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Journal

Plasma Physics and Controlled Fusion, 67(6)

ISSN

0741-3335

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Publication Date

2025-06-30

DOI

10.1088/1361-6587/addc97

Peer reviewed

Modeling laser-wakefield accelerators using the time-averaged ponderomotive approximation in a Lorentz boosted frame

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February 2025

Abstract. Future, high-fidelity simulations of multi-GeV-class Laser Wakefield Accelerators (LWFAs) will need to model the propagation of high-intensity laser drivers over meter-scale plasmas with high spatial and temporal resolutions, thus requiring high amounts of computational resources. Various techniques have been devised over the years to reduce the computational cost of such simulations, including the time-averaged ponderomotive approximation, and the use of the Lorentz boosted frame technique. In this paper we discuss the combination of these two computational techniques, highlighting the resulting significant reduction in the computational cost of LWFA simulations and the limitations of this approach. The combination of the two techniques can potentially become essential for the modeling of a multi-TeV, LWFA-based collider.

Keywords: Laser Wakefield Acceleration, Particle in Cell, Time-averaged ponderomotive approximation, Lorentz boosted frame

1. Introduction

Laser Wakefield Accelerators (LWFAs) [1] have demonstrated the production of electron beams with multi-GeV energies in 10s of cm plasmas [2], bunch durations on the order of femtoseconds [3], charges approaching nanocoulombs [4], normalized emittances $\lesssim 1 \mu\text{m}$ [5], and percent-level rms energy spreads [6], albeit not simultaneously achieved. The rapid development and the properties of LWFAs make them interesting candidates for applications to future compact radiation sources, such as Free Electron Lasers [7, 8, 9], and high-energy particle colliders [10, 11, 12].

In a LWFA, an intense laser pulse propagating in an underdense plasma ponderomotively drives an electron plasma wave (or wakefield) [1]. The plasma wave has a relativistic phase velocity and can support large fields suitable for charged particle acceleration and focusing. Optimal wake excitation requires a laser pulse duration τ_0 such that $c\tau_0 \sim k_p^{-1}$, and a laser peak intensity I_0 such that the corresponding peak normalized laser vector potential, sometimes called field strength, satisfies $a_0^2 \simeq 0.73 I_0 [10^{18} \text{ W/cm}^2] (\lambda_0 [\mu\text{m}])^2 \sim 1$. Here $k_p = (q_e^2 n_0 / m_e c^2 \epsilon_0)^{1/2}$ is the plasma wavenumber ($\lambda_p = 2\pi/k_p$ is the plasma wavelength), n_0 the ambient plasma density, m_e the electron mass, q_e the electron charge, ϵ_0 the vacuum permittivity, c the speed of light, and λ_0 the laser wavelength.

Numerical modeling of LWFAs requires self-consistently solving Maxwell's equations, describing the behavior of the laser and the electromagnetic fields in the wake, coupled to the equations of motion for the plasma particles (electrons, ions, and particle beams) and their interaction with the fields. For instance, Particle-in-Cell (PIC) codes [13] provide a numerical solution to these equations using a spatial grid (mesh) to represent the fields and an ensemble of numerical particles (or macroparticles) to sample the plasma phase-space distribution. In contrast, fluid codes represent on the grid also the average plasma quantities such as density and momentum. Plasma simulation codes are essential tools for deepening our understanding of the LWFA physics, and for designing, analyzing, and optimizing current and future LWFA experiments.

Numerical modeling of LWFAs is a computationally challenging task [14, 15, 16]. For instance, in order to study the production of the high-energy beams required for many LWFA applications, simulation codes need to quickly model the propagation of a laser pulse in plasmas over meter-scales distances. At the same time, they need to correctly represent the plasma dynamics at the scale of the laser wavelength, e.g., plasma

electrons quivering in the laser field, which is typically on the order of the micrometer for solid state lasers. Modeling a LWFA-based collider would require simulating a chain of many of such LWFA stages (e.g., hundreds of stages for a TeV-class collider, assuming a multi-GeV energy gain on each stage). Similarly, simulating the dynamics of multi-GeV beams with nanometer-scale emittances requires adequately resolving the sub-micron transverse size of the bunch. At the same time, one needs to model a spatial domain large enough to contain the wake and the laser, which have a characteristic transverse size of tens to hundreds micrometers. It is worth noting that simulations in 2D Cartesian geometry cannot accurately describe the physics of LWFAs [17], thus 3D or quasi-3D simulations are necessary [18]. Furthermore, the parameter space to explore when optimizing the performance of LWFAs is typically vast. Given the often highly-nonlinear nature of the phenomena being modeled, a fine exploration of this space is often necessary. Recently, machine learning techniques have provided valuable assistance in this task [19, 20, 21].

Start-to-end modeling of LWFAs under realistic conditions generally requires the use of supercomputers. Many high-performance computing techniques, including hybrid MPI/OpenMP parallelization [22] with dynamic load balancing [23] and different domain decompositions for macroparticle and fields operations [24], GPU computing [25, 26, 27, 28, 29], SIMD vectorization [30], and task programming [31] allowed for a more efficient use of modern computer architectures in simulations, thus granting large speed-ups and enabling the analysis of prohibitively complex physical setups.

Modeling of LWFAs can be made more readily available by using reduced physics models that lower the computational complexity of the problem. Models that, for instance, describe the problem using a reduced dimensionality, e.g., the azimuthal Fourier decomposition [18], or use temporally averaged equations for the constituents, e.g., the **time-averaged ponderomotive approximation** [14, 15, 32, 33, 34] (also known as **ponderomotive guiding center approximation** [35, 36, 37]), or use the quasi-static approximation [38, 39, 40, 37, 41, 42], or exploit the descriptions of the problem in an appropriate reference frame, e.g., the Lorentz boosted frame [43, 44], can provide computational speed-ups of orders of magnitude, and thus they are routinely used in the LWFA community.

For example, in the time-averaged ponderomotive approximation (TPA) the equations describing the motion of the plasma particles in the fields due to the laser and the wake are analytically averaged over the fast laser oscillations. The averaging removes

the need to model and resolve the details of particle motion at the laser wavelength scale, and only retains the slow motion associated with the laser envelope and the wakefield (see derivations in Refs. [38, 14]). As a consequence, the longitudinal resolution of a simulation using the TPA can be reduced by a factor $\Omega = \lambda_p/\lambda_0$, compared to the case where motion on the scale of the laser wavelength is resolved. For example, $\Omega \sim 100$ for $\lambda_0 \sim 1 \mu\text{m}$ and a plasma density $n_0 \sim 10^{17} \text{ cm}^{-3}$ (this gives $\lambda_p \sim 100 \mu\text{m}$), which is typical for multi-GeV-class LWFA. If the spatial and temporal resolutions in the simulation obey a Courant-Friedrichs-Lewy condition, i.e., the temporal step scales with the longitudinal resolution, the use of the TPA yields computational speed-ups on the order of $\sim \Omega^2$ (i.e., $\sim 10^4$ for a multi-GeV-class LWFA simulation) compared to simulations where fields on the scale of the laser wavelength are modeled.

Another technique capable of yielding considerable simulation speed-ups consists in performing the simulation in a Lorentz-boosted frame (LBF). Standard LWFA simulations are generally carried out in a reference frame where the plasma is stationary. Performing the simulation in a LBF, i.e., in a reference frame that moves in the same direction of the laser driver with a suitable velocity, can largely reduce the previously mentioned scale unbalance and, hence, significantly decrease the computational complexity of the problem [43, 45]. This is due to the relativistic contraction of the total plasma length and the corresponding dilation of the laser wavelength. This model assumes that backward propagating waves can be neglected. The maximum theoretical speed-up achievable with this technique depends on simulation details such as propagation length and dimension of the computational window. If, for instance, the propagation length corresponds to the laser depletion/dephasing length, and the size of the computational window is set based on to the plasma wavelength, the maximum speed-up can be as high as $\sim 2\Omega^2$. This speed-up, comparable to that achieved with the TPA technique, is attained in a frame moving with a velocity characterized by a relativistic Lorentz factor $\gamma_b \simeq \Omega$ [45].

In this paper, we demonstrate how the TPA and LBF methods can be combined. We show that simulations leveraging the TPA in a boosted frame produce results consistent with those obtained in the laboratory frame. Additionally, we discuss the associated limitations and the achievable speed-ups, which can be as high as $\sim (10 - 100)\Omega^2$, depending on the specific problem being modeled. The combination of the TPA and LBF methods grants significant numerical advantages of interest for the modeling of present and future multi-GeV LWFA stages, and for the modeling of a future, multi-TeV plasma-based

collider. We also discuss how, for both the TPA and the LBF methods, these theoretical speed-ups may not always be achieved, due to another limiting scale, e.g. associated to the accelerated electron bunch, or due to numerical reasons, e.g. the Courant-Friedrichs-Lewy condition dictating the maximum stable timestep of the chosen numerical solvers for the underlying equations.

The article is organized as follows. In Sec. 2 we briefly review the LBF modeling technique. In Sec. 3, we summarize the TPA approach and present an example of validation of this technique. For the validation, we compare the results obtained with the full PIC code SMILEI to those obtained using the TPA as implemented in the codes INF&RNO and SMILEI. This comparison also serves as a benchmark for both codes. In Sec. 4 we discuss the combination of LBF and TPA techniques for the modeling of LWFA. An example of an LWFA stage modeled using both techniques, along with a discussion of the speed-ups, is also provided. Conclusions are presented in Sec. 5.

2. Modeling LWFA using the Lorentz boosted frame technique

In this section, we provide a brief overview of the LBF technique for modeling LWFA.

In a typical LWFA simulation, performed in the reference frame where the plasma is stationary, i.e., the laboratory frame, one needs to model the propagation of the laser driver over the full length of the plasma. This is the maximum spatial scale of interest, and can be meter-scale for multi-GeV-class LWFA stages. Conversely, the minimum scale to be modeled is on the order of the laser wavelength, e.g., micrometer-scale for solid-state lasers, which is the typical scale of electron quivering in the laser field. The large disparity between the scales involved in the description of the LWFA physics is what renders LWFA simulations computationally expensive.

The LBF technique, where the modeling of the LWFA is done in a reference frame that moves in the same direction of the laser, i.e., the boosted frame, allows for a reduction of such scale disparity. This reduction is obtained because the ratio between the relevant maximum and minimum scales of interest is not invariant under Lorentz transformation [43]. Denoting by $c\beta_b$ the velocity of the boosted frame, whose corresponding Lorentz factor is $\gamma_b = 1/\sqrt{1 - \beta_b^2}$, the wavelength of the laser pulse in this frame is elongated by a factor $(1 + \beta_b)\gamma_b$. Besides, the plasma length is contracted by a factor γ_b , resulting in a decrease of the scale disparity. Note that we neglected backward propagating waves, e.g., Raman backscattering, as they are usually not relevant

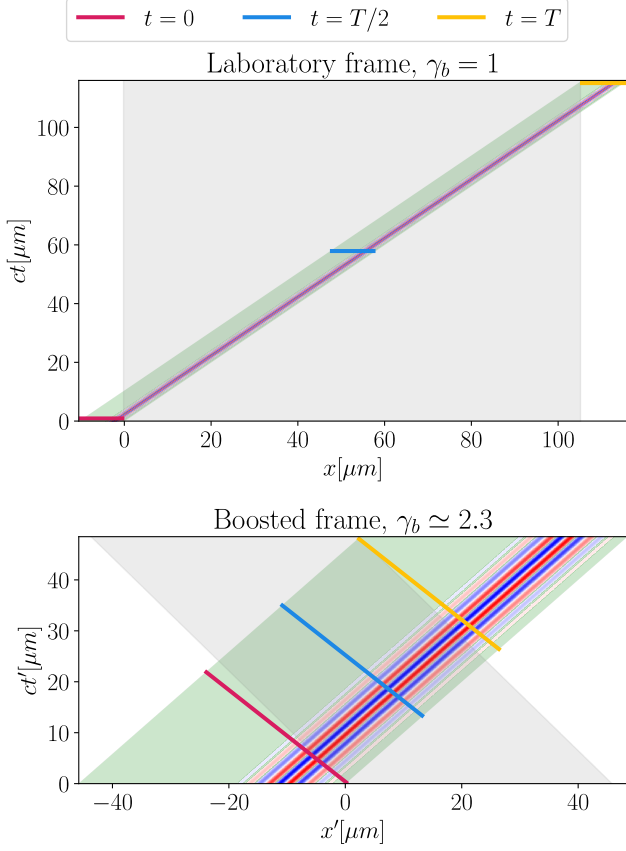


Figure 1. Space-time diagrams in the laboratory frame (top panel) and boosted frame (bottom panel) of a laser pulse propagating in vacuum for a laboratory frame distance L_{prop} , adapted from Fig. 1 of [44]. For the Figure, a 1D Gaussian laser pulse with FWHM duration in intensity in the laboratory frame of 4.45 fs and carrier wavelength $\lambda_0 = 0.8 \mu\text{m}$ has been used (the red-white-blue laser field colormap has been normalized to the interval $[-1, +1]$) in both frames. Note the different scales in the two frames. The green shaded area denotes the space-time region spanned by the simulation moving window, which moves at speed $\beta_w = 1$ in the positive z direction. In the top panel, the gray area corresponds to the space-time region between the vertical line intersecting the right border of the moving window at $t = 0$ and the vertical line intersecting the left border of the moving window at $t = T$. The same space-time region is converted to the boosted frame in the bottom panel and depicted in the gray area of that panel. The interaction time T is defined in both frames as the time needed for the crossing of the moving window and the propagation region. The lines corresponding to $t = 0, T/2, T$ in the laboratory frame correspond to lines of non-simultaneous events in the boosted frame. The moving window size in the laboratory frame is $L_w = 10.5 \mu\text{m}$, the propagation distance is $L_p = 10L_w$ and the Lorentz factor of the boosted frame in bottom panel is $\gamma_b \approx 2.3$. Please note that this choice of γ_b has been done for the sake of illustration and may not be the most suited for the resulting simulation.

in the physics of LWFAs when laser drivers with characteristic spatial extent resonant with respect to the plasma wavelength are used.

The reduction in the scale disparity yields significant computational speed-ups in the modeling of

LWFAs that can be estimated as follows. We assume that in both the laboratory and the boosted frame the modeling is performed in a computational window that moves along with the laser driver, as all the relevant LWFA physics occurs in the region surrounding the laser. We also assume that, in each reference frame, the properties of the moving window, such as its length and resolution, are defined with respect to the laser characteristics in that reference frame. Following a common convention, we will denote with a prime the quantities computed in the boosted frame. The interaction time is equal to the time needed by the trailing border of the moving window to reach the endpoint of the propagation length, as shown in Fig. 1. In the laboratory frame, the endpoint is stationary (top panel of the Figure), while in the boosted frame it moves with a speed $-c\beta_b$ (bottom panel). The length of the moving window and the propagation length in the boosted frame can be derived from the corresponding quantities in the laboratory frame as $L'_w = L_w(1 + \beta_b)\gamma_b$ and $L'_p = L_p/\gamma_b$, respectively. The interaction time in the laboratory frame T and in the boosted frame T' are (see Refs. [43, 46]):

$$cT = \frac{L_p + L_w}{\beta_w}, \quad cT' = \frac{L'_p + L'_w}{\beta'_w + \beta_b}, \quad (1)$$

where $\beta'_w = (\beta_w - \beta_b)/(1 - \beta_b\beta_w)$ is the moving window normalized velocity in the boosted frame. We assume that the spatial and temporal scales associated with the laser wavelength are the smallest scales to be modeled, and are sampled with the same number of points in the z direction in the laboratory and in the boosted frames. Hence, the longitudinal spatial resolution and the temporal step satisfy $\Delta z' = (1 + \beta_b)\gamma_b\Delta z$, and $\Delta t' = (1 + \beta_b)\gamma_b\Delta t$, respectively, i.e., $\Delta t/\Delta z = \Delta t'/\Delta z'$. The number of temporal steps N (N') for a simulation in the laboratory (boosted) frame can be obtained by dividing the interaction time T (T') by the temporal step Δt ($\Delta t'$). Using the interaction times in Eq. (1), and assuming that the moving window moves at the speed of light, i.e., $\beta_w = \beta'_w = 1$, the ratio between the number of temporal steps in the two frames, N/N' , can be expressed as a function of only L_p/L_w and the boost,

$$\frac{N}{N'} = \frac{L_p/L_w + 1}{L_p/L_w + (1 + \beta_b)\gamma_b^2} (1 + \beta_b)^2 \gamma_b^2. \quad (2)$$

It is worth noting that LWFA simulations typically use a moving window that travels at (or very near) the speed of light. This choice prevents spurious electromagnetic radiation from entering at the front of the computational window, and keeps relativistic particles from escaping at the back. A more general expression for N/N' , that does not make the assumption $\beta_w = \beta'_w = 1$, can be found in [45].

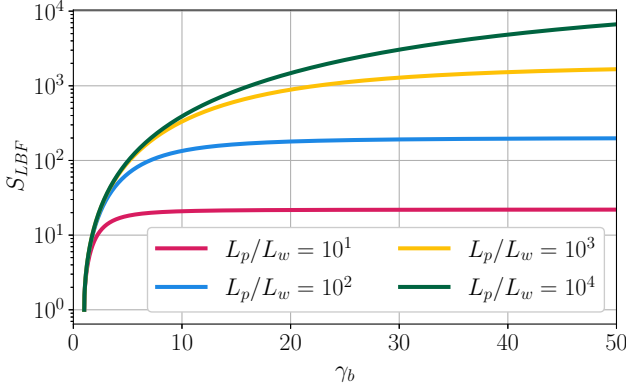


Figure 2. Theoretical speed-up $S_{LBF} = N/N'$ using Eq. (1), $N = T/\Delta t$ and $N' = T'/\Delta t'$, assuming $\beta_w = \beta'_w = 1$.

Neglecting details concerning, e.g., the definition and initialization of the macroparticles when setting up PIC simulations in different reference frames, and since the number of grid points in the z direction is the same in both reference frames, the N/N' ratio in Eq. (2) gives a measure of the speed-up provided by the LBF technique, namely

$$S_{LBF} = \frac{N}{N'}. \quad (3)$$

In Fig. 2 we plot S_{LBF} as a function of γ_b for different values of L_p/L_w . The maximum theoretical speed-up is $(S_{LBF})_{max} \simeq 2(1 + L_p/L_w)$, achieved in the limit $\gamma_b \rightarrow \infty$. However, there is no real computational advantage in considering an arbitrarily large boost velocity since, assuming $L_p/L_w \gg 1$, already for $\gamma_b \gtrsim \gamma_{b,\eta}^*$, where

$$\gamma_{b,\eta}^* \simeq \left[\frac{L_p}{2L_w} \frac{\eta}{1-\eta} \right]^{1/2}, \quad (4)$$

the speed-up is a fraction $\eta \sim 1$ (we consider $\eta = 0.9$ in this work, hence $\gamma_{b,\eta=0.9} \simeq 2.1(L_p/L_w)^{1/2}$) of the maximum speed-up. We refer to $\gamma_{b,\eta}^*$ as the optimal boost factor. For a low boost velocity, i.e. $\gamma_b \ll \gamma_{b,\eta}^*$, the speed-up is $S_{LBF} \simeq (1 + \beta_b)^2 \gamma_b^2$. Under this condition, increasing γ_b yields theoretically a significant increase in the speed-up, given its almost quadratic dependence on γ_b . The optimal boost factor scales with the propagation length and moving window length. If the plasma length is on the order of the depletion/dephasing length, $L_p \approx \lambda_p^3/\lambda_0^2$, and the moving window length scales with the plasma wavelength, $L_w \approx C\lambda_p$, where $C \gtrsim 1$, the optimal boost factor is, within multiplicative factors on the order of the unity, $\gamma_b^* \approx \lambda_p/\lambda_0 = \Omega$. As already noted in Ref. [45], for this choice of L_p and L_w the optimal boost factor corresponds to the relativistic factor of the wake, and the corresponding speed-up is $S_{LBF} \approx 2(\lambda_p/\lambda_0)^2 = 2\Omega^2$. For instance, $\Omega \sim 100$

for $\lambda_0 \sim 1 \mu\text{m}$ and a plasma density $n_0 \sim 10^{17} \text{ cm}^{-3}$, typical of multi-GeV LWFA stages, resulting in a theoretical speed-up $\gtrsim 10^4$.

Beyond the theoretical considerations outlined above, the maximum boost velocity that can be used in any given LWFA simulation depends on the details of the problem being modeled and is determined by various considerations related to, e.g., numerical convergence of the results. For instance, some kinetic aspects of physics, such as self-injection, are notoriously difficult to model in LBF simulations [44, 47] and numerical artifacts such as the **numerical Cherenkov instability** [48, 49] affect the results when the boost velocity is high. In particular, this instability has been approached through e.g. digital filtering [47, 50], modified finite-differences Maxwell solvers [51, 52, 53, 54], spectral or pseudo-spectral Maxwell solvers [55, 56, 44] or modifications in the interpolation of the fields acting on the macro-particles [57, 58]. We also note that longitudinal gradients in the background plasma distribution are enhanced for large boost velocities. Correctly resolving them in the boosted frame when the boost velocity is high might require to significantly increase the longitudinal resolution which, in turn, will increase the cost of the simulation and reduce the advantages associated with running the simulation in a boosted frame. Finally, another factor that should be considered in the choice of the boost velocity is that the dilated longitudinal resolution in the boosted frame can exceed the transverse resolution for sufficiently high values of the boost velocity. If the electromagnetic field solver used in the simulation is subject to a Courant-Friedrichs-Lewy condition, the size of the temporal step in the boosted frame will be constrained by the transverse resolution, rather than being determined by the temporal resolution in the laboratory frame as assumed in the derivation of Eq. (2) (i.e., $\Delta t' \sim \Delta x'_\perp/c < (1 + \beta_b)\gamma_b\Delta t$, where $\Delta x'_\perp = \Delta x_\perp$ is the transverse resolution). The actual value of the boost velocity, $\gamma_{b,max}$, where this effect becomes important depends on the details of the electromagnetic solver being used. A rough estimate can be given by solving $\Delta z' = (1 + \beta_{b,max})\gamma_{b,max}\Delta z \sim \Delta x_\perp$, which gives

$$\gamma_{b,max} \sim \frac{1}{2} \frac{\Delta x_\perp}{\Delta z}. \quad (5)$$

This effect increases N' (N remains the same) and, hence, reduces the computational gains provided by the LBF method. Development of special solvers that can overcome this limitation has been considered [59].

Initializing an LWFA simulation in the boosted frame, when initial conditions for the laser and particles are known in the laboratory frame, and retrieving the desired output diagnostics in the laboratory frame from a boosted frame simulation are complex tasks. This complexity arises from the loss

of simultaneity between the laboratory and boosted frames. For example, the horizontal lines in the Fig. 1 (top panel) represent the positions of the grid point data of three possible outputs at the start ($t = 0$), halfway ($t = T/2$), and at the end ($t = T$) of a laboratory frame simulation. Each of these lines is made of simultaneous points in the laboratory frame. As explained in [44], to obtain the same data, i.e., simultaneous in the laboratory time, from a boosted frame simulation, it is necessary to save sparse data points at different time steps, shown in the corresponding lines in the bottom panel obtained through Lorentz transformations.

The accuracy and reliability of the LBF method for modeling LWFAs has been extensively investigated in the past several years [47, 60, 44, 61], demonstrating its effectiveness as a robust and widely adopted computational technique in plasma physics.

3. Modeling LWFAs using the time-averaged ponderomotive approximation technique

In this section, we provide a brief overview of the TPA technique for modeling LWFAs.

In the TPA, the equations describing the motion of the electrons in the fields of the laser and the wake are analytically averaged over the fast laser oscillations. This approximation is justified by the fact that laser pulse drivers in a LWFA have a length $c\tau_0 \sim k_p^{-1}$, i.e., resonant with the plasma, that is typically much longer than the laser wavelength, and so the quivering motion of the background plasma electrons in the laser field does not couple with the wake dynamics at the scale of the plasma wavelength. Within the TPA the laser is described using the slowly-varying complex envelope $\tilde{A}(\mathbf{r}, t)$, of the transverse laser vector potential. We consider a laser propagating along the z direction and linearly polarized along x , namely

$$A_x(\mathbf{r}, t) = \text{Re}\{\tilde{A}(\mathbf{r}, t) \exp[ik_0(z - ct)]\}, \quad (6)$$

where $k_0 = 2\pi/\lambda_0$, $\mathbf{r} = (x, y, z)$ is the position vector, and t the time. The remaining components of the laser vector potential are set as $A_y = 0$, and A_z is determined in accordance with the Coulomb gauge condition, so the laser field is completely determined by the knowledge of $\tilde{A}$.

The evolution equation for the slowly-varying laser envelope is [1, 62, 15]

$$\nabla^2 \tilde{A} + 2ik_0 \left(\frac{\partial}{\partial z} + \frac{1}{c} \frac{\partial}{\partial t} \right) \tilde{A} - \frac{1}{c^2} \frac{\partial^2 \tilde{A}}{\partial t^2} = \chi \tilde{A}, \quad (7)$$

where

$$\chi = \frac{n_e q_e^2}{\varepsilon_0 m_e c^2 \bar{\gamma}}, \quad (8)$$

is the plasma susceptibility, which determines the effect of the plasma on the laser evolution, such as self-focusing, guiding by a plasma channel, etc. Here n_e is the local plasma electron density, and

$$\bar{\gamma} = \left(1 + \frac{q_e^2 |\tilde{A}|^2}{2m_e^2 c^2} + \frac{|\mathbf{p}|^2}{m_e^2 c^2} \right)^{1/2}, \quad (9)$$

where the first term accounts for the fast quivering of background plasma electrons in the laser field, and $\mathbf{p}$ is the slow local fluid electron momentum. Discussion of the limits of validity of Eq. (7) can be found in Refs. [38, 1, 62]. The second order time derivative in the left-hand-side of Eq. (7) is neglected in most codes that use the TPA [14, 38, 35, 63]. Here it is retained since it improves the description of a depleted laser pulse, and it ensures the exact Lorentz covariance of Eq. (7).

A time-explicit numerical scheme to solve Eq. (7) in Cartesian geometry is reported in Ref. [15]. These schemes can be easily parallelized with standard domain decomposition techniques. A time-implicit solution for Eq. (7), which enables the use of time-steps much larger than those in explicit schemes, is discussed in Ref. [62]. Note that since Eq. (7) is second order in time, its numerical integration requires the knowledge of the envelope field at $t = 0$, i.e., the initial condition of the laser field, and at the previous timestep $t = -\Delta t$. Alternatively, the envelope field and its temporal derivative at $t = 0$ can be used. If an exact, time-dependent analytical description of the laser field for initialization at $t = 0$ and $t = -\Delta t$ is not available, e.g., when the initial laser profile is derived from a measurement, an approximation for the envelope field at $t = -\Delta t$ can be obtained from the one at $t = 0$ by using Eq. (7) in the paraxial limit. This requires $k_0 Z_R \gg 1$, where Z_R is the characteristic Rayleigh range of the laser pulse, $Z_R = k_0 w_0^2/2$ for a laser with a transverse Gaussian mode of size w_0 , and assuming that the laser is initially in vacuum. Using a first-order temporal back extrapolation we obtain

$$\begin{aligned} \tilde{A}(t = -\Delta t) &\simeq \tilde{A}(t = 0) \\ &- \left[\frac{i}{2k_0} \nabla_\perp^2 \tilde{A}(t = 0) - \frac{\partial \tilde{A}(t = 0)}{\partial z} \right] c\Delta t, \end{aligned} \quad (10)$$

where $\nabla_\perp^2 = \partial_x^2 + \partial_y^2$ is the transverse portion of the Laplace operator.

The relativistically invariant Lorentz force that the laser exerts on plasma electrons, when averaged over the rapid laser oscillations, corresponds to the averaged ponderomotive force, which can be expressed as

$$\mathbf{F}_P = -\frac{q_e^2}{4m_e \bar{\gamma}} \nabla |\tilde{A}|^2. \quad (11)$$

When solving the equations of motion for the plasma particles, this contribution must be added to that of the Lorentz force from the wakefield. Note that, for typical LWFA parameters, background ions can be considered at rest, but the equations presented here can be easily generalized in the case of mobile ion species.

As mentioned earlier, when describing the laser-plasma interaction with the TPA particle motion and plasma/field structures on the scale of the laser wavelength are not modeled, and only the slow dynamics associated with the laser envelope and the wakefield are considered. This results in a reduction of the longitudinal resolution by a factor $\Omega = \lambda_p/\lambda_0$ compared to simulations where no approximations on the field structure are made. If the temporal step is determined by the longitudinal spatial resolution through the Courant-Friedrichs-Lewy condition of the electromagnetic field solver, the temporal resolution is also reduced by a factor Ω . This is typically the case if $\Delta z \lesssim \Delta x_\perp$. Hence, the theoretical speed-up provided by the TPA is

$$S_{TPA} \simeq \Omega^2. \quad (12)$$

For instance, for a multi-GeV LWFA stage with $\Omega \sim 100$, $S_{TPA} \sim 10^4$, comparable to the speed-up provided by the LBF technique.

The accuracy and reliability of the TPA method was established by comparing the dynamics of plasma particles and the wake properties obtained with the TPA to those obtained in the case of non-averaged particle dynamics, where the particle quiver motion in the laser field is described without approximation, computed using a standard PIC code [34]. It was found excellent agreement between TPA and non-averaged results in a broad range of laser-plasma parameters relevant for present and future LWFA experiments, namely $c\tau_0 \gtrsim 2\lambda_0$, $w_0 \gtrsim 3\lambda_0$, where w_0 is the laser spot size, and $a_0 \lesssim 10$. Additionally, it was observed that the computational savings provided by the TPA can indeed be larger than the simple estimate Ω^2 , in particular when the laser field is intense ($a_0 \gtrsim 1$). This is due to the particularly slow convergence of conventional PIC codes based on second-order numerical schemes that rely on spatial and temporal staggering of the electromagnetic fields, when modeling particle oscillations in the laser field [64, 65].

Although codes using the TPA do not model the laser field at the scale of the laser wavelength, it has recently been shown that tunnel ionization physics in LWFAs can still be included. This can be done by reconstructing the complete laser field in the vicinity of the laser peak where ionization occurs [66], or by employing averaged ionization rates and electron momentum initialization which do not require the reconstruction of the laser field [67, 68, 69].

Finally, we recall that in simulation codes that

use the quasi-static approximation [38, 39, 33, 37, 70] LWFA physics can only be modeled using an envelope description for the laser and the TPA. This results from the limitations of the quasi-static approximation, which cannot model the propagation of electromagnetic waves, i.e. the propagation of the laser field. An advanced quasi-static approximation, which removes this limitation, has been described recently in Ref. [71].

3.1. Comparing the modeling of a guided LWFA stage with and without the TPA.

In this subsection we present a comparison between the simulation results obtained with the PIC code SMILEI [22] with and without TPA, and with those obtained with the code INF&RNO using the TPA in hybrid mode [32, 72, 73]. In the hybrid mode a relativistic cold fluid description is used for the background plasma, while a PIC description is used for the particle bunch. While the computational cost of a hybrid simulation is comparable to that of a conventional PIC simulation with one particle per cell, employing a cold fluid description for the plasma has the advantage of eliminating the need for interpolation in describing plasma dynamics, thereby significantly reducing spurious numerical effects. However, only linear or moderately nonlinear LWFA regimes can be described with this modality.

The numerical schemes used to simulate the considered case study are detailed in Appendix A. We consider the propagation of a laser pulse in a plasma channel, with the acceleration of an externally injected electron beam. This type of simulations is of interest for the design of a staged accelerator [74, 75, 11]. Taking advantage of the problem's symmetry, simulations are run in 2D $r - z$ geometry.

The input laser driver is defined via the amplitude of the transverse normalized laser vector potential, defined as $a(r, z, t = 0) = q_e \tilde{A}(r, z, t = 0)/m_e c = a_0 \exp[-(z - z_{laser})^2/c^2\tau_0^2] \exp(-r^2/w_0^2)$, where r is the (transverse) radial coordinate, and z the (longitudinal) coordinate in the propagation direction. The laser pulse, linearly polarized in the x direction and whose focal plane is at the plasma entrance, has a carrier wavelength $\lambda_0 = 0.8 \mu\text{m}$, waist $w_0 = 41 \mu\text{m}$, initial duration $\tau_0 = 68 \text{ fs}$, initial peak normalized field strength $a_0 = 1$, and initially longitudinal position $z_{laser} = 0$.

The pre-formed plasma channel where the laser pulse propagates has an initial electron density distribution $n_e(r, z)$ constant in the longitudinal direction. In the radial direction, the channel has a

radially parabolic profile defined as

$$n_e(r, z) = n_0 \left[1 + \frac{4r^2}{k_p^2 R^4} \right], \quad (13)$$

where the on-axis density is $n_0 = 2.7 \times 10^{17} \text{ cm}^{-3}$. This gives $\lambda_p = 64 \text{ } \mu\text{m}$, and so $\Omega = \lambda_p/\lambda_0 = 80$. We choose $R = w_0$, following the matched condition for the laser guiding in the low-power and low-intensity limit [1].

A relativistic electron bunch is externally injected in the laser wakefield for acceleration. The electron bunch has a Gaussian charge density distribution, initial rms sizes $\sigma_z = 1 \text{ } \mu\text{m}$ and $\sigma_x = \sigma_y = 3 \text{ } \mu\text{m}$ in the longitudinal and radial directions, respectively, charge $Q = 0.65 \text{ pC}$, initial Lorentz factor $\gamma_0 = 10$, and no initial energy spread. The electron bunch initial longitudinal position z_{bunch} is set to satisfy $z_{\text{laser}} - z_{\text{bunch}} = 102 \text{ } \mu\text{m}$, which places the bunch in the second plasma oscillation behind the laser driver. The bunch is injected at waist and with initial normalized emittance and transverse momentum rms values matched to the actual transverse field in the wakefield [76], i.e. $\epsilon_x = 0.69 \text{ } \mu\text{m}$, $\sigma_{p_x} = 0.23 \text{ } m_e c$, respectively.

For the set of laser and plasma parameters under consideration, the wakefield is excited in the weakly nonlinear regime. Therefore, the depletion length is much larger than the dephasing length ($L_d \approx \pi k_0^2/k_p^3 = 20.5 \text{ cm}$), which becomes the limiting distance for the electron bunch acceleration.

To show the coherence of the results of two different implementations of the TPA and its coupling with the hybrid-fluid model for the INF&RNO simulation in this LWFA case, three simulations in the laboratory frame with different combinations of models, and related numerical schemes, are shown. The first simulation is performed with INF&RNO using the TPA in a hybrid PIC-fluid mode [32, 72, 73, 62]. The second and third simulations are performed with the full PIC code SMILEI [24] with and without the TPA. The SMILEI simulation without TPA is performed in cylindrical geometry with azimuthal modes decomposition, using two azimuthal modes [18]. The INF&RNO and SMILEI with TPA are performed in cylindrical symmetry, which is equivalent to using only one azimuthal mode.

Figure 3 shows the evolution of the peak normalized laser field strength, and of the electron bunch kinetic energy, kinetic energy spread, transverse rms size σ_x , and transverse momentum rms σ_{p_x} , obtained with the three simulations. See Appendix B for details on the calculation of the peak normalized field strength in a simulation that does not use the TPA. Despite the differences in the models and numerical schemes used by the two codes, we observe a remarkable agreement.

The residual differences in the results are coherent

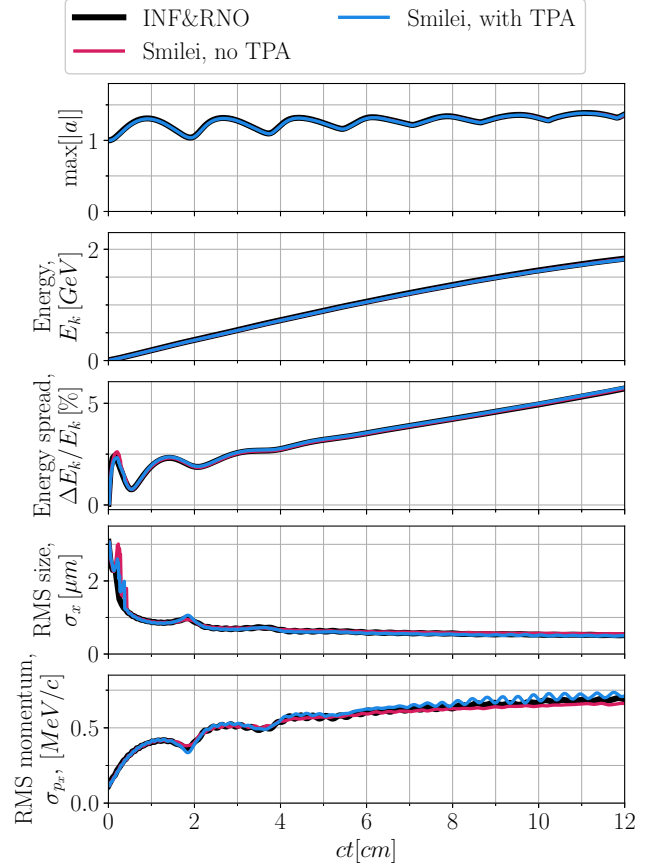


Figure 3. Comparison of the peak absolute value of the normalized envelope $a(r, z, t)$ and bunch parameters evolution obtained in the laboratory frame with INF&RNO in hybrid mode and SMILEI, with and without TPA. From top to bottom, the panels report the evolution of $\max[|a|]$, the bunch kinetic energy E_k , relative rms kinetic energy spread $\Delta E_k/E_k$, rms size σ_x along the transverse coordinate x , σ_{p_x} rms of the transverse momentum p_x .

with those observed in previous comparisons between PIC simulations without TPA, and simulations using the TPA, with and without a hybrid PIC-fluid model, performed with the codes INF&RNO, Smilei and ALaDyn [15, 75, 32, 77]. The agreement between the results with TPA and those without TPA shows that the TPA provides a reliable description of LWFA physics in the chosen regime of parameters, consistently with earlier works [78, 52, 15, 34]. Furthermore, this benchmark shows that both the implementations of the TPA in INF&RNO and SMILEI are coherent with the results obtained without TPA. In the next section, INF&RNO is used to test the validity of the TPA in simulations using the LBF technique.

4. Modeling LWFA in a Lorentz boosted frame using the time-averaged ponderomotive approximation

LBF and TPA are both well-established techniques for the modeling of LWFA [74, 79, 19]. Although, in general, the two methods are not used together, it is possible to combine them provided that the description used for the TPA is Lorentz covariant, i.e., the evolution equation for the slowly-varying laser envelope must contain the second order time derivative, as discussed in Sec. 3. If this is the case, the TPA technique can straightforwardly be integrated in a simulation code that uses the LBF technique, since no change to the structure of the TPA equations and algorithm is needed. All the input and output routines follow the same procedures used in a conventional LBF simulation, as described in Sec. 2. The field $a(z, t)$ is a transverse vector potential and so its values in the boosted and laboratory frames satisfy $a'(z', t') = a(z, t)$, where the coordinates (z, t) and (z', t') are related by a Lorentz transformation since the direction of the boost is in the same direction of propagation as the laser. In evaluating the plasma susceptibility Eq. (8) in the boosted frame one needs to consider that the bulk of the plasma is moving towards the laser with velocity $-c\beta_b$, and the unperturbed plasma density is γ_b times higher than in the laboratory frame due to relativistic contraction. Finally, the central laser wave number k_0 in Eq. (7) must be Doppler-shifted, and its value in the boosted frame is

$$k'_0 = \gamma_b(1 - \beta_b)k_0. \quad (14)$$

The initialization of the envelope field at $t' = -\Delta t'$ required to solve Eq. (7) in the boosted frame can be done using the same technique described in Eq. (10) of Sec. 3, evaluated in the boosted frame. Note, however, that for this initialization to be valid the paraxial approximation must be satisfied in the boosted frame, i.e., $k'_0 Z'_R \gg 1$, where Z'_R is the Rayleigh range in the boosted frame ($Z'_R = k'_0 w_0'^2/2$ for a laser with a transversely Gaussian mode of size $w'_0 = w_0$, and so $Z'_R = \gamma_b(1 - \beta_b)Z_R$). This poses a limit on the maximum usable value for γ_b since the Rayleigh range of a given laser pulse becomes shorter the larger is γ_b . This limitation can be removed by using in the derivation of Eq. (10) an operatorial expansion for the wave equation that goes beyond the paraxial approximation, e.g. the expansion described in [80, 78]. Similarly, if the initialization is performed using an analytical expression for the fields, this expression must be a solution of the full wave equation.

As mentioned in Sec. 3, the validity of the TPA, i.e., the error associated with the averaging of the particle dynamics over the scale of fast

laser oscillations, has been investigated only in the laboratory frame. However, since the whole TPA formalism represented by Eqs. (7), (8), (9), and (11) is exactly Lorentz invariant, we expect the averaging to be valid also in the boosted frame. Hence, if the laser and plasma parameters considered in the modeling are such that the TPA is applicable in the laboratory frame, we expect it to be applicable also in the boosted frame.

Since LBF and TPA are independent techniques, the speed-up achieved by combining them is the product of the speed-ups of the two methods. However, to determine the effective computational gain that can realistically be obtained one must account for the constraints on the maximum boost velocity discussed in Sec. 2, which can be more restrictive for a code utilizing the TPA compared to one without such approximation. In fact, LWFA simulation codes that model the complete laser field are typically characterized by grids with $\Delta z \ll \Delta x_\perp$, with Δt determined by Δz via the Courant-Friedrichs-Lewy condition. Hence, a large relativistic factor can be employed before reaching, in the boosted frame, the condition $\Delta z' > \Delta x'_\perp$ (see Eq. (5)), where $\Delta t'$ becomes constrained by $\Delta x'_\perp$ rather than being determined by $\Delta z'$, resulting in a reduction of the computational gain compared to that given in Eq. (3). On the other hand, in a simulation with TPA the computational grid is such that $\Delta z \lesssim \Delta x_\perp$, and so Eq. (5) implies the maximum boost velocity that can be utilized is lower than in a simulation that does not employ the TPA. In general, the maximum boost velocity will likely be smaller than the optimal velocity given by Eq. (4), and so an estimate for the speed-up combining LBF and TPA is

$$S_{TPA+LBF} \approx (1 + \beta_b)^2 \gamma_b^2 \Omega^2, \quad (15)$$

with $\gamma_b \lesssim (\Delta x_\perp / \Delta z) / 2$. Here $\Delta x_\perp$ and Δz refer to the grid employed in the TPA simulation. It should be emphasized that, even if the optimal boost velocity cannot be used, substantial speed-ups of $\sim 10-100$ can still be attained with very moderate boost velocities (e.g., $\gamma_b \lesssim 5$). For instance, for a multi-GeV LWFA stage with $\Omega \sim 100$ ($\lambda_0 \sim 1 \mu\text{m}$), and using $\gamma_b = 5$ we have $S_{TPA+LBF} \gtrsim 10^6$.

For the sake of comparison, neglecting the requirements on the resolution given by the presence of the accelerated electron bunch, an estimate of the speed-up of the quasi-static approximation in the same conditions is $S_{QSA} = S_{\Delta z} S_{\Delta t} \sim \Omega^3 \sim 10^6$. The factor $S_{\Delta z} \sim \Omega$ is given by the coarser spatial resolution for the laser pulse description in the comoving coordinate, while $S_{\Delta t} \sim \lambda_0 / Z_R \sim \Omega^2$ is given by the coarser time resolution for the laser pulse evolution. Despite having a larger speed-up compared to that of Eq. (15), the quasi-static approximation suffers some limitations

compared to the TPA in the LBF. For example, in the blow-out regime of LWFA the plasma behavior close to the end of the plasma wave period is not correctly described in presence of density gradients, although the advanced quasi-static approximation described in Ref. [71] slightly mitigates the errors of a purely quasi-static approach. Even with these improvements, the injection of plasma particles in the plasma waves in a quasi-static approach is possible only through the promotion of quasi-static macro-particles (or jets [71]) to standard PIC macro-particles. Presently, these approaches do not quantitatively reproduce the trapped charge and energy spectrum shape obtained in PIC simulations that do not use the quasi-static approximation [81, 82]. Finally, the transition between vacuum and plasma, which may become relevant for the study of high-energy LWFA stages with external injection, cannot be modeled at all with quasi-static approaches. Neither of these limitations is present in the TPA and LBF approaches.

In the following the same scenario described in subsection 3.1 is used to analyze the performance of a TPA simulation in the boosted frame. The results of various simulations with the hybrid mode of INF&RNO using the LBF with increasing γ_b will be shown. The simulations have been carried out up to a propagation distance of 20 cm.

Figure 4 reports the comparison between the longitudinal electric field E_z , normalized to the cold wavebreaking field $E_0 = m_e c \omega_p / q_e \approx 50$ GV/m, and the laser vector potential absolute value a on the laser propagation axis after 5.09, and 19.3 cm of propagation, in the laboratory frame (black line) and for $\gamma_b = 20, 39$ (red and blue lines, respectively). For the chosen Lorentz factors, the differences in the results are below 1%, hence not distinguishable in the plots.

Figure 5 reports a comparison of the electron density and of the laser vector potential absolute value, $|a|$, on the $z - y$ plane, showing also the position of the bunch macroparticles with red dots, after 19.3 cm of propagation, obtained in the laboratory frame (top half panel) and in the boosted frame with $\gamma_b = 39$ (bottom half panel). An excellent agreement is found as well.

Figure 6 shows a comparison of the evolution of the peak absolute value of the envelope a , and the bunch kinetic energy, kinetic energy spread, transverse rms size σ_x and transverse momentum rms σ_{p_x} , obtained in the laboratory frame (black line) and with $\gamma_b = 10, 20, 30, 39$ (colored lines). In the scales of interest for the acceleration process, the differences between the results of the shown simulations are well below 1%, even for parameters notoriously sensitive such as the electron bunch energy spread and its transverse momentum rms.

Finally, Figure 7 shows, in the top and bottom

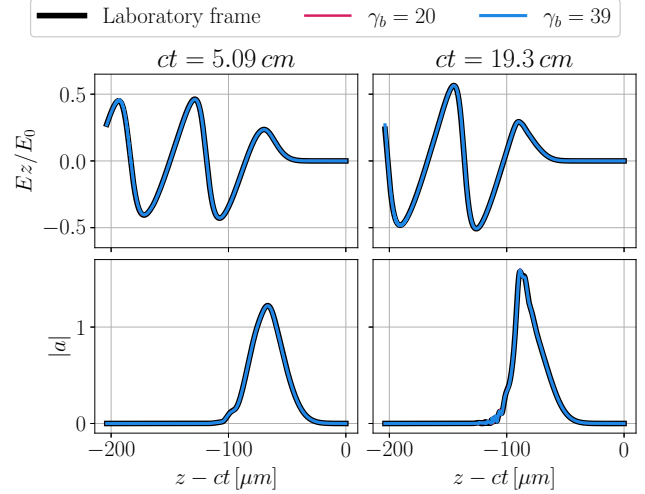


Figure 4. Comparison of E_z/E_0 and $|a|$ on the propagation axis for laboratory frame ($\gamma_b = 1$) and $\gamma_b = 20, 39$, at different times. Left panel: $ct \approx 5.09$ cm; Right panel: $ct \approx 19.3$ cm. The plots show negligible differences in the fields between the different simulations.

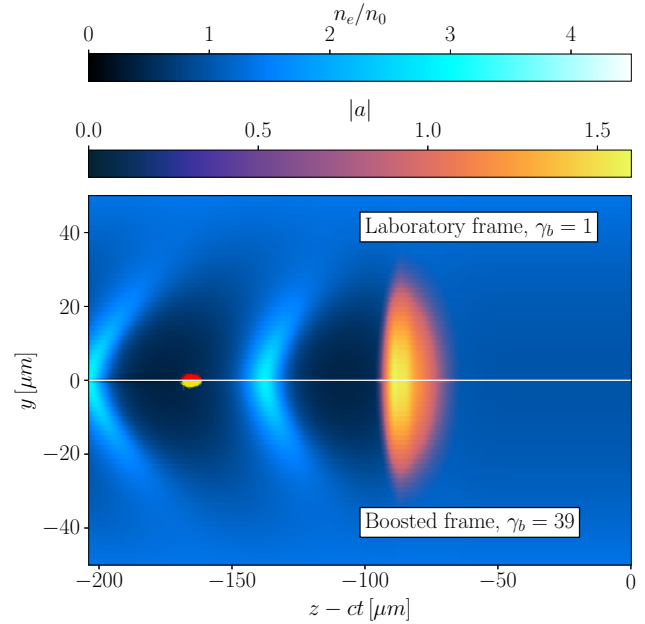


Figure 5. Comparison of the electron density n_e/n_0 and $|a|$ on the $z - y$ plane at $ct \approx 19.35$ cm. The red and yellow dots are a scatter plot the electron bunch macroparticles. Top half panel: $\gamma_b = 1$ (laboratory frame); Bottom half panel: $\gamma_b = 39$. The simulations in the laboratory and boosted frame show a remarkable agreement.

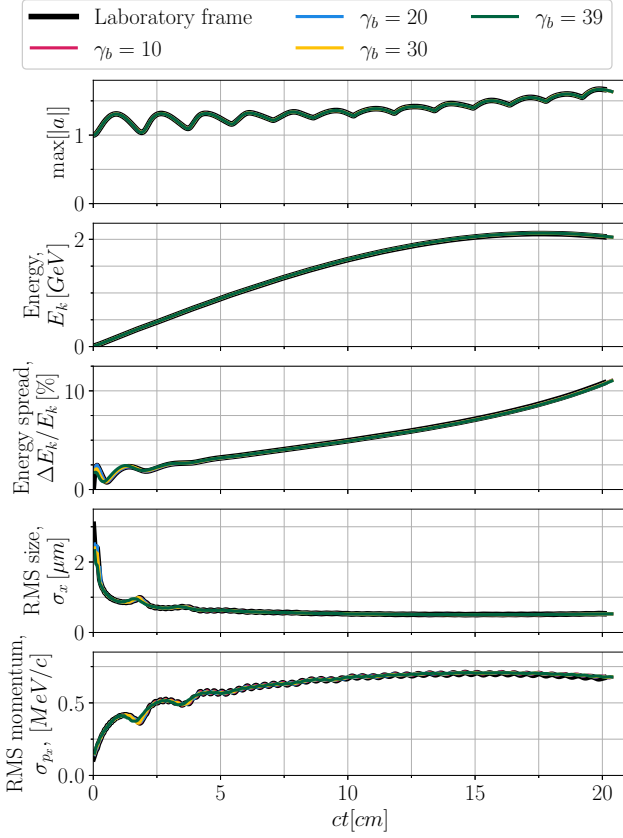


Figure 6. Comparison of the peak absolute value of the normalized envelope a and bunch parameters evolution for $\gamma_b = 1$ (laboratory frame) and $\gamma_b = 10, 20, 30, 39$. From top to bottom, the panels report the evolution of $\max[|a|]$, the bunch kinetic energy E_k , relative rms kinetic energy spread $\Delta E_k/E_k$, rms size σ_x along the transverse coordinate x , rms σ_{p_x} of the transverse momentum p_x . The plot shows that the combination of LBF and TPA is accurate and stable up to relatively high boost values.

panel respectively, the beam energy spectrum dQ/dE and the beam charge distribution along the propagation direction dQ/dz after 19.3 cm of propagation, obtained in the laboratory frame (black line) and with $\gamma_b = 10, 20, 30, 39$ (colored lines). These charge distributions obtained with different γ_b are almost superposed, the difference between the results of the simulations being below 1%.

The agreement between the TPA results in the laboratory frame and those obtained with the TPA in the LBF shows that, using the fully covariant TPA formalism described in Sec. 4, the two techniques can be combined without physical inconsistencies, even with relatively high Lorentz factors. However, the maximum attainable speed-up will be limited by numerical constraints.

Table 1 reports the spatial and temporal resolution of the shown simulations, as well as the computing time needed to execute them. The theoretical speed-up in Table 1 is computed using S_{LBF} given by Eq. (2) with

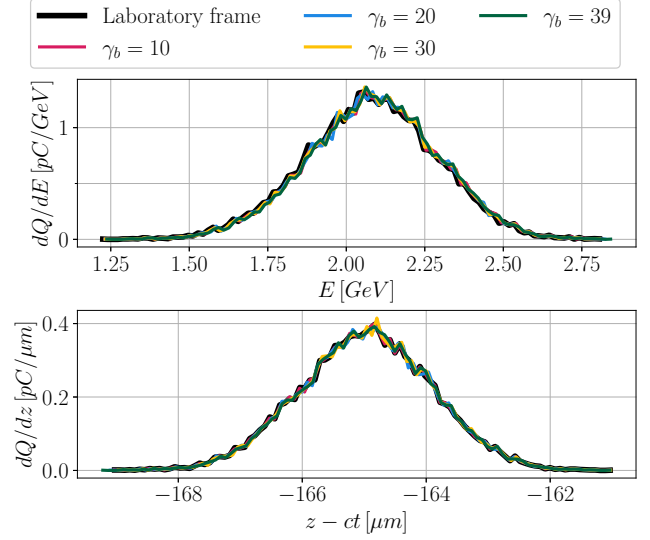


Figure 7. Comparison of bunch energy and longitudinal position spectra for laboratory frame and $\gamma_b = 10, 20, 30, 39$ at $ct \approx 19.3$ cm.

the inclusion of a factor that takes into account the different longitudinal and temporal resolutions used in different simulations, namely

$$S_{LBF}^{Effective} = \frac{\eta}{\eta_{ref}} \left(\frac{\Delta z}{\Delta z_{ref}} \right)^2 S_{LBF}, \quad (16)$$

where $\eta = c\Delta t/\Delta z$, and the reference simulation is the one in the laboratory frame. Note that the numerical parameters chosen for the simulations listed in Table 1 ensure that the Courant-Friedrichs-Lewy condition for the INF&RNO fluid plasma solver is always satisfied in the boosted frame. The measured speed-ups are in relatively good agreement with the theoretical ones. The speed-up reaches a maximum and then decreases with γ_b , since the Δz , Δt , and their ratio must be decreased to satisfy the stability condition, and so, for high values of γ_b , the speed-up given by the LBF technique does not compensate the increase in computing time caused by using smaller Δz and Δt . However, even with relatively small values of γ_b , the resulting speed-up compared to the TPA simulation in the laboratory frame reaches two orders of magnitude, e.g. 136 for $\gamma_b = 6$ and 237 for 8.

Introducing the LBF technique in a TPA simulation provides a two-order-of-magnitude speed-up in execution times. A lab-frame TPA simulation in a given geometry, e.g. 3D, reduces the computing time by four orders of magnitude compared to a simulation without TPA in the same geometry. The combined benefit of the LBF and TPA techniques may therefore provide speed-ups on the order of 10^6 , which can reach an order of 10^8 if we compare simulations in cylindrical geometry with 3D simulations. **The**

relative differences in the electron beam parameters and spectrum obtained with different γ_b are below 1%, coherently with the LBF convergence study on LWFA simulations with self-injection described in [61], which did not use the TPA. This suggests that the combined use of TPA and LBF does not add additional sources of error for the external injection scheme considered in this article. The reported results highlight the potential of coupling the TPA with the LBF techniques for the simulation of long distance propagation.

5. Conclusions

This article demonstrates the possibility of coupling the time-averaged ponderomotive approximation (TPA) and the Lorentz boosted frame (LBF) techniques to reduce the computational cost of LWFA simulations.

After a brief review of both techniques, we have discussed the implementation of the TPA in the boosted frame. We showed that, when a fully Lorentz-invariant envelope equation and an accurate laser pulse initialization are used, the results obtained with the TPA in the laboratory frame are in excellent agreement with those obtained combining the TPA with the LBF technique. This has been validated through the long distance propagation of a laser pulse in a plasma channel with the acceleration of an electron bunch externally injected in the laser wakefield. The benchmark is particularly relevant for high-energy multi-stage LWFA. The laboratory frame results have been validated by comparing a simulation without TPA with two simulations using different implementations of the TPA in two PIC codes, INF&RNO and SMILEI. The results obtained with INF&RNO combining the TPA and LBF with Lorentz factors ranging from 2 to 39 showed no significant differences compared to the base case.

Numerical constraints limit the choice of the maximum Lorentz factor of the LBF. However, we have shown that even with relatively small Lorentz factors, e.g. of the order of $\lesssim 10$, a speed-up of two orders of magnitude can be obtained, compared to a TPA simulation in the laboratory frame. For long-distance laser propagations typical of simulations of high-energy LWFA stages, the total speed-up of a cylindrical simulation using both the TPA and the LBF technique can easily reach eight orders of magnitude compared to a 3D simulation without the TPA carried out in the laboratory frame. This speed-up is comparable to the ones attainable with the quasi-static approximation, with the advantage of enabling the modeling of kinetic physics effects such as self-injection.

The presented results will pave the way to the implementation of non quasi-static PIC codes for

LWFA with considerable reductions in the required computational resources.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Acknowledgements

F. Massimo would like to thank A. Sablon for his input during the early stages of this work.

This work was supported by the Director, Office of Science, Office of High Energy Physics, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and used the computational facilities at the National Energy Research Scientific Computing Center (NERSC).

This work was granted access to the HPC resources of TGCC under the allocation 2023-A0150510062 (Virtual Laplace) made by GENCI. Most of the development of SMILEI relative to this article was made on the meso-scale HPC “3Lab Computing” hosted at École polytechnique and administrated by the Laboratoire Leprince-Ringuet, Laboratoire des Solides Irradiés et Laboratoire pour l’Utilisation des Lasers Intenses. Most of the simulation results obtained with SMILEI were obtained on the same cluster.

Appendix A. Numerical schemes used in the simulations

The numerical schemes and settings of the simulations shown in this article are detailed in the following. To summarize the main requirements to conduct long-distance simulations like the ones shown in the sections 3.1 and 4: a solver (for the envelope equation [62, 15] or Maxwell’s equations) with low numerical dispersion is necessary to accurately describe the laser propagation and reduce the numerical dephasing of the accelerated electron bunch. Techniques to reduce the numerical Cherenkov radiation (or its effects) are necessary to avoid an artificial increase of the bunch emittance [51]. Additionally, in cylindrical geometry charge conserving shape functions [84] for the reduction of artifacts near the propagation axis are used, to avoid an inaccurate calculation of the transverse force acting on the bunch. **The continuity equation for the charge and current density is satisfied through a charge conserving current deposition scheme [85].** These requirements were met with different techniques in INF&RNO and SMILEI.

In both codes the electron bunch is modeled with 20000 macroparticles, using the same charge

	$k_p \Delta z$	$\eta = c\Delta t / \Delta z$	$k_p \Delta r$	Time [hours]	Measured speed-up	Theoretical speed-up
laboratory frame	1/80	0.24	1/8	99.5	–	–
$\gamma_b = 2$	1/80	0.24	1/8	7.02	14	14
$\gamma_b = 4$	1/80	0.24	1/8	1.60	62	60
$\gamma_b = 6$	1/80	0.24	1/8	0.73	136	133
$\gamma_b = 8$	1/80	0.24	1/8	0.42	237	225
$\gamma_b = 10$	1/120	0.24	1/8	0.63	158	148
$\gamma_b = 20$	1/120	0.10	1/8	0.57	175	165
$\gamma_b = 30$	1/120	0.05	1/8	0.72	138	119
$\gamma_b = 39$	1/120	0.05	1/8	0.60	166	139

Table 1. Longitudinal cell size, integration time step, transverse (radial) cell size resolution and execution time for INF&RNO simulations. All the values are cited in the laboratory frame. The spatial and temporal resolutions in the boosted frame are given by $\Delta z' = \gamma_b(1 + \beta_b)\Delta z$, $\Delta r' = \Delta r$, and $\Delta t' = \gamma_b(1 + \beta_b)\Delta t$. The simulation times are measured on NERSC Perlmutter using an AMD EPYC 7763 CPU node [83]. The theoretical speed-up $S_{LBF}^{Effective}$ is given by Eq. (16).

and initial macroparticle coordinates in all the simulations. The bunch macroparticles are evolved as PIC macroparticles using their coordinates in the 6D phase space.

For the the INF&RNO simulations, the size of the computational window is $L_z = 204 \mu\text{m}$ and $R_{max} = 193 \mu\text{m}$ in the longitudinal and radial direction, respectively. For the laboratory frame simulation, the mesh resolution in the two directions $\Delta\zeta$ and Δr is set to $k_p \Delta\zeta = 1/80$ and $k_p \Delta r = 1/8$, where $\zeta = z - ct$ is the comoving coordinate and the on-axis plasma wavenumber $k_p = 9.8 \times 10^{-1} \mu\text{m}^{-1}$ for the chosen density. The integration timestep is $c\Delta t = 0.24\Delta\zeta$. The values of $\Delta\zeta$, Δr and Δt used in the boosted frame simulations are reported in Table 1. The high-accuracy numerical scheme used to solve the envelope equation in INF&RNO is described in [62]. The simulations are performed in a hybrid mode. The electron bunch is modeled as a set of macroparticles interacting with the grid fields as in a PIC code and advanced in the phase space with a **relativistic** Boris Pusher [86]. Charge conserving interpolation/projection shape functions are used to avoid numerical artifacts near the propagation axis [84]. The plasma electrons are modeled as a relativistic cold fluid, whose density and momentum evolution equations (described in [72]) are solved using second order upwind longitudinal derivatives, second order centered transverse derivatives, and a second order Runge-Kutta for their time integration. The use of a fluid model for the plasma allows to obtain accurate results with the computational cost comparable to using one macroparticle per cell in a PIC simulation for this case study where the kinetic effects in the plasma evolution are negligible [77]. The initialization of the wakefield is performed adiabatically, while maintaining the laser and the bunch frozen, until a stationary configuration is reached. This configuration is used as the initial

condition. **The initialization of the electron beam in the boosted frame simulations follows the algorithm described in Appendix B of [45]. In these simulations, the plasma at rest in the laboratory frame is initialized as moving at speed $-\beta_b c$ in the z direction and with a density higher by a factor γ_b compared to the laboratory frame density. In the boosted frame simulations, the number of grid points and resolution Δr along the transverse direction are unchanged, as well as the number of grid points in the longitudinal direction. As described in Sec. 2, the longitudinal cell size Δz and the integration timestep Δt are increased by a factor $\gamma_b(1 + \beta_b)$ compared to their value in the laboratory frame. Apart from the described changes and numerical schemes, the operations implementing the interaction between the macro-particles and the grid, e.g. the force interpolation and field source projection, are the same as in a PIC simulation in the laboratory frame.**

The fully kinetic PIC simulations performed with SMILEI use a similar simulation window size, with the same transverse resolution used in the INF&RNO simulation. The effects of numerical Cherenkov radiation have been significantly reduced by using the B-TIS3 interpolation scheme [58], adapted to support the azimuthal Fourier decomposition [18]. This allows to reduce an artificial growth of the bunch transverse momentum and size [51, 57, 58], that would be detrimental in the simulation of long simulation distances. Using this scheme instead of a spectral solver allows to maintain a high degree of scalability due to the easier parallelization of finite difference electromagnetic solvers. To avoid numerical artifacts near the propagation axis, we adopted charge conserving shape functions defined on two points following [84] (also implemented in FBPIC [55]). Given the focusing of the electron bunch with increasing energy in the shown simulations, avoiding these artifacts was essential to avoid an

inaccurate interpolation of the transverse force acting on the macroparticles.

For the SMILEI PIC simulation using the TPA, the longitudinal mesh resolution is set to $k_p \Delta z = 1/160$ and the integration timestep is $c\Delta t = 0.99\Delta z$. The laser envelope is evolved through the explicit solver with reduced dispersion for Eq. (7) described in [15], adapted to cylindrical geometry with one azimuthal mode [18]. The macroparticles are advanced in the phase space using the **relativistic** Boris-like pusher with the addition of the ponderomotive force described in [15, 75]. The plasma is sampled with [1, 2, 1] macroparticles initially distributed regularly in the z , r directions and along the azimuthal angle interval $\theta = [0, 2\pi)$ respectively.

For the SMILEI PIC simulation not using the TPA, the longitudinal mesh resolution and the integration timestep were respectively $k_p \Delta z = 1/640$, (keeping $c\Delta t = 0.99\Delta z$). The **relativistic** Boris pusher was used to advance the macroparticles. The plasma was sampled with [1, 4, 8] macroparticles.

To evolve the electromagnetic fields (or their low-frequency part in the simulation with TPA), both SMILEI simulations used the optimized longitudinal derivative stencil described in [15] for the Yee-like solver in quasi-cylindrical geometry, using 2 azimuthal modes (1 azimuthal mode for the simulation with TPA) [18]. This solver considerably reduces the numerical dispersion to describe the laser propagation more accurately. One of the main consequences is a more accurate numerical propagation speed for the laser pulse, which reduces the numerical dephasing that would change the energy evolution of the electron bunch.

The results shown in this article, which used the numerical schemes reported in this Appendix, were obtained on CPUs. Almost all these numerical schemes are explicit schemes with a high degree of locality in the data dependencies, that can be efficiently parallelized on GPU with techniques well-known in the PIC development community [25, 26, 27, 29]. The only exception, i.e. the implicit laser envelope solver scheme used in INF&RNO [62], solves an elliptic equation in each transverse plane corresponding to a grid coordinate z . This solver has been shown to be parallelizable on GPU even in 3D in the code HiPACE++ [42].

Appendix B. Extracting the envelope of the vector potential from the simulation without TPA

To compare the evolution of $\max[|a|]$ in Fig. 3, this value has been obtained directly from the simulations with TPA. In the case of the simulation without TPA,

which does not use the vector potential in the definition of the electromagnetic fields, its value has been obtained through an *ad-hoc* postprocessing. Without loss of generality, the $\max[|a|] = \max[|q_e \tilde{A}/m_e c|]$ is assumed to be found on the propagation axis. At each diagnostic timestep t , from the value of the transverse electric field on the propagation axis $E_x(z, r = 0, t)$, the envelope $\tilde{E}_x(z, r = 0, t)$ of this component of the electric field can be found. This can be obtained through a multiplication of $E_x(z, r = 0, t) = \text{Re}[\tilde{E}_x(z, r = 0, t)e^{ik_0(z-ct)}]$ by $e^{ik_0(z-ct)}$. The real and imaginary part of this product, after the use of a low-pass filter to remove the harmonics centered around $2k_0$, are proportional to the real and imaginary parts of $\tilde{E}_x$, except for a constant phase term that does not change its absolute value. The complex envelopes $\tilde{E}_x$ and $\tilde{A}$ are related through (see Eqs. A4 and A5 of [69]):

$$\begin{aligned} \tilde{E}_x(z, t) = - \left(\frac{\partial}{\partial t} - ik_0 c \right) \tilde{A}(z, t) \approx \\ c \left(\frac{\partial}{\partial z} + ik_0 \right) \tilde{A}(z, t), \quad (\text{B.1}) \end{aligned}$$

where $r = 0$ has been dropped for the sake of simplicity of notation.

A simple discretization of Eq. B.1 through the lowest order centered finite differences yields:

$$\tilde{E}_x(z, t) \approx c \left[\frac{A(z + \Delta z, t) - A(z - \Delta z, t)}{2\Delta z} + ik_0 \tilde{A}(z, t) \right]. \quad (\text{B.2})$$

Using Eq. B.2, starting from a position z sufficiently far from the laser pulse on its right, where it can be assumed that $E_x(z, t) \approx 0$ and $\tilde{A}(z, t) \approx 0$, the value of $\tilde{A}(z - \Delta z, t)$ can be found from $\tilde{A}(z + \Delta z, t)$, $\tilde{A}(z, t)$ and $\tilde{E}_x(z, t)$. Repeating this step iteratively towards decreasing z , the whole $\tilde{A}(z, t)$ on the propagation axis ($r = 0$) can be found, except for a constant phase term that does not change its absolute value.

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