WAND-PIC: A three-dimensional quasi-static particle-in-cell code with parallel multigrid solver and without predictor-corrector

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(Dated: December 3, 2020)

We introduce the first quasi-static particle-in-cell (PIC) code: WAND-PIC which doesn’t require the commonly used predictor-corrector method in solving electromagnetic fields. We derive the field equations under quasi-static approximation and find the explicit form of the “time” derivative of transverse plasma current. After that, equations for the magnetic fields can be solved exactly without predicting the future quantities. Algorithm design and code structure are greatly simplified. With the help of explicit quasi-static equations and our adaptive step size, plasma bubbles driven by the large beam charges can be simulated efficiently without suffering from the numerical instabilities associated with the predictor-corrector method. In addition, WAND-PIC is able to simulate the sophisticated interactions between high-frequency laser fields and beam particles through the method of sub-cycling. Comparisons between the WAND-PIC and a first-principle full PIC code (VLPL) is presented. WAND-PIC is open-source \([1]\), fully three-dimensional and parallelized with the in-house multigrid solver. Scalability, time complexity, and parallelization efficiency up to thousands of cores are also discussed in this work.

I. INTRODUCTION

Plasma-based accelerators represent one of the most exciting concepts in high-gradient particle acceleration. Plasmas with density \(n_0\) can sustain a high accelerating gradient: \(E_\parallel \sim \sqrt{n_0/10^{18}\text{cm}^{-3}} \text{[GV/cm]}\), thereby enabling compact particle accelerators that are much smaller than the present-day conventional accelerators. Accelerating structures are excited either by ultra-intense laser pulses for a laser wakefield accelerator (LWFA) \([2–4]\), or by relativistic electron bunches for a plasma wakefield accelerator (PWFA) \([5]\). GeV-level electron accelerations have been demonstrated in recent experiments for both LWFA \([6–9]\) and PWFA \([10, 11]\).

In LWFA, the energy gain of the witness bunch over a dephasing distance \(L_d \propto n_0^{-3/2}\) \([12–14]\) can be estimated as \(\Delta W_{\text{LWFA}} = E_\parallel L_d \propto n_0^{-1}\) which favors the use of low density plasma and long propagation distance. Plasma densities \(n_0 \sim 10^{17}\text{cm}^{-3}\) are employed in recent experiments \([15]\) with energy gain reaching 8 GeV over an acceleration distance of 20 cm. In PWFA, the energy gain of the witness bunch is largely governed by the transformer ratio \([16]\) and the initial energy of the driver beam \(\gamma_0 mc^2\), where \(\gamma_0\) is the relativistic factor of the driver particles. The maximum energy gain of an accelerated (witness) electron beam is limited to \(\Delta W_{\text{PWFA}} = 2\gamma_0 mc^2\). Energy doubling of 42 GeV electrons in a meter-scale plasma has been demonstrated \([17]\). Therefore, either in LWFA or PWFA, increasing the energy gain would inevitably require more energy in the driver and longer propagation distance. With the rapid development of the ultra-intense multi-petawatt laser systems \([18, 20]\) and the ultra-short, high-current compact electron beam sources \([21, 22]\), we could envision an increasing number of the practice of the meter-scale LWFA and PWFA at single stages. The difficulty of simulating meters long propagation distance of plasma-based accelerators must be overcome. For example, a decent 3D simulation of LWFA driven by a 0.8 μm laser pulse would take more than \(10^4\) core-hours to accomplish for a propagation distance of just a few millimeters. Numerical challenges escalate even more when hundreds of meter-scale stages are involved in developing TeV-scale linear lepton colliders \([23]\).

There are two major approaches to simulate the plasma-based accelerators, one is to use the first-principle fully explicit particle in cell (PIC) code \([24, 25]\) where the Maxwell equations are solved by finite-difference time-domain (FDTD) method \([26]\) and the source terms: currents of macroparticles are deposited on the grid. However, the Courant–Friedrichs–Lewy (CFL) condition \([27]\) must be satisfied to ensure convergence, in short: the time step size must be smaller than the spatial step size which is chosen to be much smaller than the smallest length scale \(\Delta L_{\text{min}}\) in the simulation domain. For example, in the LWFA, the smallest length scale is normally the laser wavelength: \(\Delta L_{\text{min}}^{\text{LWFA}} = \delta \lambda_0\) therefore a time step size \(\delta t \ll \omega_0^{-1}\) is required, where \(\omega_0 = 2\pi c/\lambda_0\) is the laser frequency. And for PWFA in the nonlinear regime, the smallest length scale normally equals the sharpness of the nonlinear wakefield: \(\Delta L_{\text{min}}^{\text{PWFA}} \ll k_p^{-1}\), where \(k_p = \omega_p/\sqrt{4\pi e^2 n_0/m}\) is the plasma frequency, \(e\) and \(m\) are the electron charge and mass. However, the evolution of the envelopes of the drivers are much slower in both cases: at a rate of \(\sim \omega_p^2/\omega_0\) for the LWFA and a rate of \(\sim \omega_p/\sqrt{2}\gamma\) for the PWFA. Therefore a great amount of computational time would be saved if we can decouple the two distinct time scales and separate the "slower" evolution of the driver from the generation of the wakefield. This is done by the so-called quasi-static approximation (QSA) proposed by Springle \textit{et al} \([28]\) and...
first implemented in PIC code by Mora et al. [29, 30] and Whittum [31]. The QSA assumes the envelope of the driver is unchanged or "frozen" during the time when cold plasma electrons are passed over by the driver, enables a time step size which is much bigger compared with the full PIC code and not subject to CFL condition. Several quasi-static PIC codes have demonstrated the reduction of computational time more than two order-of-magnitude, like the WAKE [29, 30], LCODE [32, 33], QuickPIC [34–36] and HiPACE [37]. The WAKE and LCODE are two-dimensional (2D) codes with cartesian or cylindrical geometry, and QuickPIC and HiPACE are fully 3D and fully parallelized.

However, a great saving in time comes with more numerical intricacies: unlike the FDTD method where the fields are natural discretized both in time and in space on staggered "Yee lattice" [26] and can be updated locally from the previous step, a quasi-static PIC code must regenerate new wakefields at every time step because the generation of the wakefields and time evolution of the driver are decoupled. Moreover, a bigger challenge is that in some equations of wakefields under QSA, the time derivative of transverse current is involved and is not explicit i.e., the equation for transverse magnetic field is never explicit and closed-form. To our knowledge, all the existing quasi-static codes (WAKE, LCODE, QuickPIC, HiPACE) solve the wakefields by the so-called "predictor-corrector" method [38]. Although an improved iteration loop [36] has been developed to improve the stability and convergence of the predictor-corrector method, current quasi-static codes are still experiencing difficulties in simulating the extremely nonlinear wakefield i.e., the plasma bubble excited by a large beam charge or ultra-intense compact laser pulse. The reason is that the predictor-corrector method often fails to converge at the back of the large bubble where the plasma electrons are highly relativistic and the wakefields are sharp. This long-standing issue of quasi-static codes prevents people from studying the accelerating structure driven by the extremely powerful and compact drivers which are already within the reach of present-day laser systems and particle accelerators.

In this work, we present the first quasi-static code: WAND-PIC (Wakefield AcceleratioN and Direct laser acceleration) which doesn’t use the predictor-corrector method (an early, single-core version is first published by us in 2017 [39]). A new set of quasi-static equations are developed and the source terms of all partial-differential equations are explicit. Therefore, all fields can be solved directly without predicting the future quantities, and great stability can be achieved when simulating large bubbles. WAND-PIC is also a full 3D, parallel code that can run on the distributed systems of over thousands of cores. Several new features are also developed in WAND-PIC, include adaptive mesh refinement which enables us to simulate large bubbles effectively, and sub-cycling technique which enables us to simulate the direct laser acceleration (DLA) of electrons in quasi-static code for the first time.

The rest of the paper is organized as follows. First, we briefly summarize the advanced features in WAND-PIC. Then, the quasi-static equations for fields and particles are described in sec. III and the implementation of different drivers and the interactions between drivers are presented in sec. IV. In sec. V we compare the results of WAND-PIC and a 3D full PIC code VLPL [40]. The algorithm design and parallel scalings are shown in sec. VI followed by future development and conclusion.

II. SUMMARY OF THE ADVANCED FEATURES

![FIG. 1: (a) The 3D simulation domain in WAND-PIC. The 2D transverse plane is partitioned into square subdomains. In the longitudinal direction, the adaptive step size is shown by the red ticks which are denser at the back of the bubble. (b) A hierarchy of grids in one subdomain with different mesh sizes.](image-url)
In this section, we briefly introduce the four advanced features of WAND-PIC.

1. Explicit source terms for all wakefield equations
In quasi-static codes, the particles’ distribution and the fields depend on $t$ and $z$ only through a "time-like" variable $\xi = ct - z$. In the 3D domain, fields are solved at every 2D $\xi$ slice with step size $d\xi$ and particles are pushed only in positive $\xi$-direction due to the causality: $d\xi/dt = c - v_z > 0$. Therefore, when solving the fields at one $\xi$ step, information only at the current ($\xi$) step and the past ($\xi - d\xi$) step are known. It would be ideal if the source terms of all field equations are explicit such that no "future" information at ($\xi + d\xi$) step is needed. Several papers [30, 32, 36, 37] have presented the derivations of Maxwell equations under QSA, and the results are largely similar: equations are not completely explicit for all fields. $\partial j_L/\partial \xi$ is implicit either in the equations of $B_{\perp}$ solved in QuickPIC [36] and HiPACE [37], or in the equation of wakefield potential $\psi$ solved in WAKE [30], or in the equations of $E_{\perp}$ solved in LCODE [32]. In WANDPic, $\partial j_L/\partial \xi$ is explicitly given, as a result, all field equations are now closed-forms and "static" (since $\xi$ is a time-like variable) and can be solved at once easily with a Poisson solver and without predictor-corrector iterations. More details will be provided in sec. III.

2. Adaptive mesh refinement
With an increasing need for simulating plasma wakefield driven by the tightly-focused laser pulses with power exceeds PW and beam drivers with current exceeds tens of kA, we need to accurately model the nonlinearity of the wakefield/bubble structure over tens of centimeters even meters. In WAND-PIC we have implemented the technique of adaptive mesh refinement in the longitudinal ($\xi$) direction to handle the steep structure at the back of the bubble. As shown in Fig. 1, the longitudinal step size $d\xi$ (red tick) is automatically adjusted based on the speeds of plasma trajectories, meshes are much finer near the back of the bubble where the plasmas trajectories are fast. More details and simulation examples can be found in sec. VI A.

3. Full description of driver particles in fast laser fields
Like other quasi-static codes, the driver particles (in some cases witness particles) are not subject to quasi-static approximation: they are governed by the full equations of motion in the electromagnetic fields produced by themselves and in plasma. Since the laser pulses are modeled quasi-statically, the interaction between the laser pulse and particles are normally modeled through the averaged ponderomotive approach. In WAND-PIC, we improve the modeling of driver particles by including the fast oscillating laser fields into their equations of motion. While the laser pulse is still described by its envelope, the fast oscillating fields on one particle are calculated from the laser envelope and the phase of the particle with respect to the laser. Then using the subcycling method [31], the particles are advanced with a small enough time step. Details and simulation examples are shown in sec. IV and V A.

4. Parallel geometric multigrid solver
In quasi-static code, fields are solved at every 2D $\xi$ slice, and particles are advanced in positive $\xi$-direction. For the fields, a 2D Poisson solver is needed. In order to make WAND-PIC compatible with the present-day high-performance computing systems, we parallelized the two transverse directions: $x$ and $y$ by applying a square partitioning on it. As shown in Fig. 1, the transverse plane is divided into subdomains. An in-house parallel multigrid solver [42, 43] is developed alongside WAND-PIC. This geometric multigrid solver naturally fits into the 2D partitioning of the domain and does iterative relaxation of the solution on a hierarchy of grids with different mesh sizes, therefore, residual errors with different wavelength are effectively smoothed out at different layers. Details and performance evaluation can be found in sec. VI.

III. QUASI-STATIC EQUATIONS FOR WAKEFIELDS AND PLASMA PARTICLES

The quasi-static equations we used are first derived in [39]. For convenience, we briefly show the derivation again in this work.

Under the QSA, distribution function $f_e$ of plasma electrons and electromagnetic fields depend on $t$ and $z$ only through a combination $\xi = t - z$, where the speed of light $c$ is normalized to 1. First, we start with the kinetic equation:

$$\frac{\partial f_e}{\partial t} + \frac{\partial H}{\partial \mathbf{P}} \cdot \frac{\partial f_e}{\partial \mathbf{R}} - \frac{\partial H}{\partial \mathbf{R}} \cdot \frac{\partial f_e}{\partial \mathbf{P}} = 0,$$

where $H = [1+(\mathbf{P}+\mathbf{A})^2]^{1/2} - \phi$ is the Hamiltonian, $\mathbf{P} = \mathbf{p} - \mathbf{A}$ is the canonical momentum, $\phi$ is the electric potential, and $\mathbf{R} = (x,y,z)$ is the electron position vector. The trajectory of an individual electron in phase space $(\mathbf{R}, \mathbf{P})$ is determined by the equations of motion:
\[
\frac{d\mathbf{P}}{dt} = -\frac{\partial H}{\partial \mathbf{R}}, \quad \frac{d\mathbf{R}}{dt} = \frac{\partial H}{\partial \mathbf{P}},
\]  
\tag{2}

From the dependence of \( H \) on \( \xi = t - z \), we derive that \( dH/dt = \partial H/\partial \dot{\xi} = \partial H/\partial \dot{\xi} \) and \( dP_z/dt = -\partial H/\partial z = \partial H/\partial \dot{\xi} \). Hence, \( H - P_z = \text{const} \). Since all electrons start their motion from cold homogeneous plasma where \( H = 1 \) and \( \mathbf{P} = 0 \), the integral of motion takes the form: \( H - P_z = 1 = 0 \). And the distribution function of electrons can be expressed in the form

\[
f_\ast(t, \mathbf{R}, \mathbf{P}) = f_\ast(\xi, \mathbf{r}, \mathbf{P}_\perp)\delta(H - P_z - 1),
\]  
\tag{3}

where \( f_\ast \) represent a distribution function of macroparticles performing two dimensional motion in the \((x, y)\)-plane and \( \mathbf{r} \equiv (x, y) \). Substituting Eq. (3) into (1), we find that \( f_\ast \) satisfies the Vlasov equation:

\[
\frac{\partial f_\ast}{\partial \xi} + \frac{\partial H_\ast}{\partial \mathbf{P}_\perp} \cdot \frac{\partial f_\ast}{\partial \mathbf{r}} - \frac{\partial H_\ast}{\partial \mathbf{r}} \cdot \frac{\partial f_\ast}{\partial \mathbf{P}_\perp} = 0,
\]  
\tag{4}

where

\[
H_\ast = \frac{1 + (\mathbf{P}_\perp + \mathbf{A}_\perp)^2 + (1 + \psi)^2}{2(1 + \psi)} - \psi - A_z
\]  
\tag{5}

is the Hamiltonian for the two-dimensional motion in the \((x, y)\)-plane and \( \psi = \phi - A_z \) is the wakefield potential. The trajectory of an individual particle in the phase space \((\mathbf{r}, \mathbf{P}_\perp)\) is determined by Eq. (2) and by replacing \( \mathbf{P}_\perp = \mathbf{p}_\perp - \mathbf{A}_\perp \), these equations can be written in the form

\[
\frac{d}{d\xi} \mathbf{P}_\perp = \frac{\gamma}{1 + \psi} \mathbf{V}\mathbf{E} + [\mathbf{e}_z \times \mathbf{V}] \mathbf{B}_z + [\mathbf{e}_z \times \mathbf{B}_\perp],
\]  
\tag{6}

\[
\frac{d}{d\xi} \mathbf{r}_\perp = \mathbf{V} = \frac{1}{1 + \psi} \mathbf{P}_\perp
\]  
\tag{7}

where \( \gamma = [1 + \mathbf{p}_\perp^2 + (1 + \psi)^2]/2(1 + \psi) \) is the relativistic factor, and \( \mathbf{V} \equiv \mathbf{p}_\perp/(1 + \psi) \) is the particle ”velocity” in \((x, y)\)-plane. Integration of Eq. (4) over \( P_x \) and \( P_y \) gives the continuity equation:

\[
\frac{\partial}{\partial \xi} n_\ast = -\nabla \cdot (n_\ast(\mathbf{V})),
\]  
\tag{8}

where \( n_\ast = \int dP_x dP_y f_\ast \) is the density of macroparticles and the brackets denote averaging over transverse momentum \( \langle \mathbf{V} \rangle = n_-^{-1} \int dP_x dP_y f_\ast \mathbf{V} \). As seen from Eq. (8), that the total number of macroparticles is the conserved at each \( \xi = \text{const} \) slice. We also note that the density and the current density of plasma electrons can be expressed through the distribution function \( f_\ast \) as:

\[
n_e = \frac{n_\ast(\gamma)}{1 + \psi}, \quad j_\perp = n_\ast(\mathbf{V}), \quad j_z = \frac{n_\ast \langle p_z \rangle}{1 + \psi},
\]  
\tag{9}

where \( \langle p_z \rangle = \langle \gamma \rangle - \psi - 1 = [1 + \langle \mathbf{p}_\perp^2 \rangle - (1 + \psi)^2]/(2(1 + \psi)) \). Besides, \( n_e - j_z = n_\ast \).

We now show that the wakefield potential \( \psi \) and the fields \( E_z, B_z \) at a ”time” \( \xi \) are determined only by positions and momenta of macroparticles at the same time, that is, by \( f_\ast(\xi, \mathbf{r}, \mathbf{P}_\perp) \). Using \( \xi \) as a time-like variable, Maxwell’s equations in dimensionless variables take the following form:

\[
\nabla \times \mathbf{E} = -\frac{\partial}{\partial \xi} \mathbf{B},
\]  
\tag{10}

\[
\nabla \times \mathbf{B} = \frac{\partial}{\partial \xi}(\mathbf{E} - \mathbf{j}).
\]  
\tag{11}

Combined with Gauss’s law \( \nabla \cdot \mathbf{E} = -n_e + 1 \), we obtain the following equations

\[
\Delta_\perp \psi = n_\ast - 1, \quad \Delta_\perp E_z = -\nabla_\perp \cdot \mathbf{j}_\perp, \quad \Delta_\perp B_z = \mathbf{e}_z \cdot [\nabla_\perp \times \mathbf{j}_\perp], \quad \Delta_\perp \mathbf{B}_\perp = -[\mathbf{e}_z \times \nabla_\perp j_z] - \left[ \mathbf{e}_z \times \frac{\partial}{\partial \xi} \mathbf{j}_\perp \right].
\]  
\tag{12}
Note that the source term $n_*(V)$ in the equation for $\psi$ is fully determined by macroparticles’ positions while the source term $n_*(V)$ in the equation for $E_z$ and $B_z$ requires knowledge of the macroparticles’ positions and momenta.

To obtain a closed-form of the Eq. [15] for transverse magnetic fields, we establish a relationship between the time derivative of the transverse current and the electromagnetic fields. Such a relationship is well-known for cold weakly perturbed plasma [24]: $\partial_j/\partial t = (ω_0^2/4π)E$. To generalize it to strongly perturbed relativistic plasma, we multiply the Vlasov Eq. [4] by the “velocity” $V_\perp = \partial H/\partial P_\perp$ and integrate it over momentum. After straightforward calculations we find

$$\frac{\partial}{\partial ξ}J_\perp = n_*(a) - \frac{\partial}{\partial x}n_*(V_x V_\perp) - \frac{\partial}{\partial y}n_*(V_y V_\perp),$$

(16)

where $a = d^2r_\perp/dξ^2$ is the particle “acceleration”:

$$a = \frac{[e_\perp \times B_\perp]}{1 + \psi} + \frac{[e_\perp \times V_\perp B_z]}{(1 + \psi)} + \dot{a},$$

(17)

$$\dot{a} = \frac{γν_\perp}{(1 + \psi)^2} - \frac{V}{1 + \psi}(E_z + V \cdot V_\perp)$$.

(18)

Substituting $\partial J_\perp/\partial ξ$ from Eq. [16] to Eq. [15] we obtain Helmholtz equation describing the transverse magnetic field:

$$Δ_\perp B_\perp = \frac{n_*(a)}{1 + \psi} B_\perp - [e_\perp \times S]$$

(19)

with the source

$$S = \frac{[e_\perp \times n_*(V)]B_z}{(1 + \psi)} + \frac{n_*(a)}{1 + \psi} - \frac{\partial}{\partial x}n_*(V_x V_\perp) - \frac{\partial}{\partial y}n_*(V_y V_\perp) + \nabla_\perp j_z.$$

Thus, in quasi-static approximation all fields are determined from static Eqs. [12] - [14] and [19] by positions and momenta of macroparticles in the plane $(x, y)$ at given $ξ$. The source terms in these equations do not have “time” derivatives of the fields or currents. In the codes QuickPIC [36] and HiPACE [37], equations similar to Eqs. [12] - [15] are also derived, but the explicit form of $\partial J_\perp/\partial ξ$ were never given.

IV. IMPLEMENTATION OF DIFFERENT DRIVERS AND INTERACTIONS BETWEEN DRIVERS

Two types of drivers are implemented in WAND-PIC: laser pulse and beam driver. For a laser pulse with vector potential $A_\perp = A_\perp \exp[-ik_0ξ]$, we solve the following equation for the envelope $A_\perp$ [45] in paraxial approximation:

$$\left(ik_0 \frac{2\partial}{\partial t} - \frac{2\partial^2}{\partial ξ^2} + \nabla_\perp^2 \right)A_\perp = k_0^2 \chi_a A_\perp.$$

(20)

The effective plasma susceptibility $\chi = \langle n_e/γ \rangle$ is a local-averaged quantity.

For the beam drivers, different types of macroparticles are available including electrons and a variety of ions. Driver particles are different from plasma trajectories in two ways: (i) driver particles are not subject to quasi-static approximation, instead, four independent dimensions $(x, y, z, t)$ will be used to describe them; (ii) unlike the plasma trajectories which experience averaged pondermotive push from the laser pulses, we include the high frequency laser fields $(E^L, B^L)$ to advance the driver particles. For example, consider a laser pulse which is polarized in $x$-direction has two potential components $A_x, A_z$ and $|A_x| >|A_z|$. The laser fields are we keeping in the code are:

$$\dot{E}^L_x = -\frac{\partial A_z}{\partial t} = -(\frac{\partial A_x}{\partial t} + \frac{\partial A_z}{\partial ξ}) - ik_0 A_x \exp(-ik_0ξ),$$

(21)

$$\dot{E}^L_z = \frac{\partial A_x}{\partial t} - \frac{\partial A_z}{\partial z} \approx \frac{\partial A_x}{\partial ξ} + ik_0 A_x \exp(-ik_0ξ),$$

(22)

$$\dot{E}^L_z \approx -\frac{\partial A_x}{\partial ξ} + ik_0 A_x \exp(-ik_0ξ) = -\frac{\partial A_x}{\partial x} \exp(-ik_0ξ),$$

(23)

$$\dot{B}^L_y = -\frac{\partial A_x}{\partial y} \exp(-ik_0ξ).$$

(24)
In deriving the above equations for the laser components we have used Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ and assumed $|\mathbf{E}_y| < < |\mathbf{E}_x|$ and $|\mathbf{B}_z| < < |\mathbf{B}_y|$.

Therefore, for a linear polarized (in $x$-direction) laser pulse, two electric and two magnetic components are determined from one dominant envelope $\tilde{A}_x$ (if a second polarization exists, we just need to solve one more envelop equation for $\tilde{A}_y$). For every particle, we calculate and interpolate the four (for a circularly polarized laser: six) laser field components and six wakefield components onto it. Then we use a Boris-like pusher to push particles and use the sub-cycling method to ensure the high-frequency fields are properly resolved in a small-enough time step.

Thus, when we have both laser driver and beam driver overlapped inside the bubble, i.e., in the case of DLA of witness bunch [46–52] or hybrid-driven plasma wakefield accelerator [53], the interaction between laser and particles can be accurately reproduced.

V. COMPARISON WITH FULL 3D PIC SIMULATIONS

A. Bubble driven by a beam driver with large charge

In this section, we assess the performance of WAND-PIC in simulating the wakefield driven by a beam driver with a "large" charge. In general, in the context of PWFA, we consider a normalized charge $Q \gg 1$ to be a large driver charge where $Q = k_0^2q/(4\pi e \epsilon_0)$ [39,44], and $q$ is the beam charge. Unlike the spherical model developed for a laser driver [55], the bubble boundary driven by a compact (size $\sigma < k_p^{-1}$) charge driver with $Q \gg 1$ can be described by the following equation [39,56]:

$$r_b \frac{d^2r_b}{d\xi^2} + 2 \left( \frac{dr_b}{d\xi} \right)^2 + 1 = 0, \quad (25)$$

where $r_b$ is radius of bubble as a function of $\xi$. Due to the fast-growing of $dr_b/d\xi$ term, the back of the bubble consists of very fast trajectories and a steep wakefield. The maximum momentum of a trajectory in a bubble described by Eq. (25) can be solved by the normalized bubble model [55] which yields: $p_x \approx Q$ and $p_z \approx p_z^2/2 = Q^2/2$. This calculation illustrates the challenge of simulating such a bubble in a quasi-static code: the longitudinal "velocity" in the co-moving frame: $v_x = 1 - p_z/\gamma \approx 2/Q^2$ is much smaller than the transverse velocity: $v_z \approx 2/Q$. Therefore, to have converging solutions for trajectories’ motion and wakefields, the longitudinal step size $\delta \xi$ should be smaller than transverse step size $\delta x$ and we find that $\delta \xi \leq \delta x/Q$ would be a good choice to accurately capture the steepness of back of the bubble. To make the calculation more efficient, we calculate the required $\delta \xi$ adaptively at every $\xi$ step according to the maximum transverse velocity of all trajectories: $\delta \xi \propto 1/\max(|V_\perp|)$, in this way, we make sure that finer meshes are deployed only near the back of the bubble.

In the following simulation, we choose an uniform plasma density $n_0 = 6.5 \times 10^{17} \text{cm}^{-3}$ and a 10GeV electron beam with Gaussian charge distribution: $n_e = 10n_0 e^{-x^2/\sigma_x^2 - y^2/\sigma_y^2 - z^2/\sigma_z^2}$, where $\sigma_x = \sigma_y = 6.6 \mu m$ and $\sigma_z = 8 \mu m$. The total charge of the electron beam is $q = 2nC$ which corresponds to a normalized charge $Q = 5.34$ and a peak current $I_{ph} = 45.5\,kA$. This kind of beam is not beyond the reach since a 10GeV electron beam with $q = 2nC$ and $I_{ph} = 15\,kA$ is already available at FACET-II facility at SLAC National Accelerator Laboratory [22] and electron beams with currents of 50–150 kA and durations of 3 $fs$ will soon be available in the near future [24].

We conduct the same simulations in both WAND-PIC and VLPL-3D and their results are compared in Fig. 2. The simulation box size in both codes are: $L_x \times L_y \times L_z = 4\lambda_p \times 4\lambda_p \times 2.7\lambda_p$ and the spatial resolution is 0.01$\lambda_p$ in both three directions. In Fig. 2(a), the plasma bubbles generated by WAND-PIC and VLPL-3D are compared side by side and they are in good agreement in terms of bubble length, radius, and steep closing of the bubble. Small differences are noticeable, for example, the electron sheath which closes the bubble is narrower in WAND-PIC and the beginning of the second bubble in WAND-PIC is slightly bigger. One of the most important features of the large bubble is the extremely nonlinear wakefield, an accurate reproduction of the accelerating field is essential for the estimate of final energy gain of witness and control the beam quality. In Fig. 2(b), we compare the on-axis $E_z$ from VLPL-3D and four different WAND-PIC simulations with different levels of mesh refinement: WAND-PIC (k) in the figure means the smallest step size $\delta \xi_{\min}$ will not be smaller than $1/k$ of the original step size, therefore WAND-PIC (1) means mesh refinement is turned off.

From Fig. 2(b) and its inset, we can see that WAND-PIC with mesh refinement $k \geq 4$ and VLPL-3D produce close results (difference $\approx 5\%$). Lower mesh refinement ($k = 2$) generates $15\%$ smaller peak $E_z$ and WAND-PIC without mesh refinement ($k = 1$) generates $40\%$ smaller peak $E_z$. A higher level of mesh refinement helps to calculate the trajectories’ speeds and wakefield accurately, and convergence will be reached when we increase the level mesh refinement: the WAND-PIC with $k = 4$ and $k = 8$ generate the same results as one can see from Fig. 2(b). In practice, $k = 4 \sim 8$ would be a sufficient number in most of the PWFA simulations. Because trajectories only acquire
FIG. 2: Comparison of simulation results from VLPL-3D and WAND-PIC. (a) Side-by-side comparison of plasma bubbles from VLPL-3D (upper half) and WAND-PIC (lower half). (b) Comparison of the longitudinal wakefield: $E_z$ on-axis from VLPL-3D and WAND-PIC (k) where k stands for the maximum level of mesh refinement: when the adaptive size is smaller than the $1/k$ of original step size, mesh refinement will stop automatically. (c) Comparison of the transverse focusing wakefield $E_x - B_y$ as a function of $x$ at the center of the bubble. (d) Normalized runtime of WAND-PIC (k) for different levels of mesh refinement k.

relativistic speed at the back of the bubble, most of the mesh refinement process will take place at a small region where the electron sheath is very narrow. Therefore, the wakefields everywhere other than the back of the bubble will still be solved accurately even without the mesh refinement. As shown in Fig. 2(c), the focusing fields $E_x - B_y$ at the bubble center from VLPL-3D and WAND-PIC are almost identical regardless of the level of mesh refinement. Due to the same reason, the overall runtime of the code will not increase too much even for very large $Q$ as we increase the level of mesh refinement. Fig. 2(d) shows the runtime of WAND-PIC with different k, most of the change in runtime happens when we increase from $k = 1$ (no refinement) to $k = 2$ and the runtime increased by 20%. As $k$ increases to 14 the runtime only increases a little since $k = 4$ is enough to get the desired trajectory speed.

This example shows that the adaptive mesh refinement in WAND-PIC is a useful and necessary technique to simulate the big bubble in PWFA. During the investigation, we found that the effectiveness of adaptive mesh refinement largely relays on the development of "$\partial_\xi$-free" sources for all wakefield equations: without using the predictor-corrector, straightforward integration of trajectories in $\xi$ direction is always stable as long as enough mesh downsizing is performed. In fact, quasi-static codes with predictor-corrector show unstable performance when $Q \gg 1$. It’s common that even with a small enough step size $d\xi$ and a large number of predictor-corrector iterations, the predictor-corrector would still fail to converge due to numerical instability at the back of the bubble. Sometimes in such code, one can use fairly large $d\xi$ and 1st order predictor-corrector to work around this issue since in this way trajectories’ speeds would be underestimated at the back of the bubble. Another workaround people normally use in quasi-static codes with predictor-corrector is adding speed limitation on trajectories or truncating the size of the domain to avoid simulating
the back of bubble, none of these methods can produce accurate wakefield at the back of bubble as WAND-PIC does when drive charge is large. Driver charge as big as $Q = 100$ has been simulated in WAND-PIC \[39\].

B. Direct laser acceleration of electrons in quasi-static code

![Comparison of direct laser acceleration (DLA) in VLPL-3D and WAND-PIC. (a) Side-by-side comparison of plasma bubbles and injected electron bunches from VLPL-3D (upper half) and WAND-PIC (lower half) at propagation distance $z = 1.15\text{mm}$. (b) Phase space ($W_\parallel, W_\perp$) of the injected electrons color-coded by their relativistic factor $\gamma$ at the propagation distance $z = 1.15\text{mm}$. (c) For VLPL-3D and (c) for WAND-PIC. Insets: energy spectra. Dashed black curve in (b) encloses the phase space obtained from VLPL-3D simulation with lower resolution $P_{\text{pump}} = P_{\text{DLA}} = 21\text{TW}$. The pump pulse and DLA pulse have the same power and wavelength: $\lambda_{\text{pump}} = \lambda_{\text{DLA}} = 0.8\mu\text{m}$. The duration and spot size of pump pulse: $\tau_{\text{pump}} = 16.6\text{fs}$, $w_{\text{pump}} = 8.7\mu\text{m}$. The duration and spot size of DLA pulse $\tau_{\text{DLA}} = 9.4\text{fs}$, $w_{\text{DLA}} = 5.5\mu\text{m}$.](image)

In this section, we use WAND-PIC to simulate the direct laser acceleration of electrons in the bubble regime and compare the results with a 3D full PIC code. In the context LWFA, the electrons inside a plasma channel or plasma bubble can gain energy directly from the laser through the DLA mechanism if the driver pulse overlaps with them \[48, 49\], or, when an additional DLA pulse is added to the location of electron bunch \[40, 47, 50\]. The DLA mechanism can happen in a long plasma channel where longitudinal wakefield is zero \[58\], or in the accelerating portion of the bubble \[46, 48\], or even in the decelerating portion of the bubble \[51\], as long as the Doppler-shifted frequency $\omega_D = \omega_L (1 - v_z / v_{ph})$ of the laser field matches the electrons’ betatron frequency $\omega_\beta = \omega_p / \sqrt{2\gamma}$ in the channel/bubble. Here $\omega_L$ and $v_{ph}$ are the laser frequency and phase velocities, respectively, and $v_z$ is the longitudinal particle velocity. The actual description is complicated by the fact that the $\langle \omega_D \rangle = \langle \omega_\beta \rangle$ relationship is only satisfied on average \[48, 55\] because of the rapid nonlinear variation of $v_z$ during one betatron period $T_\beta = 2\pi / \omega_\beta$. The result of such relativistic nonlinearity of the laser-particle interaction is an irregular (stochastic) motion of the accelerated electrons \[59\] and high sensitivity of the gained energy to the spatial-temporal resolution \[51\].

In order to understand whether or not the WAND-PIC can capture accurately and efficiently the details of DLA in bubble regime. We design following simulation setup: a leading pump pulse and a trailing DLA pulse separated by a distance of $\Delta \tau = 33\text{fs}$ are launched into a tenuous plasma with density $n_0 = 7.7 \times 10^{18}\text{cm}^{-3}$ (more pulse parameters can be found in the caption of Fig. 3). Both pulses are polarized in $x$ direction. A short electron bunch with negligible charge is injected to the center of the DLA pulse with initial momentum $p_z = 15mc$, duration $\tau_0 = 4\text{fs}$ and transverse size $w_{\text{bunch}} = 3\mu\text{m}$. We propagate the pulses and electron bunch up to the dephasing distance $z = L_{\text{deph}} = 1.15\text{mm}$ and check the energy gain of the electrons from both wakefields and laser fields. Two simulations are conducted in VLPL-3D with two sets of resolutions: (1) $\delta x = \delta y = \lambda_L / 5$, $\delta z \approx c \delta t = \lambda_L / 100$ and (2) $\delta x = \delta y = \lambda_L / 25$, $\delta z \approx c \delta t = \lambda_L / 50$. Same simulation is conducted in WAND-PIC, the resolutions are: $\delta x = \delta y = \lambda_L / 6.28$, $\delta z = \lambda_L / 16.7$, $c \delta t = \lambda_L / 2$ with number of sub-cycling $N_{\text{sub}} = 50$. In WAND-PIC the longitudinal step size and time step size are much bigger.

This setup is particularly interesting because the tightly focused/guided DLA pulse in the back of the bubble will have a non-vanishing longitudinal electric field component: $|E_0^\parallel| \propto x|E_0^\perp| / (k_0 R^2)$ \[52, 50\], where $x$ is the transverse coordinate. For bubble radius $R \sim k_0^{-1}$ and a relativistic laser pulse $\epsilon |E_0^\perp| / mc\omega_L > 1$, the electrons undulating with betatron amplitude $\sim R$ will experience comparable longitudinal laser electric field and longitudinal bubble electric field. An accurate simulation of direct laser acceleration of electrons in this setup would help to understand the energy transfer from different components of fields to the electrons.

Simulation results of VLPL-3D and WAND-PIC are presented in Fig. 3. Fig. 3(a) shows the side-by-side comparison...
of plasma bubbles and electron bunches at propagation distance $z = 1.15$mm from VLPL-3D (resolution set (1)) and WAND-PIC. The bubble sizes are similar in both simulations. However, in WAND-PIC simulation, there is no self-injection at the back of the bubble and the bubble boundary is more clear and defined. The electron bunches in VLPL-3D and WAND-PIC have similar transverse sizes under the action of DLA and have both advanced to the same positions inside the bubble. The electron bunch in WAND-PIC shows less stretching in longitudinal direction. To evaluate the reproduction of DLA in both codes, we plot the workdone phase space $(W_{||}, W_{\perp})$ for all electrons in Fig. 3 (b) for VLPL-3D (resolution set (1)) and in Fig. 3 (c) for WAND-PIC, respectively. The workdone $W_{||}$ and $W_{\perp}$ are defined as follows:

$$W_{||} = -e \int (E_{z}^{L} + E_{z}^{W}) \cdot v_{z} dt,$$

$$W_{\perp} = -e \int E_{\perp} \cdot v_{\perp} dt \approx -e \int E_{z}^{L} \cdot v_{z} dt,$$

where $E_{z}^{L}$ and $E_{z}^{W}$ are longitudinal and traverse laser electric field respectively and $E_{z}^{W}$ is the longitudinal wakefield. As shown in Fig. 3 (b) and (c), the results from VLPL-PIC and WAND-PIC are very close to each other. Not only the absolute gains in longitudinal and traverse directions are close in two codes, but also the distributions in phase space are in good agreement, indicating that the WAND-PIC is accurately modeling the components of the laser and the interaction between the laser and electrons through the sub-cycling method. The insets in Fig. 3 (b) and (c) show the energy spectrum of all electrons obtained from VLPL-3D and WAND-PIC, they are in good agreement in terms of energy range and shapes (three-peak feature). Note that the black-dashed contour in Fig. 3 (b) encloses the phase space $(W_{||}, W_{\perp})$ obtained from VLPL-3D with a lower resolution (resolution set (2)): $\delta z \approx \delta t = \lambda_{L}/50$. In that simulation, the energy gain from the traverse electric field of the laser is underestimated by 30%, this will influence the final energy distribution of the electrons as well as the radiation output associated with betatron oscillation. Fig. 3 (b) tells us, to capture the sophisticated interactions between electrons and laser fields, a normal PIC code needs a longitudinal/time resolution around $\lambda_{L}/100$. However, the WAND-PIC is able to simulate the bubble evolution and DLA mechanism separately by using coarse resolution for the former and sub-cycling for the latter. For comparison, in this particular setup, the WAND-PIC uses two order of magnitude less core-hours compare to the VLPL-3D.

VI. ALGORITHM, EFFICIENCY AND SCALING

Since we have developed explicit source terms for all equations which don’t need a predictor-corrector, the algorithm design and code structure are greatly simplified and straightforward. The whole algorithm consists of two main loops: i) time loop and ii) $\xi$ loop. At every time step in the first loop, the driver is “frozen” in the moving frame and plasma trajectories and fields are advanced in positive $\xi$-direction. In the inner $\xi$ loop, at each $\xi$ slice, the source terms: currents and number densities of the plasma trajectories are deposited onto the grid, and fields are solved exactly at the same slice using the multigrid solver. Then the fields are interpolated to trajectories’ positions and a Boris-like pusher is used to advance trajectories (1st, 2nd, and 4th-order Runge-Kutta are also available). After the $\xi$ loop is finished, driver particles are advanced in time using a volume-preserving algorithm (VPA) [61] and their currents are also collected and deposited. In the case of laser driver, the envelop equation is similar to the time-dependent Schrodinger equation, it can be rearranged to a Poisson-like equation and solved also by our multigrid solver.

The multigrid solver is chosen in WAND-PIC instead of the commonly used FFT solver (used by QuickPIC and HiPACE) for several reasons. First, it naturally fits into the 2D square partitioning of the domain and the communication between subdomains are local: one subdomain only communicates with four adjacent neighbors as shown in Fig. 1. However, a 2D FFT solver requires a complicated global communication scheme and a huge amount of overheads. Second, multigrid solver potentially has better time complexity: $O(n)$ compare to an ideal FFT method: $O(n \log(n))$, where $n$ is the problem size. Third, since multigrid is an iterative method, a good initial guess of the solution can be applied to accelerate the solving process, for example, in WAND-PIC we use the field at the previous $\xi$ step or previous time step as the initial guess. We found that in WAND-PIC, a multigrid solver with an initial guess is two times faster compared with a zero initial guess.

To assess the overall performance of the WAND-PIC under parallelization, benchmarking is conducted and the strong scaling, weak scaling, and time complexity are obtained and shown in Fig. 4. Note that scalings and efficiency may vary with the different problems we are solving, for example, a linear regime and a blowout regime would generate different loads on cores. Therefore we concentrate on a common situation: a fully-blowout spherical bubble driven by the laser pulse and we choose the domain size to be three times of bubble size — the characteristic length of the solution is fixed. Fig. 4 (a) shows the strong scaling where the transverse problem size is fixed to be $1000 \times 1000$. WAND-PIC shows a good linear speedup up to 3000 cores (there was run-to-run variance due to the hardware). Fig. 4 (b)
shows the overall time complexity of the WAND-PIC (where approximately 80% of the runtime are consumed by the multigrid solver), the number of cores is fixed to be 64 and we change the normalized problem size $n$ by changing the transverse resolution, the base problem size ($n = 1$) is $320 \times 320$. The time complexity of WAND-PIC shows $O(n)$ at a smaller problem size but deviates from $O(n)$ at a larger problem size. Overall, WAND-PIC shows a time complexity between $O(n)$ and $O(n \log(n))$. At last, Fig. 4(c) shows the weak scaling where the problem size per core is fixed. The parallel efficiency remains 83.3% at 500 cores and becomes 62% at 3000 cores. Efficiency decreases due to the increased overheads when more cores are added. Sources of overheads include i) fast trajectories cross more subdomains when more cores are included therefore require more send/receive operations; ii) increased inter-nodes communication of the hardware (Lonestar 5 has 24 cores per node). There is still a lot of space for us to improve the efficiency of the WAND-PIC when load balancing is implemented in the future.

![Graphs showing WAND-PIC benchmarking](image)

**FIG. 4**: WAND-PIC benchmarking: the benchmarking are conducted on the Lonestar 5 Architecture (Xeon E5-2690 v3). (a) Strong scaling of WAND-PIC, transverse problem size (number of cells) is fixed to be $1000 \times 1000$. (b) The algorithm time complexity of WAND-PIC. While changing the problem size, the number of cores we used is fixed. (c) Weak scaling of WAND-PIC, transverse problem size per core is fixed.

## VII. FUTURE DEVELOPMENT AND CONCLUSION

Since the first release of WAND-PIC in 2019 [1], it has been under continuous improvement. The new features we are developing now include i) parallelization in longitudinal dimension though the pipeline technique [35, 37] which would extend our scalability to hundreds of thousands of cores; ii) automatic load balancing which would reduce the overheads and improve the efficiency; iii) transverse local mesh refinement which would improve the level of details in the physical region we are interested in, for example, the back of the bubble and witness beam; iv) better multigrid cycles and smoothers which would improve the multigrid solver performance. These changes will be applied in the near future and be released to the open-source community.

In conclusion, a new quasi-static 3D parallel PIC code: WAND-PIC has been introduced in this work. With the advanced quasi-static equations which are fully explicit and static, wakefields driven by the relativistic beams or laser pulses are solved without using the predictor-corrector method. WAND-PIC has implemented different types of drivers as well as the interactions between the drivers and is able to simulate various scenarios in the plasma-based accelerators. Comparison between the results of WAND-PIC and a 3D full PIC code (VLPL) show that the WAND-PIC is efficient and accurate in modeling the large bubble driven by a large beam charge and the direct laser acceleration of electrons in the bubble. Good parallel scalings and time complexity are achieved by the use of parallel multigrid solver and the simplified, explicit field-solving procedures.

## VIII. ACKNOWLEDGMENTS

This work was supported by the DOE grant DE-SC0019431. The authors thank the Texas Advanced Computing Center (TACC) at The University of Texas at Austin for providing HPC resources. The authors would like to also
thank Dr. Roopendra Singh Rajawat for inventing the name "WAND-PIC" and Ji Hoon Kim for useful discussions.

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