QuickPIC: a highly efficient fully parallelized PIC code for plasma-based acceleration

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Abstract. A highly efficient, fully parallelized, fully relativistic, three-dimensional particle-in-cell model for simulating plasma and laser wakefield acceleration is described. The model is based on the quasi-static approximation, which reduces a fully three-dimensional electromagnetic field solve and particle push to a two-dimensional field solve and particle push. This is done by calculating the plasma wake assuming that the drive beam and/or laser does not evolve during the time it takes for it to pass a plasma particle. The complete electromagnetic fields of the plasma wake and its associated index of refraction are then used to evolve the drive beam and/or laser using very large time steps. This algorithm reduces the computation time by 2 to 3 orders of magnitude without loss of accuracy for highly nonlinear problems of interest. The code is fully parallelizable with different domain decompositions for the 2D and 3D pieces of the code. The code also has dynamic load balancing. We present the basic algorithms and design of QuickPIC, as well as comparison between the new algorithm and conventional fully explicit models (OSIRIS). Direction for future work is also presented including a software pipeline technique to further scale QuickPIC to 10,000+ processors.

1. Introduction
Particle accelerators play important roles in scientific discovery. Due to their versatility, they have found many applications in science and technology. For example, they are the major components of linear colliders which probe the fundamental structure of elementary particles. In the state-of-the-art linear collider, i.e., the Stanford Linear Collider (SLC), 50 GeV electron and positron beams are collided. For the next ambitious world-class collider, i.e., the International Linear Collider (ILC), the electron and positron beams will collide with center of mass energies from 500 GeV up to 1 TeV. Synchrotron light sources, which are invaluable tools for studying objects at the molecular and atomic level, also depend on particle accelerators to generate high quality multi-GeV electron beams. Since
conventional and superconducting RF technology can support a maximum accelerating field < 50MeV/m, the required length for acceleration is several tens of kilometers for a TeV collider and more than hundreds of meters for a synchrotron light source.

It is well known that plasmas can sustain very high acceleration gradients on the order of \( \sqrt{n_0 (cm^{-3})} \) eV/cm, where \( n_0 \) is the plasma density. When an intense short electron or laser pulse is propagated into an underdense plasma, the plasma electrons are evacuated by the space charge force or the light pressure, forming an ion column. Plasma electrons are then drawn back by the stationary ions making a sphere-like wake structure. The plasma wakefield excited by the electron/laser beam has a longitudinal component which also scales as \( \sqrt{n_0 (cm^{-3})} \) eV/cm and a transverse component which provides a linear focusing force for the electrons. The wake moves at the speed of the driver, therefore it can be used to accelerate an externally or self-injected trailing electron beam. Such plasma/laser wakefield accelerator (PWFA/LWFA) concepts have shown tremendous progress over the past few years. In the recent E167 experiment conducted at SLAC, 3 ~ 4 GeV energy gain over 10 cm long plasma section was reported [1]. The substantial energy gain is obtained by sending a 28.5 GeV electron beam into a Lithium vapor with a density of \( 3 \times 10^{17} cm^{-3} \). The beam is strong enough to ionize Lithium atoms and the tail of the beam experiences an accelerating field on the order of 10GeV/m in the Lithium plasma wake. In 2004, three independent groups reported on generating quasi-monoenergetic electron beams with a central energy around 100~200MeV in LWFA experiments in millimeter-long gas jets [2]. These experiments have affirmed the feasibility of compact plasma-based accelerators.

Despite the success of recent PWFA/LWFA experiments, much nonlinear beam (laser)-plasma interaction physics issues need to be understood and controlled in order to scale the current experiments up to a future high gradient accelerator. These problems include, the efficient transfer of energy from the driver to a trailing beam, the transverse dynamics and stability of ultra-relativistic beams, the X-ray radiation loss, the beam erosion in the self-ionized plasma, the guiding and pump depletion of the laser driver, and the external injection of particle beam into the wakefield structure.

To understand these issues, especially in a complicated experimental setup, significant advances in both the theory and computer modeling are required. Accurate 3D particle-based computer models are now routinely used to simulate past experiments conducted at the Stanford Linear Accelerator Center(SLAC), Lawrence Berkerley National Laboratory(LBNL), Rutherford Appleton Laboratory (RAL), and Laboratoire d'Optique Appliquée(LOA), and they provide many insights into the experiments. These computer models, such as OSIRIS [5], VORPAL [6], turboWAVE [7], and VLPL [8], are based on the Particle-In-Cell method [9] and include a full electromagnetic field model. However, the vast time scale differences between the beam/laser evolution and the plasma response make such a full electromagnetic model inefficient and impractical to simulate a 100~1000GeV PWFA afterburner [10] stage or a 1~10GeV LWFA stage. Under SciDAC I, we have developed a fully non-linear quasi-static parallel PIC code, QuickPIC, which enabled us to conduct the first full scale simulations for a TeV PWFA stage with 100~1000 times less CPU resources as compared to the full PIC model. Recently, we have also included the capability to model a laser driver in QuickPIC using the ponderomotive guiding center description. The QuickPIC code represents a significant improvement in simulating plasma-based acceleration and it is now an essential tool for making important quantitative predictions of PWFA/LWFA experiments.

2. QUASI-STATIC PIC MODEL

2.1. Particle-In-Cell method

In a full electromagnetic PIC algorithm, the simulation domain is divided into grids. These grids are usually uniform and the charge and current densities are defined at the grid points. Plasma particles are represented by macro-particles. They are loaded onto the grid and their current and charge are assigned to the nearby grid points. The Maxwell’s equations
\[ \frac{1}{c} \frac{\partial B}{\partial t} = -\nabla \times E \quad \text{and} \quad \nabla \times B = \frac{4\pi}{c} j + \frac{1}{c} \frac{\partial E}{\partial t} \]

are discretized on the grid with \( E \) and \( B \) defined on the Yee-mesh \([11]\). These two equations are also time-centered to allow consecutive updates of \( E \) and \( B \) respectively. The updated fields are used to advance the particles to new positions and velocities via the relativistic equation of motion

\[ \frac{dP}{dt} = q \left( E + \frac{V \times B}{c} \right), \quad \frac{dx}{dt} = v \frac{m}{\gamma} \]

2.2. Computational challenge

The finite difference form of the full electromagnetic PIC algorithm described above is usually second order accurate, but the grid size has to resolve the smallest wavelength in the simulation. For PWFA, this typically requires \( \Delta x < 0.05 \frac{c}{\omega_p} \), where \( \Delta x \) is the grid size and \( \omega_p \) is the plasma frequency. For LWFA, the longitudinal grid size has to resolve the laser wavelength, \( \Delta z < 0.05 \lambda \). The time step \( \Delta t \) is subject to the numerical stability requirement, i.e., the Courant condition \( \Delta t < \Delta x \sqrt{3} \), for 3D simulations with cubic cells.

Due to the accuracy and stability requirements, a 3D simulation using a full electromagnetic PIC code is computationally challenging. For the typical simulation parameters in Table 1 and 2, to simulate a 1 GeV PWFA/LWFA stage on Seaborg (IBM SP3 platform) requires 5,234/1.2E5 node-hours, and to model a 50 GeV PWFA experiment requires 261,712 node-hours. Even with the fastest supercomputer today, it will be impractical to simulate a TeV PWFA or a 10 GeV LWFA stage.

The root of the challenge is the full electromagnetic field solver. A reduced description model for LWFA, called the ponderomotive guiding center model, takes advantage of the fact that particles oscillate in the laser field but their averaged motion does not contain high frequency oscillations. The averaged orbit can be determined by the envelope function of the laser field. Therefore the requirement that the longitudinal grid size has to resolve the laser wavelength can be relaxed. The ponderomotive guiding center approach reduces the computation need by roughly a factor of \( \frac{22}{20} \) but it will still take \( \sim 5,000 \) node-hours to model a 1GeV LWFA stage.

2.3. Quasi-static approximation

There are two intrinsic time scales associated with the PWFA and LWFA. For a PWFA the drive beam is ultra-relativistic (the Lorentz factor of the beam \( \gamma_b > 2000 \)), so it evolves on the scale of the betatron wavelength \( \frac{c}{\sqrt{2\gamma_b \omega_p}} \), which is much longer than the plasma wavelength. For a 50 GeV beam this is a factor of \( \sim 500 \) times longer. While for a LWFA, the laser beam evolves on the scale of
Rayleigh length \( z_R = \frac{\pi w_0^2}{\lambda} \), where \( w_0 \) is the laser spot size and \( \lambda \) is the laser wavelength. For the laser parameters in Table 2, the Rayleigh length is \( \sim 70 \) times longer than the plasma wavelength. Therefore, it is possible to separate the time scales of the particle/laser beam and the plasma evolution and assume that the driver does not evolve during the time a plasma electron takes to pass the driver beam. The plasma response can then be calculated by “freezing” the driver and the fields associated with it. This approach is called the quasi-static approximation. We have successfully implemented it in a parallel PIC code, QuickPIC [12].

QuickPIC solves a reduced set of Maxwell’s equations in the Lorentz gauge, which results from the quasi-static approximation. In the moving window coordinates \((x, y, s = z, \xi = ct - z)\), for which \( s \) denotes the propagation distance of the moving window and \( \xi \) denotes the position in the window, the reduced Maxwell’s equations can be expressed as,

\[
-\nabla_z^2 \phi(x, y, s, \xi) = 4\pi \rho(x, y, s, \xi),
\]

\[
-\nabla_z^2 A(x, y, s, \xi) = 4\pi J(x, y, s, \xi)/c.
\]

Where \( \phi \) and \( A = A_z + A_\xi \hat{z} \) are the scalar and vector potential in the Lorentz gauge respectively, and they are related to each other by \( \nabla_z \cdot A(x, y, s, \xi) = -\frac{\partial \psi(x, y, s, \xi)}{\partial \xi} \), where \( \psi \equiv \phi - A_z \). It is worth noting that the quasi-static approximation implies \( \rho, J, \phi \) and \( A \) depend weakly on the variable \( s \), hence \( s \) can be dropped from the expressions. Therefore these two equations are Poisson-like equations whose sources and solutions are defined on each transverse slice with \( \xi \) being a parameter.

For the plasma particles, \( \xi \) can be viewed as the fast time variable. The corresponding equations of motions are

\[
\frac{dP_{p,\perp}}{d\xi} = \frac{q_p}{c - V_{pe}}\left[ E_{\perp} + \left( \frac{V_p}{c} \times B \right)_{\perp} \right],
\]

\[
\frac{dX_{p,\perp}}{d\xi} = \frac{V_{p,\perp}}{1 - V_{pe}/c}.
\]

The longitudinal momenta are related to the transverse momenta and \( \psi \) through the following relation [13],

\[
P_{p,\xi}/(m_ec) = \frac{1 + P_{p,\perp}/(m_ec^2)}{2[1 - q_p \psi/(m_ec^2)]^2} - [1 - q_p \psi/(m_ec^2)]^2
\]

It is further assumed that the longitudinal displacement of the plasma particle is small during the time for the driver to pass by. QuickPIC uses a 2D PIC algorithm for updating the plasma particles and the electric and magnetic fields are solved for in each slice. Then the driver can be updated using the appropriate equations for the beam or for the laser. Figure 1. illustrates the loop for the quasi-static algorithm.

For the slowly evolving beam, \( s \) can be viewed as the slow time variable. The equations of motion for a beam particle are,

\[
\frac{dP_{b,\perp}}{ds} = -\frac{q_b}{c} \nabla_b \psi, \quad \frac{dP_{b,\xi}}{ds} = \frac{q_b}{c} \frac{\partial \psi}{\partial \xi}
\]
\[
\frac{dX_{b\perp}}{ds} = \frac{P_{b\perp}}{\gamma m_c}, \quad \frac{d\xi}{ds} = 1 - \frac{P_{b\perp}}{\gamma m_c}.
\]

For a laser driver, the ponderomotive guiding center description is used. The envelope of the laser is updated using the following paraxial equations,

\[
2 \frac{\partial}{\partial s} \left(-ik_0 + \frac{\partial}{\partial \xi}\right) \hat{a} - \nabla^2 \hat{a} = \frac{4\pi e}{m_c^2 c^2} \hat{J} = k_0^2 \chi_\rho \hat{a}
\]

where the plasma modification to the susceptibility is

\[
\chi_p = -\left(\frac{\omega_p^2}{\omega_0^2 + \omega_p^2}\right) = -\frac{4\pi e^2}{m_e \omega_0^2} \frac{1}{\text{Volume}} \sum \frac{1}{f_p (1 - V_{pe} / c)}.
\]

The plasma electrons now respond to the laser through the ponderomotive force,

\[
\frac{dP_{p\perp}}{ds} = \frac{q_p}{c - V_{pe}} \left( E_{\perp} + \left( \frac{V_p}{c} \times \mathbf{B}_{\perp}\right) - \frac{m_e c^2}{\gamma_p} \nabla_{\perp} \frac{|\mathbf{p}|^2}{4}\right).
\]

![Diagram](image)

**Figure 1.** The driver evolves slowly and can be updated on a slow time scale; the plasma response is solved for in a transverse 2D slice with the fast time scale. Both algorithms for the driver and the plasma are fully parallelized.

2.4. Code features

QuickPIC is constructed on an object-oriented PIC Framework UPIC [14] based on the modern Fortran language. UPIC provides high level objects such as scalar field and vector field objects for high performance computing. These objects support 1D domain decomposition and dynamic load-balancing. The Framework includes spectral field solvers and also contains fast Sin/Cos transforms to allow optimal performance for conducting boundary conditions.

As new ideas in plasma-based accelerator experiments appear, new physics models have been integrated into QuickPIC. Recently, it has been suggested that an intense electron beam can ionize Lithium vapor and create the plasma along the beam path [15]. To study the self-ionized PWFA
experiments, an ionization module based on the ADK model has been developed and successfully benchmarked against a similar package in the full PIC code OSIRIS. The synchrotron radiation damping effect from the betatron motion of the beam electron is found to be important in recent PWFA experiments. Radiation damping effect has recently been included in QuickPIC providing better agreement between the simulation results and the experimental data. A third area of improvement is the addition of a plasma channel in the code which is required to model cutting-edge experiments on channel-guided LWFA experiments.

Furthermore, we have developed the capability to study ion motion in PWFA. This effort will provide better understanding of future PWFA experiments.

3. Benchmarks
QuickPIC has been tested in many scenarios and the results are in good agreement with the full PIC code OSIRIS. Here we present four different benchmarks in figure 2. The first benchmark is done for an electron beam driver. The transverse and longitudinal profile of the electron beam are Gaussian with $\sigma_r = 7\mu m$ and $\sigma_z = 45\mu m$ respectively. The total number of electrons is $N = 1.8 \times 10^{10}$. The beam is ultra-relativistic with $\gamma = 55800$. The plasma density is $n_0 = 2.0 \times 10^{16} \text{cm}^{-3}$. The peak beam density is $n_b / n_0 = 25.9$. The second benchmark is for a positron beam driver, it has $N = 1.8 \times 10^{10}$ positrons with $\gamma = 55800$. The beam spot sizes is $\sigma_r = 25\mu m$ and $\sigma_z = 600\mu m$ respectively. The plasma density is $n_0 = 2.0 \times 10^{14} \text{cm}^{-3}$, the peak density ratio is $n_b / n_0 = 15.2$.

The third benchmark shows the comparison of the longitudinal wakefield in a plasma ionized by the electron beam driver. The beam has $N = 2 \times 10^{10}$ electrons with $\sigma_r = \sigma_z = 20\mu m$. The neutral gas density is $n_0 = 1.25 \times 10^{17} \text{cm}^{-3}$. The last benchmark is done for a laser driver with normalized...
vector potential \( a = 2 \). The laser has \( t_{\text{rise}} = t_{\text{fall}} = 30 \, \text{fs} \) and the wavelength is 800 nm. The plasma density is \( n_0 = 1.38 \times 10^{19} \, \text{cm}^{-3} \). The transverse profile is Gaussian and the focused spot size is \( w_0 = 13.66 \, \mu\text{m} \) FWHM at the plasma entrance.

In all four benchmarks the plasma responses are in the highly nonlinear regime, thus these benchmarks indicate of the validity and robustness of the quasi-static model.

### 4. Modeling PWFA and LWFA experiments

QuickPIC has been used to model a series of PWFA experiments conducted at SLAC. Among these experiments, the recent E167 experiment was carried out in the self-ionization regime [1]. In this experiment, 28.5 GeV electron bunches each with a charge of 3nC \( (1.8 \times 10^{10} \, \text{electrons/positrons}) \) are generated in the SLAC linear accelerator. The electron bunches are tuned to have an energy chirp before entering the chicane. They are subsequently compressed to 12 \( \mu\text{m} \) in two stages through the chicane and a double bend. The peak beam current reaches more than 10kA and the beam space charge force is strong enough to ionize the Lithium vapor in an oven. The beam propagates in the Lithium plasma created by itself and excites plasma wakefields. The length of the Lithium oven is varied from 10cm to 30cm and the energy of the part of the beam which feels the accelerating field is measured against the length of the plasma.

In the QuickPIC simulation, the experimentally measured profile of the Lithium vapor is used. The observed energy gain in the simulation is plotted against the propagation distance for different Lithium profiles in figure 3. The maximum energy gain in the simulation is in good agreement with the experiment data. QuickPIC simulations have also helped to identify beam head erosion as a key physics process limiting the energy gain in an energy doubling PWFA experiment.

![Figure 3](image-url)

Figure 3. QuickPIC simulation result for the energy gain versus the plasma length for different Lithium oven lengths in the E167 PWFA experiment. Red diamonds/green squares/ blue diamonds are the Lithium oven profile with three different lengths and red crosses/green crosses/blue triangles are the corresponding energy gain of the beam.

Recently, QuickPIC has also been applied to study a state-of-the-art LWFA experiment with channel guiding. The laser in this experiment has a modest power so relativistic self-focusing effect is
weak. The plasma channel then acts as an optical fiber to confine the laser while it propagates. The plasma channel is created using a capillary discharge and is modeled as a parabolic profile for which the center of the channel has a lower density than the edge. We have added a module which is able to generate a plasma channel with an arbitrary profile in QuickPIC. Figure 4 shows a snapshot from the simulation at a propagation distance for which the laser beam is focused such that it blows out plasma electrons at the center of the channel.

Figure 4. QuickPIC simulation of a LWFA experiment with a plasma channel that demonstrates laser guiding. The laser is shown in orange color in the 2D projection on the bottom and at the right hand side wall. The plasma density is shown in 3D contours.

QuickPIC has also been used to study a design of self-guided LWFA with a 200TW laser. Such lasers are just becoming available. Combining QuickPIC and OSIRIS simulations allow the derivation and testing of scaling laws to extrapolate LWFA towards parameters of interest to high-energy physics. The QuickPIC simulation took 192 node-hours to run which is more than 200 times faster than the 3D OSIRIS simulation with the same parameter. The results are being compared to the OSIRIS simulation and so far the agreement for both the wakefields and the laser evolution are excellent.

5. Scaling quasi-static model to peta-scale platform
The quasi-static algorithm currently only scales to ~100 processors for large problems because of the 2D plasma solver. In the QuickPIC 2D plasma solver, $\xi$ is viewed as a time variable so the calculation is sequential in $\xi$. The plasma slice is updated for every $\Delta \xi$ as the driver pass through. An analogy can be made to the processing of an instruction stream in a CPU, where the plasma slice is similar to an instruction and the plasma solver can be viewed as an execution unit. Furthermore there is no information being passed backward in $\xi$, this feature will allow QuickPIC to adopt a software pipelining technique to achieve much greater parallelism. Using this technique multiple copies of the code can be started simultaneously, each one works on a different part in $\xi$ of the beam and passes the results to the one working on the part which immediately follows. Figure 5 shows a diagram of a 4-stage pipeline in QuickPIC. Speedup is achieved by adding more pipeline stages to the workflow, which is similar to the case of a modern CPU where pipelining increase throughput.
If the number of pipelined stages is $N$, the code speeds up by approximately $N$ times over its current speed. For a high resolution run with $1024 \times 1024 \times 1024$ grids, this number can be as large as 128. Since the 2D plasma solver in the code will run efficiently on 128 processors with $1024 \times 1024$ grids, it would be possible to scale QuickPIC to 16,384 processors with high parallel efficiency.

![Diagram of the software pipeline design in QuickPIC](image)

Figure 5. The software pipeline design in QuickPIC. A 4-stage pipeline is shown, each stage consists of a plasma solver and a beam solver.

6. Conclusions

We have developed a highly efficient parallel PIC code, QuickPIC, for modeling plasma-based acceleration. This code is based on the quasi-static model which takes advantage of the vast time scale difference in the problem (For a PWFA/LWFA, this is the difference between the time scales for the plasma and for the electron/laser beam to evolve; in the case of a LWFA, there is an additional difference between the time scales of the laser oscillation and plasma oscillation) and greatly reduce the amount of computation needed to simulate current and future PWFA/LWFA experiments. QuickPIC has been successfully benchmarked against the 3D full electromagnetic PIC code OSIRIS. QuickPIC simulations have also been validated against recent PWFA experiments and helped to identify the key physics which saturates the energy gain in the experiment. QuickPIC is 100–1000 times more efficient than a full electromagnetic PIC code, therefore it enables scientific discovery by exploring the parameter space which is not easily accessible for full PIC codes. To scale QuickPIC to future peta-scale computing platforms, we have proposed (and begun to implement) a software pipelining technique which exploits another level of parallelism in the quasi-static model. Preliminary result shows good scalability of this approach. In the near future, we also plan to add adaptive mesh refinement by incorporating it into the UPIC framework. Appropriate algorithms for including self-trapped particles under the quasi-static model are essential for studying “dark currents” in PWFA/LWFA and we are currently addressing this need.

We acknowledge useful conversations with the E167 team and the rest of the SciDAC accelerator team. This work was supported by the US Department of Energy through grants DE-FC02-01ER41179, DE-FG03-92ER40727, and DE-FG02-03ER54721, DE-FG02-03NA00065, DE-FG02-97ER41039, DE-FG02-92ER40745 and DE-FC02-01ER41192, by ILSA at LLNL under W-07405-ENG48 and by NSF under NSF-PHY-0321345. Simulations were done at NERSC and on the DAWSON Cluster.
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