}{2} \left( B_{i+\frac{1}{2}}^{n+\frac{1}{2}} + B_{i-\frac{1}{2}}^{n-\frac{1}{2}} \right) \quad (2.26)$$

It is important to note though that it is not a simple temporal averaging as is used in LTI, both the time index and the spatial index are different. This new method, that we call B-TIS3, then introduces the following error on  $B$ :

$$\varepsilon_{\text{B-TIS3}} = \frac{1}{2} \varepsilon_{\text{B-TIS}} + \frac{1}{2} \varepsilon_{\text{r-B-TIS}} \quad (2.27)$$

$$= -B_0 \cos(\varphi) \left( 1 - \cos(\widehat{\delta\varphi}) \right) \quad (2.28)$$

The second term involving  $\sin(\varphi)$  has indeed disappeared as we expected. The expression

of this error is similar to the one introduced by LTI with the important difference though that we have  $\widehat{\delta\varphi} < \delta\varphi$ , which should point to an improvement of accuracy.

To illustrate this point, let us consider a forward propagating wave in vacuum with  $\omega = \omega_0$  and  $k_x = k = \frac{\omega_0}{c}$ . We thus have,  $\delta\varphi = \frac{\omega_0 \Delta t}{2}$  while  $\widehat{\delta\varphi} = \frac{1}{2} \frac{\omega_0}{c} (\Delta x - c\Delta t)$ . Then, per the equation 2.8, 2.9, 2.10 and 2.28, with our numerical parameters we get:

$$\varepsilon_{LTI}^{\text{las}} = -B_0 \cos(\varphi) \times 2.77 \cdot 10^{-3} \quad (2.29)$$

$$\varepsilon_{LTI}^{\text{las}} = -B_0 \cos(\varphi) \times 1.15 \cdot 10^{-5} - B_0 \sin(\varphi) \times 2.06 \cdot 10^{-4} \quad (2.30)$$

$$\varepsilon_{B-TIS}^{\text{las}} = -B_0 \cos(\varphi) \times 1.25 \cdot 10^{-7} - B_0 \sin(\varphi) \times 5 \cdot 10^{-5} \quad (2.31)$$

$$\varepsilon_{B-TIS3}^{\text{las}} = -B_0 \cos(\varphi) \times 1.25 \cdot 10^{-7} \quad (2.32)$$

On the other hand, let us consider a wave, propagating forward in the simulation at the Nyquist frequency so that  $\omega = \frac{\pi}{\Delta t}$  and  $k_x = k = \frac{\pi}{\Delta x}$ . Then, as  $\delta\varphi = \frac{\pi}{2}$  and  $\widehat{\delta\varphi} = 0$ :

$$\varepsilon_{LTI}^{\text{Nyq}} = -B_0 \cos(\varphi) \quad (2.33)$$

$$\varepsilon_{LTI}^{\text{las}} = -B_0 \cos(\varphi) - B_0 \sin(\varphi) \quad (2.34)$$

$$\varepsilon_{B-TIS}^{\text{las}} = 0 \quad (2.35)$$

$$\varepsilon_{B-TIS3}^{\text{Nyq}} = 0 \quad (2.36)$$

Both of these simple cases show the immense improvement in accuracy that B-TIS3 brings to our simulations regarding the magnetic field over all the previously considered methods.

A comparison of the results from the B-TIS3 method and the previous one is presented in figure 5. We can see that this improved B-TIS3 eliminate the troublesome compounding error impacting B-TIS1 and lead to computed values of  $p_x$  even closer to the theoretical ones than those obtained using LTI. Results on transverse momentum  $p_y$  are just as good as before, the improvement margin being already very slim even with LTI.

At this point, the reader should note, that we have focused on forward propagating waves, as they are what is most commonly encountered in VLA and LWFA and what this scheme was designed for. Counter-propagating radiation, however, can be present in a few situations, because of back-scattering for instance or even in the case of colliding laser pulses. It is thus of interest to check the robustness of our new scheme in such scenarios.

The accuracy of both LTI and QTI is not impacted for a counter-propagating wave, as we still have  $\delta\varphi = \frac{\omega \Delta t}{2}$ . For B-TIS and B-TIS3 however, with  $k_x = -k$ , we now get  $\widehat{\delta\varphi} = \frac{1}{2} (k\Delta x + \omega \Delta t)$ . With this, for a counter-propagating laser pulse we get:

$$\varepsilon_{B-TIS3}^{\text{back las}} = -B_0 \cos(\varphi) \times 1.11 \cdot 10^{-2} \quad (2.37)$$

And for a wave propagating backward at the Nyquist frequency:

$$\varepsilon_{B-TIS3}^{\text{back Nyq}} = -2B_0 \cos(\varphi) \quad (2.38)$$

While these results appear much worse than in the case of forward propagation, it should be noted that they are not that different from the accuracy level of LTI, with a factor of 2 to 4 between them. Therefore, the presence of counter-propagating radiation in the simulation, although not the ideal use case for B-TIS3, should not prove physics breaking and the overall gains might be well worth this trade-off.

From these results, it appears that we have successfully solved the initial problem encountered in the computation of the longitudinal momentum  $p_x$  and that B-TIS3

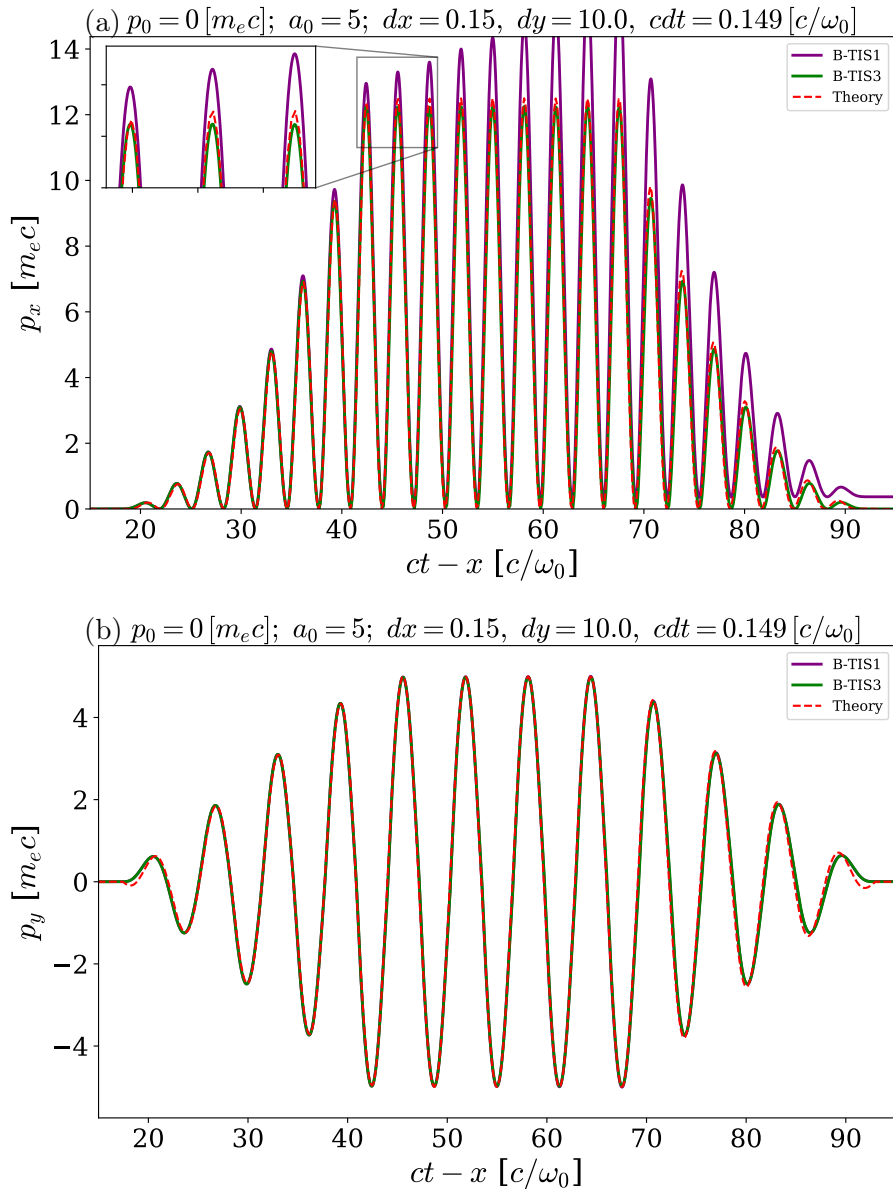


FIGURE 5. Evolution of the electron normalised momentum  $p_x$  (a) and  $p_y$  (b) with respect to the normalised coordinate  $ct - x$  for the considered different methods. The red dashed line shows the theoretical  $p_x$  (respectively  $p_y$ ) given by equation (2.11) (respectively equation (2.12)).

appears well suited to reproduce the physics of vacuum laser acceleration contrary to B-TIS1 and QTI.

As LTI is by far the most common method used in PIC codes, it seems an appropriate method to compare to. We will then only present simulation results for both of these methods. A summary of results for LTI and B-TIS3 is presented in figure 6. The better reproduction of the momentum with B-TIS3 shown in Figures 6.a and 6.b leads to an

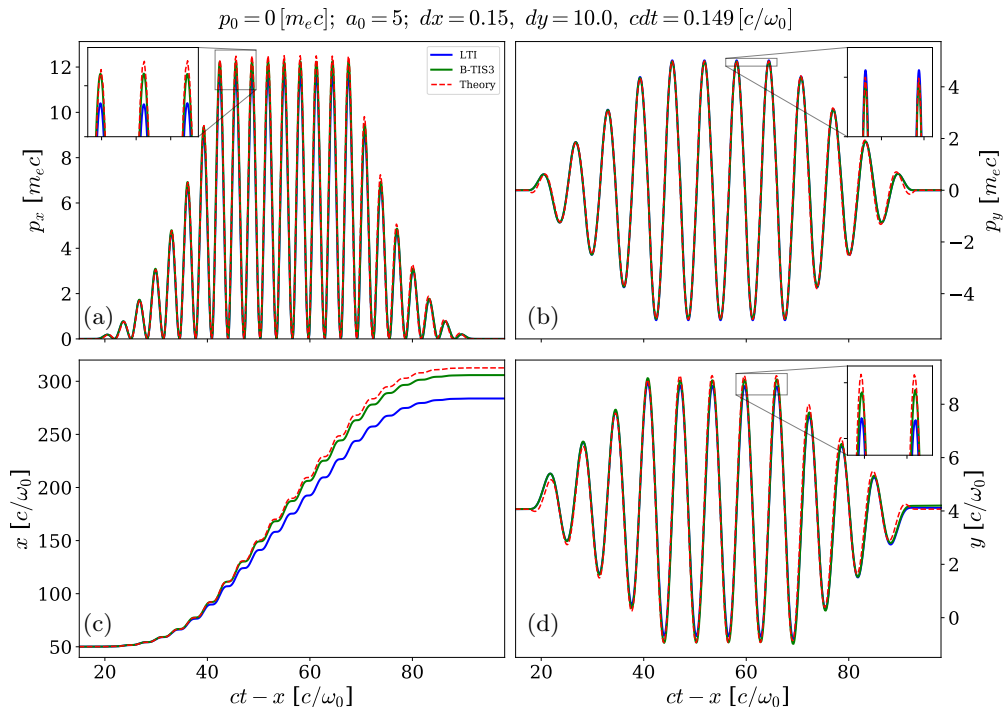


FIGURE 6. Evolution of the electron normalised momentum: (a)  $p_x$ , (b)  $p_y$  and normalised position: (c)  $x$ , (d)  $y$  with respect to the normalised coordinate  $ct - x$  for LTI and B-TIS3. The red dashed line shows the theoretical values expected from analytical model introduced earlier.

electron trajectory more faithful to the theoretical predictions as can be seen in figures 6.c and 6.d.

### 2.5. Simulations with initial longitudinal momentum

We have so far investigated only the case of an electron initially at rest but, in practice, electrons are far more likely to have a non zero initial momentum. Going back to the analytical model developed in 2.1, with  $p_{x,0} \neq 0$  and  $\gamma_0 \neq 1$  we now get:

$$\gamma = \gamma_0 + \frac{p_x}{m_e c} - \frac{p_{x,0}}{m_e c} \quad (2.39)$$

Which leads to the three following equations now describing the electron motion:

$$\frac{p_x}{m_e c} = \frac{p_{x,0}}{m_e c} + \frac{1}{2} \left( \gamma_0 + \frac{p_{x,0}}{m_e c} \right) \left( \frac{e\mathbf{A}}{m_e c} \right)^2 \quad (2.40)$$

$$\frac{\mathbf{p}_\perp}{m_e c} = \frac{e\mathbf{A}}{m_e c} \quad (2.41)$$

$$\gamma = \gamma_0 + \frac{1}{2} \left( \gamma_0 + \frac{p_{x,0}}{m_e c} \right) \left( \frac{e\mathbf{A}}{m_e c} \right)^2 \quad (2.42)$$

Figure 7 show results from two simulations where the electron had an initial longitudinal momentum  $p_0$ : The first one with  $p_0 = m_e c$  and the second one with  $p_0 = 5m_e c$ . All other numerical and physical parameters are the same as previously. The two methods results in much more noticeable differences than previously.

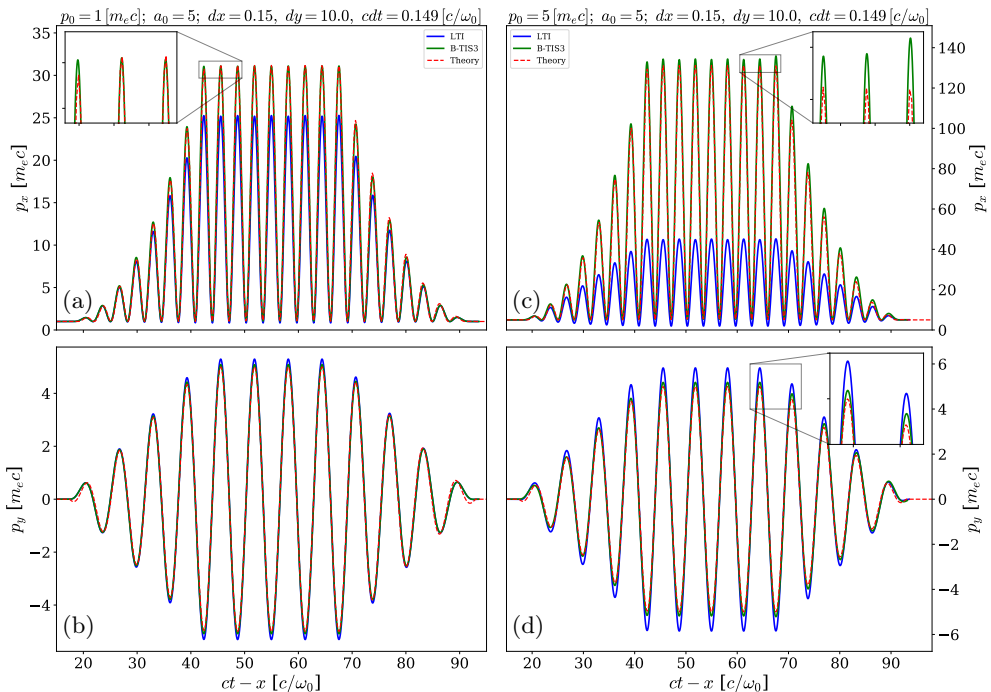


FIGURE 7. Evolution of the electron normalised momentum: (a) (*resp.* (c))  $p_x$ , (b) (*resp.* (d))  $p_y$  with respect to the normalised coordinate  $ct - x$  for LTI and B-TIS3 with  $p_0 = m_e c$  (*resp.*  $p_0 = 5 m_e c$ ). The red dashed line shows the theoretical values expected from analytical model introduced earlier.

It is apparent that the greater the initial velocity of the electron, the more LTI underestimate the longitudinal momentum. The maximum longitudinal momentum  $p_{x,max}$  being underestimated by at least a factor of 3 compared to the theoretical value when using LTI with a an initial momentum  $p_0 = 5 m_e c$ . B-TIS3, on the other hand, slightly overestimates  $p_x$  but overall produces results much closer to the predictions of the analytical model.

Looking at the transverse momentum  $p_y$  now, both methods reproduce fairly well the theoretical results though both tend to overestimate it. Once again, B-TIS3 results appear closer to those of the model and, though the error increases when the initial momentum  $p_0$  increases, this increase appears much smaller for B-TIS3 than LTI.

Note that all of the presented simulations have been realised using the Boris pusher (Boris 1970). We found very negligible differences between simulations using Boris' scheme and simulations using the scheme proposed in (Vay 2008) to correct the Boris pusher inaccuracies at relativistic speed and we observed the same inaccuracies with LTI and the same improvements with B-TIS3, irrespective of the choice of pusher.

### 3. Interaction with a gaussian beam

In order to get to more realistic cases, we now consider, as our incident wave, a laser pulse with a gaussian spatial profile instead of plane wave with an infinite transverse size.

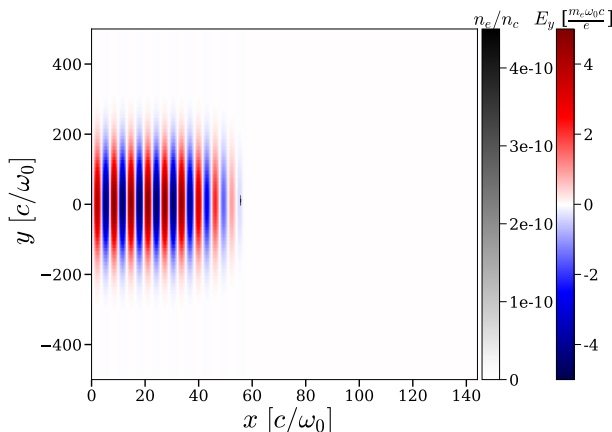


FIGURE 8. Initial situation with a spatially gaussian wave.

### 3.1. Theoretical description

We keep the same trapezoidal temporal profile for our laser pulse so as to make comparisons with earlier results easier, however its transverse size is now finite and given by a gaussian profile with a width (FWHM of the intensity profile) of  $160 \omega_0/c$ . The figure 8 shows this initial situation.

We can come back to the equations introduced in section 2.1 but considering now the more general case of a wave polarised along the  $y$  axis and propagating along the  $x$  axis such that  $\mathbf{A}(x, y, t) = A(x, y, t)\mathbf{e}_y$ . The laser waist is assumed here much bigger than the wavelength and as such we can neglect the existence of a vector potential component along  $x$  (We will discuss this approximation later). The energy conservation equation then leads to:

$$\frac{d}{dt} (\gamma mc^2) = ev_y \frac{\partial A}{\partial t} \quad (3.1)$$

And the motion equation (2.1) gives us:

$$\frac{dp_x}{dt} = -ev_y \frac{\partial A}{\partial x} \quad (3.2)$$

$$\frac{d}{dt} (p_y - eA) = -ev_y \frac{\partial A}{\partial y} \quad (3.3)$$

Using the fact that  $\frac{d\mathbf{A}}{dt} = \frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{A}$ , we finally get to:

$$\frac{dp_x}{dt} = -ev_y \frac{\partial A}{\partial x} \quad (3.4)$$

$$\frac{dp_y}{dt} = e \left( \frac{\partial A}{\partial t} + v_x \frac{\partial A}{\partial x} \right) \quad (3.5)$$

$$\frac{d}{dt} (\gamma mc^2) = ev_y \frac{\partial A}{\partial t} \quad (3.6)$$

This system is much more complex than the previous one and we will not attempt to solve it analytically here. We can still gather though that the ponderomotive force of the laser will push aside the electron and that it will gain a residual momentum, both longitudinal and transverse. For an exact solution of the motion and acceleration of electrons by the laser fields, we would have to consider the longitudinal component of  $\mathbf{A}$  ( $\mathbf{A} = A_x \mathbf{e}_x + A_y \mathbf{e}_y$ ) which would modify equations (3.1) from (3.6) above. For simplicity's

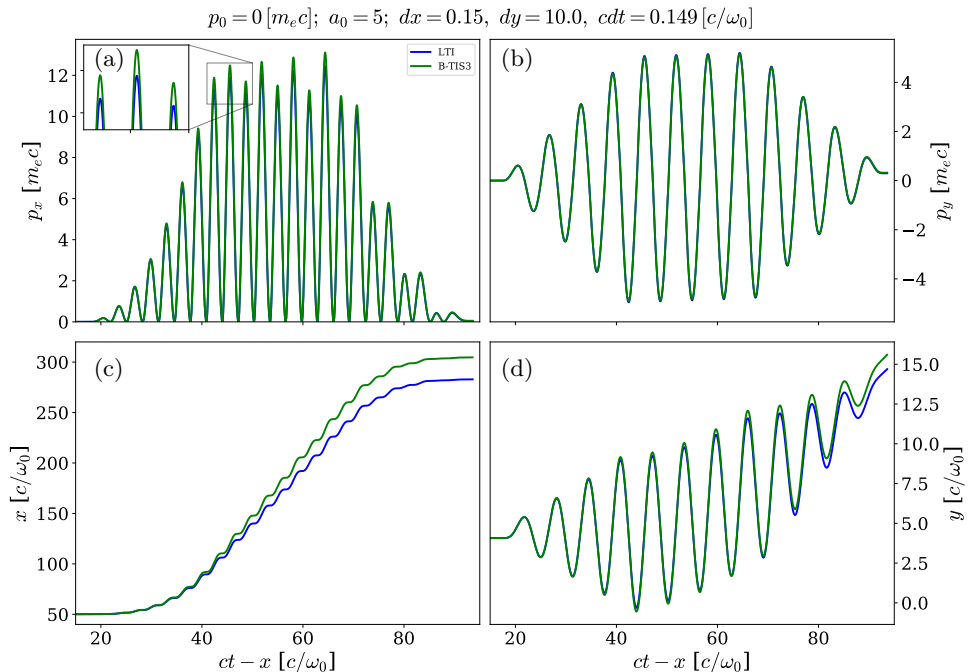


FIGURE 9. Evolution of the electron normalised momentum: (a)  $p_x$ , (b)  $p_y$  and normalised position: (c)  $x$ , (d)  $y$  with respect to the normalised coordinate  $ct - x$  for LTI and B-TIS3 with a transversely gaussian laser beam and an electron initially at rest ( $p_0 = 0$ ).

sake, however, we do not consider the component  $A_x$  which is negligible in our case. More comprehensive descriptions and computations on this subject can be found in (Mora & Antonsen 1997; Quesnel & Mora 1998).

### 3.2. Numerical results

The figures 9 and 10 sum up the simulation results for an electron initially close to the propagation axis and, respectively, with no initial longitudinal momentum ( $p_0 = 0$ ) or with  $p_0 = m_e c$ .

The behaviour observed in the simulations is in accordance with our expectations: the electron drift transversely as it is being accelerated and thus ends up with residual non-zero longitudinal and transverse momentum,  $p_x$  and  $p_y$ , even after it has exited the laser beam. This residual extra momentum is quite small when the electron is initially at rest but it quickly becomes more important when the electron has some initial velocity as we can see in figures 10.a and 10.b.

Both methods predict overall a similar behaviour for the electron though we can observe notable differences on final momentum and positions. Indeed as the electron is sensibly more accelerated in the B-TIS3 case, it travels a much longer distance while inside the laser pulse. This difference is especially apparent in the case with a non-zero initial momentum, which is coherent with our previous observations.

As we cannot compare to an analytical model here, we will use a numerical method to estimate the theoretical result. When reducing both the spatial grid size and the time step duration, both numerical methods should converge on a unique solution corresponding to the physical solution.

We look at the results of three pairs of simulation where we chose respectively:  $\Delta x =$



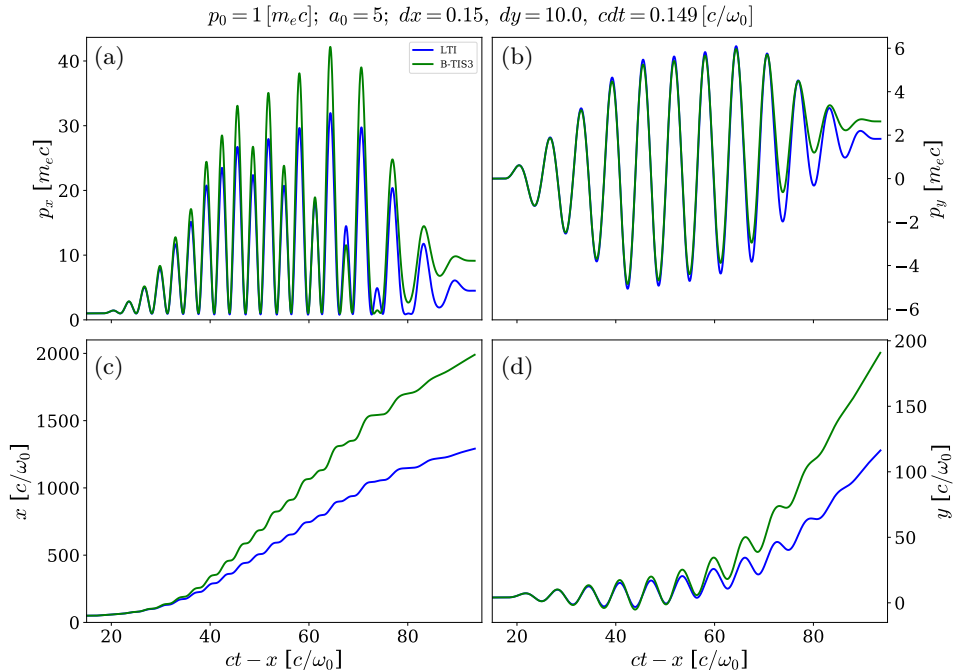


FIGURE 10. Evolution of the electron normalised momentum: (a)  $p_x$ , (b)  $p_y$  and normalised position: (c)  $x$ , (d)  $y$  with respect to the normalised coordinate  $ct - x$  for LTI and B-TIS3 with a transversely gaussian laser beam and an electron with an initial longitudinal momentum ( $p_0 = m_e c$ )

$0.15c/\omega_0$  and  $c\Delta t = 0.149c/\omega_0$  for the first one,  $\Delta x = 0.10c/\omega_0$  and  $c\Delta t = 0.099c/\omega_0$  for the second one and  $\Delta x = 0.05c/\omega_0$  and  $c\Delta t = 0.049c/\omega_0$  for the third. Observed momenta are shown in figures 11. Those results clearly show that both methods are converging on the same solution which appears fairly close to the one obtained initially through B-TIS3. We thus observe once again that B-TIS3 tends to slightly overestimate the electron momentum while LTI noticeably underestimate it.

It is important to note however, that even when dividing by 3 both  $\Delta t$  and  $\Delta x$  (thus increasing the computation time by a factor nine), LTI still does not give better results than B-TIS3 with a worse resolution. B-TIS3 appears, in that light, as a fairly good improvement on the standard LTI.

### 3.3. Influence of the initial position

The ponderomotive force acting on the particle depends on the laser pulse intensity gradient which varies widely depending on the transverse position.

We show in this section that we can indeed observe this behaviour in our simulations. We present here in figure 12, the momenta of electrons with different initial positions  $y_0$ .

Both methods tend to predict similar final momentum for the electron as long as it is outside of the stronger field region of the laser pulse. Indeed differences in results between LTI and B-TIS3 are less important the farther the electron initially from the propagation axis.

As we showed that the error introduced by LTI was bigger when the electron was

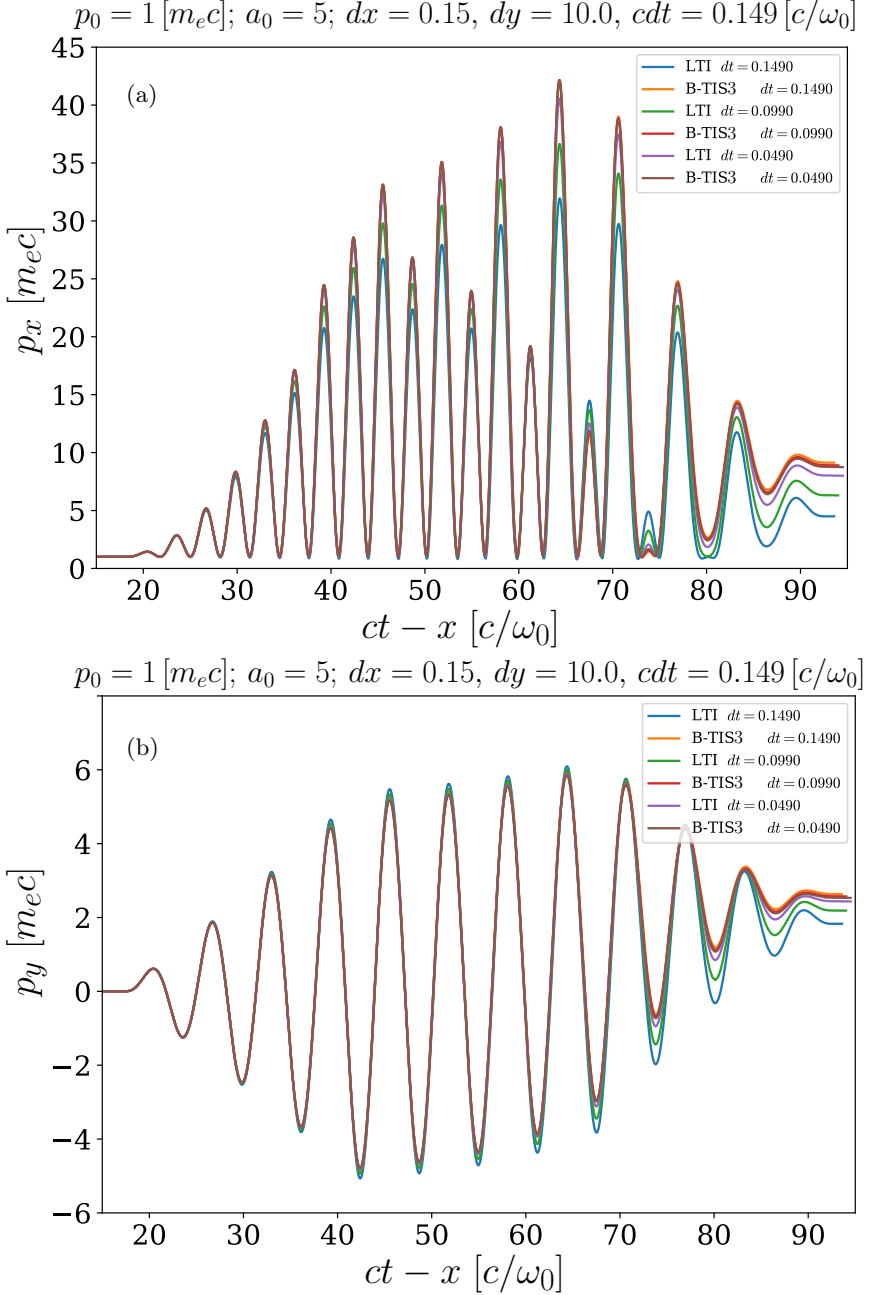


FIGURE 11. Evolution of the electron normalised momentum: (a)  $p_x$ , (b)  $p_y$  with respect to the normalised coordinate  $ct - x$  for LTI and B-TIS3, with  $p_0 = m_e c$  and varying cell sizes and time steps.

strongly accelerated, it thus seems logical that its predictions are better - thus more in accordance with B-TIS3 - when the electron is far from the high intensity region near the propagation axis and less accelerated.

Though final momentum may appear similar, the small differences can have a big impact on the particle trajectory. Furthermore, when trying to study VLA we are of

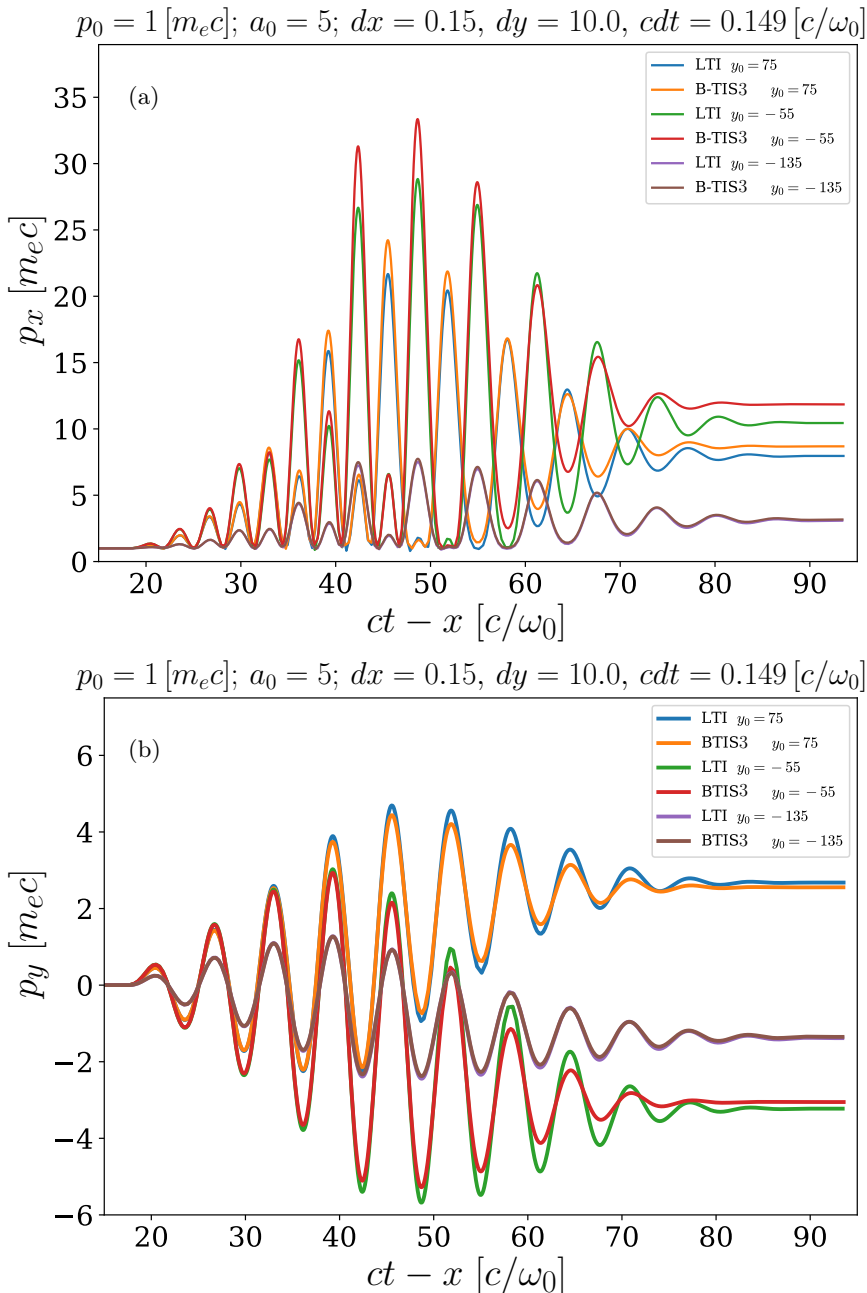


FIGURE 12. Evolution of the electron normalized momentum: (a)  $p_x$ , (b)  $p_y$  with respect to the normalised coordinate  $ct - x$  for LTI and B-TIS3, with  $p_0 = m_e c$  and varying initial transverse position  $y_0$  of the electron. Note that the transverse profile of the laser is centered on  $y = 0$ .

course more interested in the strongly accelerated electrons. Thus the usage of the B-TIS3 method appears better suited to these simulations than the standard LTI.

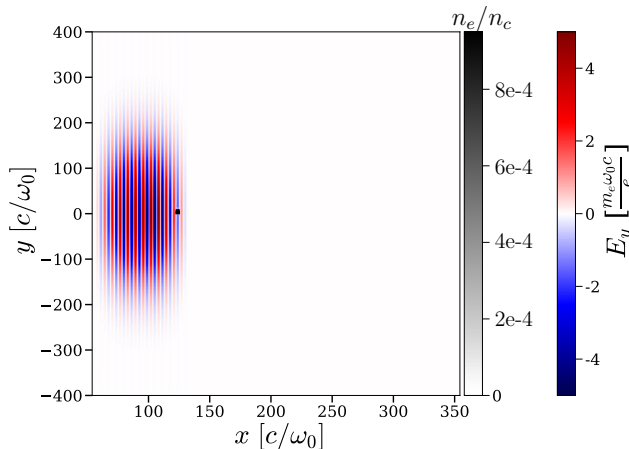


FIGURE 13. Initial situation with a spatially gaussian laser beam and an electron bunch.

## 4. Results for VLA and DLA simulations

### 4.1. VLA simulations

Now that we have determined that B-TIS3 gives more accurate results than LTI for a single electron, we want to simulate a bunch of electrons and see the impact of the different methods on more realistic cases. We thus introduce in our simulation a full electron beam instead of a single particle while keeping the same laser profiles as described in section 3. The initial situation is presented in figure 13. Note that we chose here to initialise the electron beam directly in the laser field so as to maximise electron acceleration. The (2D-) charge of the beam is quite low ( $\approx 4.5 \text{ pC } \mu\text{m}^{-1}$ ) so as to limit space charge effects and both the longitudinal and transverse spatial extensions are chosen to be close to a laser wavelength of 800 nm.

Still comparing results of simulations using either LTI or B-TIS3, in both simulations we observe the electron beam being longitudinally accelerated with the laser ponderomotive force making it gradually blow up. The electrons then exit the laser pulse, mostly through the sides without making it through longitudinally from end to end. Electrons are, however, accelerated for much longer in the B-TIS3 simulation, resulting in the charge being contained in the simulation box for a much longer propagation distance as we can see in figure 14.

Figures 15 and 16 give a comparison of the spatial positions of the electrons within the laser beam as well as their phase space  $(x, p_x)$  for two different time of the simulation. As expected, we can see that the beam is progressively bursting apart due to the laser ponderomotive force. The asymmetry in the explosion of the beam is due to the fact that the electron bunch is initially not exactly on the propagation axis but in fact slightly above it, hence the drift mostly towards positive values of  $y$ . Also, as the electron beam is initially about as long as a laser wavelength, the back-end and the front-end are not in phase. They interact initially with fields of different values - thus feel different forces which explains the progressive separation of the two ends of the beam.

We can see in figures 15.a and 15.b. that the beam is dispersed much more quickly in the simulation using LTI compared to the one using B-TIS3, and it is even more apparent in figure 16.a where there is almost no electron left in the laser beam while the electron bunch is, at the same time, still clearly present in figure 16.b for B-TIS3. The periodic evolution of  $p_x$  that we saw in earlier section is also visible on the map of the  $(x, p_x)$

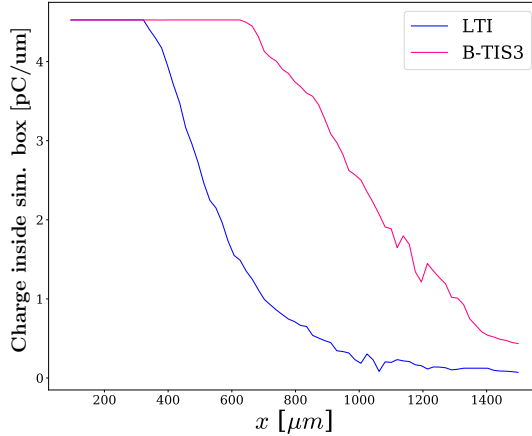
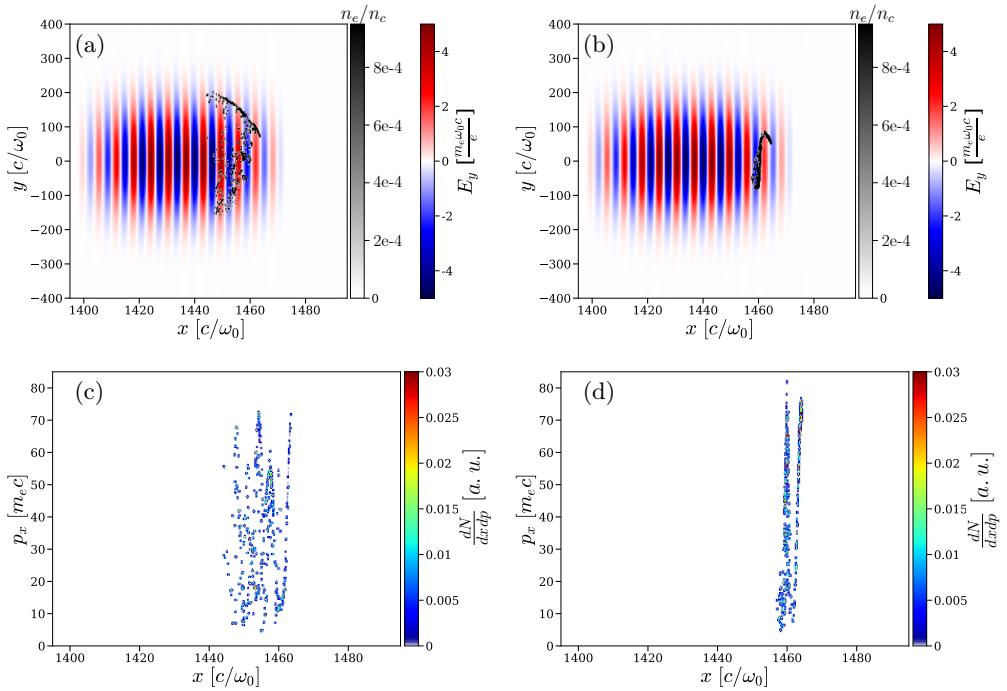


FIGURE 14. Charge inside the simulation box with respect to travelled length.

FIGURE 15. Top: electronic density map (greyscale) superimposed to the electric field  $E_y$  map (colours) after a propagation of  $570 \mu\text{m}$  for (a) LTI and (b) B-TIS3. Bottom: phase space  $(x, p_x)$  after a propagation of  $570 \mu\text{m}$  for (c) LTI and (d) B-TIS3.

phase space, especially in figures 15.d and 16.d. Though this structure is quickly masked in the case of LTI, we can still make it out in figure 15.c.

Figure 17 show a comparison of the electron energy spectrums after two different propagation length. The remaining charge inside the simulation window is much more important in the case of B-TIS3 and reaches higher energies which is coherent with previous observations.

In the end, it appears that B-TIS3 produce results significantly different from LTI. Considering those results and the previous comparison to theoretical models, LTI appears

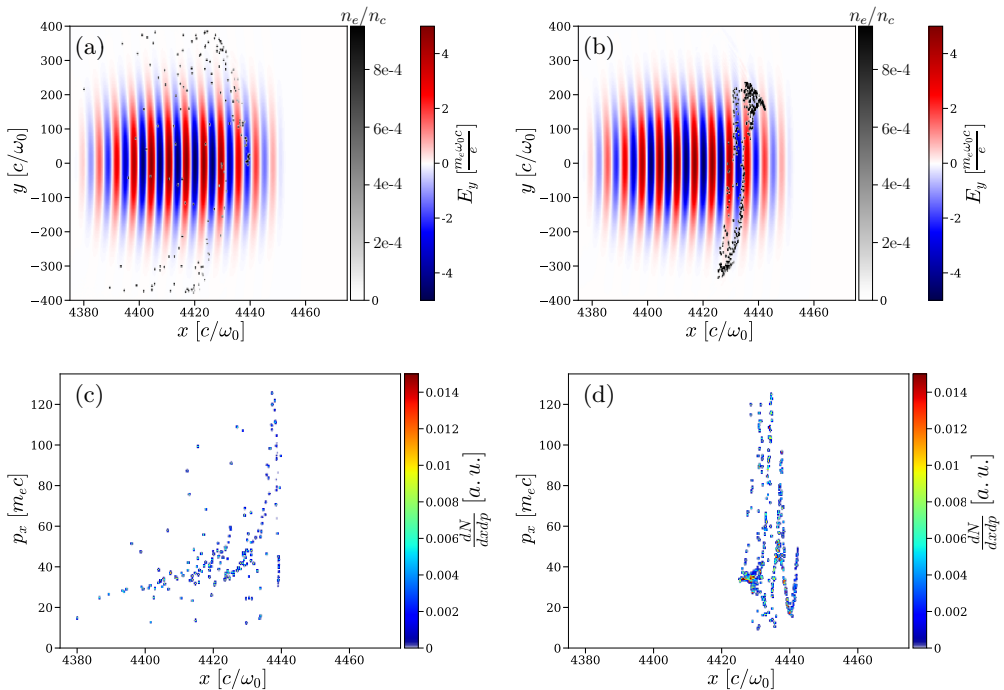


FIGURE 16. Top: electronic density map (greyscale) superimposed to the electric field  $E_y$  map (colours) after a propagation of 950  $\mu\text{m}$  for (a) LTI and (b) B-TIS3. Bottom: phase space ( $x, p_x$ ) after a propagation of 950  $\mu\text{m}$  for (c) LTI and (d) B-TIS3.

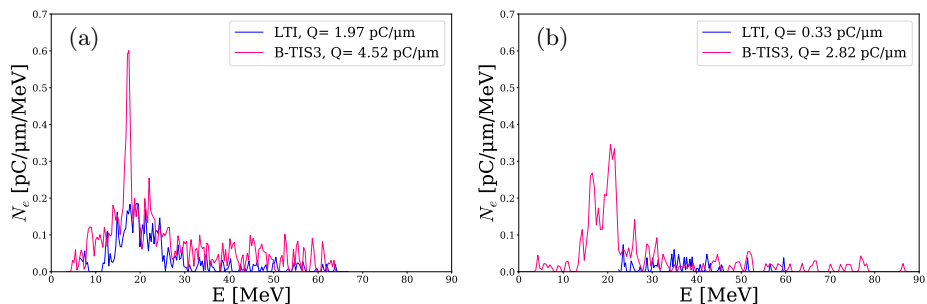


FIGURE 17. Energy spectrum of the accelerated electrons after a propagation of (a) 570  $\mu\text{m}$  and (b) 950  $\mu\text{m}$ .

- barring a prohibitively costly refining of the grid - to not be well suited to the study of VLA though B-TIS3 may be an easy to implement substitute to solve this problem. LTI may indeed lead to an inadequate estimation of the accelerated charge and of the beam energy, two key characteristics in electron acceleration.

#### 4.2. DLA simulations

Investigating the use of B-TIS3 for VLA simulation has allowed us to highlight its improvement compared to LTI. However, as VLA as so far shown to be quite limited as a reliable source of accelerated electrons, it is interesting to also study the use of B-TIS3 in simulations of other acceleration methods.

We already demonstrated the usefulness of B-TIS to mitigate impact of numerical

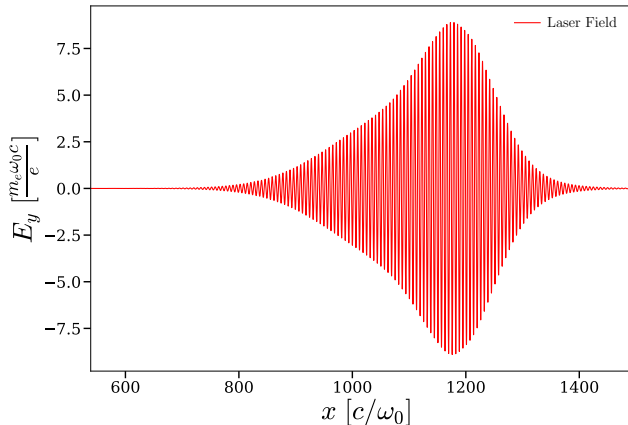


FIGURE 18. Temporal profile of the electric field  $E_y$ .

artefacts such as numerical Cherenkov radiation in LWFA simulations (Bourgeois & Davoine 2020) and those results still apply with B-TIS3. In addition to this, our new interpolation technique B-TIS3 should also bring great improvements to simulations of another situation: Direct Laser Acceleration.

In LWFA, DLA occurs when the laser beam is long enough to encompass part of the bubble where electrons are being accelerated which brings about a coupling between electrons and laser fields (Pukhov *et al.* 1999). Those electrons are then subject not only to the electromagnetic wake fields but also to those of the laser pulse and their energy gain is, in part, due directly to the laser wave and not only to the plasma wave.

To investigate this setting, we performed two 2D simulations (one using LTI, the other B-TIS3), choosing laser and plasma's parameters leading to the creation of a wakefield with efficient electron acceleration but with a purposefully elongated temporal profile for the laser, facilitating interaction between the accelerated electrons and the laser field so as to get DLA. Figure 18 shows the temporal profile of the laser used in the simulation which is made by adding two gaussian temporal profiles with different amplitudes, lengths and delays ( $a_0 = 6$ ,  $\tau = 42$  fs for the first profile, where  $\tau$  is the laser intensity profile FWHM, and  $a_0 = 4$ ,  $\tau = 85$  fs for the second one with a 42 fs delay between the two maximums). This results in an asymmetric temporal profile with duration of around a hundred femtoseconds: the high intensity pulse front generates the wakefield while the low intensity pulse tail fills the back of the bubble and interact with the electron beam as shown in figure 19. This laser profile was specifically designed to favour laser interaction with an accelerated electron beam and DLA in a fast 2D simulation.

This laser is propagating in a 6 mm long and fully ionised plasma with an electron density of  $n_e = 0.0025n_c$ . We used a density gradient injection technique (Bulanov *et al.* 1998; Suk *et al.* 2001; Ekerfelt *et al.* 2017) to facilitate electron injection in the bubble. The simulation is performed inside a moving window of  $6400 \times 400$  cells with  $c\Delta t = 0.149c/\omega_0$ ,  $\Delta x = 0.15c/\omega_0$  and  $\Delta y = 3c/\omega_0$ .

Figure 19 gives an example of DLA in a numerical simulation. As in all LWFA cases, the laser propagating inside the plasma excites a plasma wave in its wake which creates a cavity positively charged in which electrons can be accelerated. The borders of this cavity or bubble are delimited by a higher electron density and easily visible on the greyscale map. A beam of electrons has already been injected and is being accelerated inside of the bubble around  $y = 0$   $c/\omega_0$  and  $x = 20350$   $c/\omega_0$ . The laser oscillations are easily visible

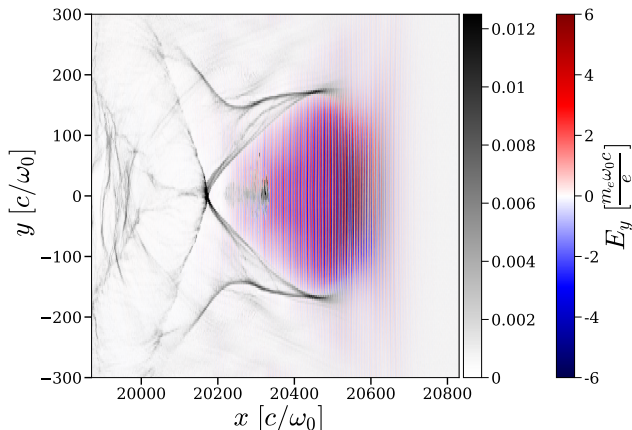


FIGURE 19. Electron density map normalised to the critical density  $n_c$  (greyscale) superimposed to the electric field  $E_y$  map.

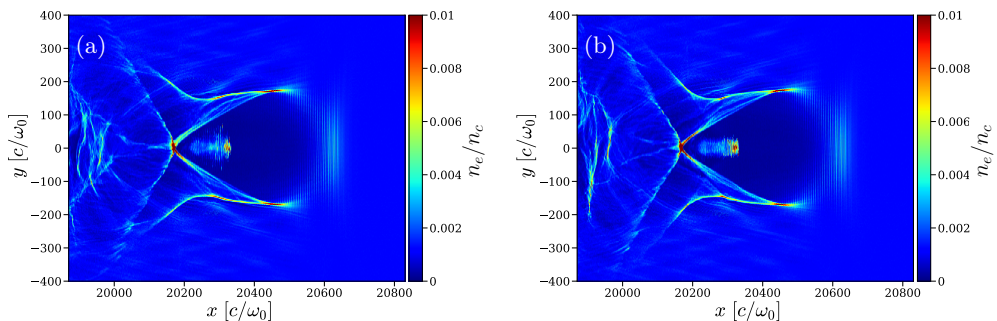


FIGURE 20. Electron density map after 2.65 mm of laser propagation in the plasma: (a) LTI simulation, (b) B-TIS3 simulation.

and present over the whole length of the bubble meaning all of the injected electrons are directly influenced by the laser field.

Both simulations predict the formation of an accelerating bubble in the wake of the laser beam and the injection and subsequent acceleration of a similar charge of electrons. Note that contrary to what was done in our previous paper (Bourgeois & Davoine 2020), B-TIS3 is now applied to all electrons in the simulation, irrespective of their energy.

There are nevertheless significant differences between the two simulations. The electron beam appears much more focused in the B-TIS3 case. This effect is visible directly on the transverse size of the beam as can be seen in figure 20, but also on the transverse momentum of the accelerated electrons as shown in figure 21. It is important to note that numerical Cherenkov radiation is quite weak in those 2D simulations and thus this numerical artefact is not responsible for this variation in beam transverse size and divergence in the way we observed in (Bourgeois & Davoine 2020). In the present case, the difference is indeed due to the improved modelisation of the laser-electron interaction in the B-TIS3 simulation. Comparing the electrons phase space  $(p_x, p_y)$  of both simulations, we can see that both beams have a similar structure but with a much higher dispersion in the LTI case, especially for the transverse momentum of the most energetic electrons. This seems in accordance with previous observations suggesting LTI tends to overestimate  $p_y$



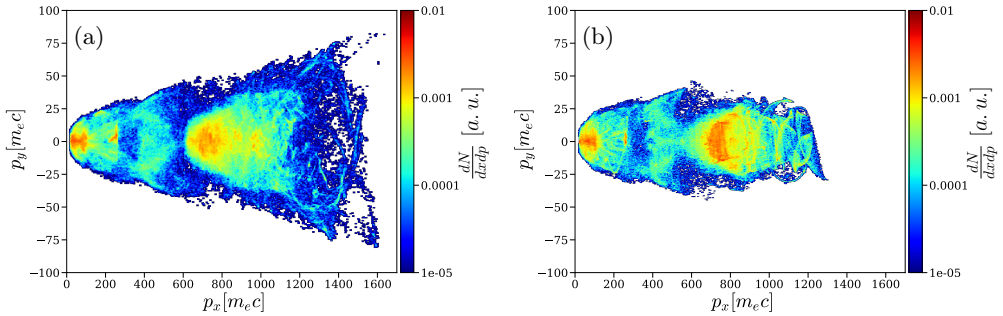


FIGURE 21. Phase space map  $(p_x, p_y)$  after 2.65 mm of laser propagation in the plasma: (a) LTI simulation, (b) B-TIS3 simulation.

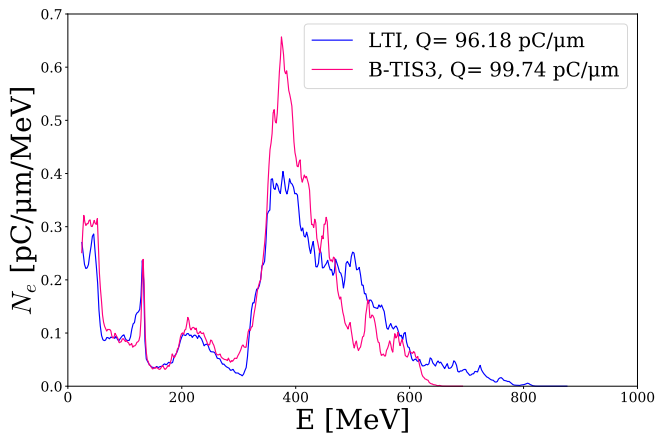


FIGURE 22. Energy spectrum of the accelerated electrons after 2.65 mm of laser propagation in the plasma.

and thus the beam divergence. However, somewhat contrary to what could be expected, LTI also predicts higher longitudinal momentum than B-TIS3 despite the fact that we showed in our previous VLA simulations that LTI tends to underestimate  $p_x$  when B-TIS3 slightly overestimate it. This difference may be explained by the fact that electrons are not accelerated only by laser fields as was previously the case. Direct laser acceleration is the result of a complex coupling between the laser and the plasma fields and a small error on the laser fields effect can lead to an important perturbation of this coupling, leading to the overestimation of both  $p_y$  and  $p_x$ .

Looking at the energy spectrums of both beams (figure 22), we can again observe the previously noted similarities and differences: LTI present a broader spectrum which reaches to higher energies whereas B-TIS3's spectrum is much more peaked.

The overall similarity of those two simulations leads us to think that B-TIS3 does not introduced adverse effects to the modelisation of DLA in our simulation. To the contrary in fact, the previous results on the VLA simulations make us confident in the fact that the modelisation of laser-electron interaction is improved by the use of B-TIS3 over LTI leading to a better reproduction of the electrons behaviour in both VLA and DLA.

Note that DLA simulations presented here had relatively low electronic densities. Simulations with higher densities were also performed and we found that differences between simulations using LTI or B-TIS3 are less and less prevalent with higher electronic

densities ( $n_e \approx 0.01n_c$  or higher) to the point of becoming almost negligible. We can assume that, in those regimes, the plasma impacts the laser propagation sufficiently so that there are real, physical differences in amplitude between the electric and magnetic fields of the laser, making the error on the  $B$  amplitude introduced by LTI negligible.

## Conclusion

In this paper we improved upon the already introduced technique of B-TIS making it more robust and accurate. We then demonstrated its usefulness, not only to mitigate adverse effects of NCR, but also to better model laser-electron interaction phenomena, getting more faithful results, especially in terms of momentum, than the traditional PIC methods. These improvements appear particularly important in the case of VLA simulations or simulations involving DLA with low electron densities where those small differences lead to more realistic values of charge and energy for the accelerated electron beams.

With the benefit of this technique established, it could now be used to study more complex cases of LWFA, DLA, VLA or other situations where electron beam or plasma co-propagates with an electromagnetic pulse in a PIC simulation box. For instance, VLA with radially polarised laser (Zaïm *et al.* 2017), could benefit from this improved modelisation to better understand the polarisation impact and effects of other properties on the acceleration process.

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## Declaration of Interests

The authors report no conflict of interest.

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