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Three-Dimensional Particle-in-Cell Simulations of Laser Wakefield Experiments

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Abstract. Plasma accelerator methods offer the potential to reduce the size of moderate and high energy accelerators by factors of 1000. In the past few years great advances have been made in the production of low emittance, high quality (i.e., monoenergetic) electron beams with energies between .1 and 1 GeV using ultra-fast (< 50 femtoseconds), high power (> 10TW) lasers. The most noticeable of these advances were the experimental results presented in the "Dream Beam" issue of Nature and in a recent issues of Physical Review Letters, Nature, and Nature Physics. The experimental progress have been made due to advances in lasers, diagnostics, plasma sources, and the knowledge of how to control of this highly nonlinear acceleration process. And this experimental progress has occurred simultaneously with and been in part due to advances in modeling capabilities. Using a hierarchy of particle-in-cell (PIC) codes OSIRIS, VORPAL, and QuickPIC, we have performed numerous full scale 3D simulations using parameters quoted from the *Nature* and *Nature Physics* articles. Our simulations have predicted results, provided agreement between simulations and experiments (within the shot-to-shot variations of the experiments), and provided insight into the complicated physics of the experiments. Most importantly, as our confidence in the fidelity of our methods increases we can now guide the planning of new experiments, and probe parameters that are not yet available. Thereby providing a "road map" for generating high quality, high-charge 10 to 100 GeV electron beams for use in high-energy physics and light sources.

1. Introduction

The quest to understand the fundamental nature of matter and energy requires ever higher energy particle collisions, which in turn leads to ever larger and more expensive particle accelerators. The international community has identified a TeV center of mass electron-positron collider, the ILC [1], as the highest priority concept for the next high-energy physics facility. Because the ILC will require two 20 km long superconducting linear accelerators, it is reasonable to conclude that this collider will be the last such facility ever built using "conventional" technology . Orders of magnitude higher accelerating electric fields will be required for the field of experimental high-energy physics to continue exploring the energy frontier in the ensuing decades.

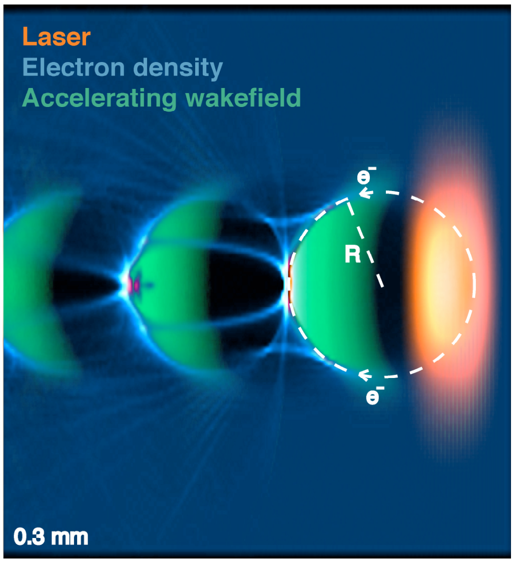

Figure 1. Schematic representations of the LWFA (above) in the so called blowout regime is shown above.

The maximum achievable accelerating gradient is orders of magnitude larger when sustained by the collective fields of a plasma, rather than an evacuated metal structure. This has been demonstrated for electrons in both laser wakefield acceleration (LWFA) [2,3,4] and plasma wakefield acceleration (PWFA) [5] experiments. Figure 1 provides a schematic representation of how the laser or beam driver creates a density modulation in the plasma electrons, which in turn creates accelerating and focusing electric fields that propagate with a velocity close to the speed of light, *c*.

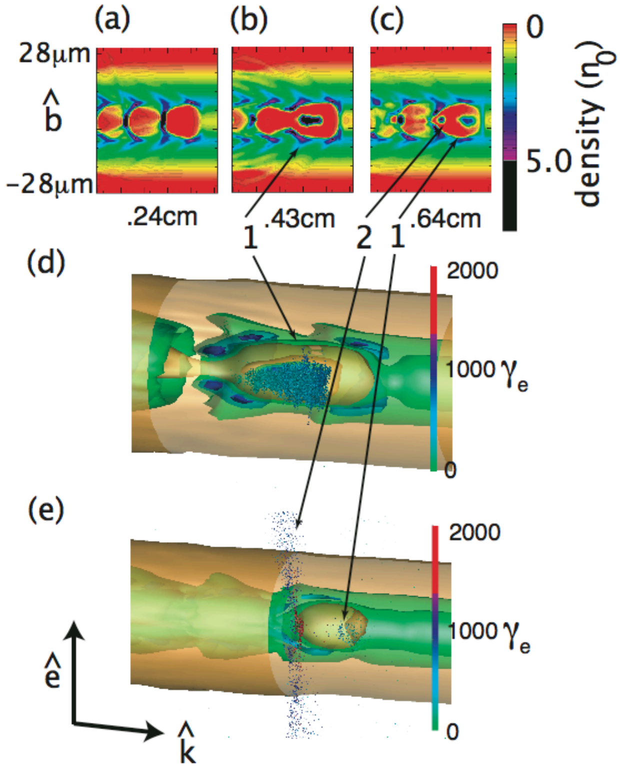

Figure 2: OSIRIS simulation of the LWFA concept, showing the 3D contours (in panels (d) and (e)) of the electron density in the blowout regime after .43cm and .64cm of propagation in a plasma channel described in ref. [6].

In the LWFA, diffraction of the laser pulse limits the effective interaction of the accelerated electrons with the plasma wake to a few Rayleigh ranges, unless the laser is guided. For sufficient laser intensity and power, relativistic electron dynamics within the laser field can self-guide much of the pulse. A plasma channel with an electron density minimum on axis and roughly parabolic shape transversely can guide laser pulses with no requirements on power [2,5]. Figure 2 shows visualizations of OSIRIS [6] simulations of the LWFA concept, where in each case the surface shows the electron density. The upper image overlays some of the accelerated electrons, while the lower image shows the plasma wake generated inside a plasma channel. One of the findings from the simulation is that there are significant differences between two and three dimensional simulations, particularly in the self-injection of relativistic electrons. And since number and energy spectrum of accelerated electrons is one of the few diagnostics available in current LWFA experiments, three dimensional PIC simulations of these experiments is the currently the only tool available to study LWFA experiments in a quantitative fashion.

Nonetheless, beam energy and emittance is only a small part of the entire LWFA system. Other considerations, such as the nonlinear self-guiding of lasers in a uniform plasma, or the nonlinear interactions between a high intensity laser and a perform channel are also important issues that can be studied either with a fully explicit PIC code in 2D, or with a PIC code with a reduced equation for the fields. Furthermore, the quality of the accelerated bunch, such as the energy spread and emittance, can be controlled through external injection, which is another open area of LWFA research. The ability for codes to make quantitative comparisons with current and future experiments, and the ability to explore a wide range of new concepts demand a hierarchy of codes capable of satisfying the various needs.

This paper is organized as follows. In the next section, the various of algorithms and codes from the entire SciDAC advanced accelerator (AA) community are introduced. In section 3, recent accomplishments from the SciDAC team are highlighted. Finally, in section 4, future challenges and new ideas, both computational and theoretical, are discussed.

2. Present software and algorithms

State of the art simulations of plasma based accelerator concepts are based on the electromagnetic PIC algorithm [8], in which Maxwell's equations are advanced in the time domain with a compact 2^{nd}-order stencil on a Cartesian mesh [9], while particles are advanced with 2^{nd}-order accuracy through free space [10]. The gridded fields are interpolated to particle locations to calculate the Lorentz force, while the current is deposited from the particles in appropriate locations of the mesh [11] for the next Maxwell update. The particle shape can be a simple tent-like function (area weighting), with a size one of two grid cells (in each direction), or it can be higher-order (i.e. smoother and larger) [8,12,13]. A higher-order shape (typically based on splines) must be matched by higher-order field interpolation for the Lorentz force, to minimize self-forces on the particles and numerical heating, and care must be taken to satisfy conservation of charge. This step is critical as it eliminates the need to solve Poisson's equation, and makes this type of code highly scalable. The particle advance and field update are time-centered to yield global 2^{nd}-order accuracy,. Higher-order particle shapes can greatly reduce the numerical heating, as can digital filtering of the currents on the simulation mesh.

VORPAL [7] and OSIRIS [14] are two such codes, both parallelized with a domain decomposition that allocates Cartesian subsets of the full mesh among multiple processors. To make effective use of cache, particles are advanced by the processor holding the local mesh, and the particle arrays are also sorted periodically so that proximity in space leads to proximity in the array. The message passing interface (MPI) is used to communicate field data between the "guard" cells of neighboring meshes and also to transfer particles that move from one mesh to another. High-parallel efficiency has been obtained through pre-fetch, i.e., posting a non-blocking receives prior to the corresponding (blocking) send, or by using a separation between updates along the mesh boundaries and the interiors, combined with non-blocking sends of field and particle data, allowing for effective overlap of communication with computation. Also, the inherently local field update and particle push, as well as use of locally charge conserving current deposition, means there is no need for global communication, which allows both codes to scale effectively up to several thousand processors.

The time step for explicit electromagnetic codes is constrained by the usual Courant stability criterion for electromagnetic waves in vacuum, plus the stability conditions imposed by the 2^{nd} order integration method. As a result, 3D simulations of LWFA experiments with a 3 mm interaction length require ~10^5 processor hours. Simulations of PWFA experiments are in principle ~100x less demanding, because it's not necessary to resolve the small time and space scales of the laser pulse; however, in ongoing experiments the interaction lengths are ~100x longer, so the computational requirements are comparable. Hence, there is a strong need for reduced models that approximately capture the relevant dynamics of the system with less computational effort. The 3D quasistatic code

QuickPIC [15], which is built on the UPIC software framework [16], is an extremely successful example, which accurately simulates PWFA and LWFA systems in relevant parameter regimes with >100 x speed-up over OSIRIS or VORPAL.

3. Recent Accomplishments from the SciDAC Team (Need to add VORPAL results and rewrite section so that it appears more unified).

The three codes described above have been verified through code benchmarking exercises and, where possible, by comparison with theory; validation is done via comparison with experimental data. In previous simulation works[6,17], it has been shown that for a majority of LWFA's, 2D and 3D simulations can yield different results. Therefore, 2D validation exercises are at best qualitative.

Using reasonable laser power (17TW) and pulselength (< 50fs), fully explicit PIC (OSIRIS) simulations of the LWFA concept in 3D predicted the creation of well-defined electron beams of moderate energy spread [6] that was seen independently by three initial experimental teams [2,3,4]. Since that time, OSIRIS was used to support one of those experimental efforts [3], to model all three experiments in greater detail [17], as well as more recent experiments [18]. Similarly, simulations using the fully explicit VORPAL code have been used to closely model LBNL experiments on 100 MeV and 1 GeV laser wakefield accelerator stages in 2 and 3D [2,19,20], and to model controlled injection [21,22] and guiding [23] and other topics [24]. The simulations access internal dynamics of the accelerator not available to experimental diagnostics for optimization and projection of possibilities for new experiments. These simulations are further detailed in [20]. Agreement between 3D PIC results and the published experimental data is sometimes within ~10% for some parameters like total accelerated charge and beam energy, while the agreement for other quantities like energy spread is more qualitative, and the developers of OSIRIS and VORPAL are constantly improving the numerical aspects of these codes to improve the agreement. In any case, this extensive validation of fully explicit PIC is a major step forward.

Both quasi-static (QuickPIC) and fully explicit (OSIRIS) PIC have been validated successfully in 3D via comparison with data from recent PWFA experiments [29]. These two algorithms have also been successfully benchmarked [15] on both PWFA and LWFA, with quasi-static PIC showing two or more orders of magnitude speed-up in some problems. The agreement between these two models gives much confidence in each because they are based on different physics algorithms and numerical methods.

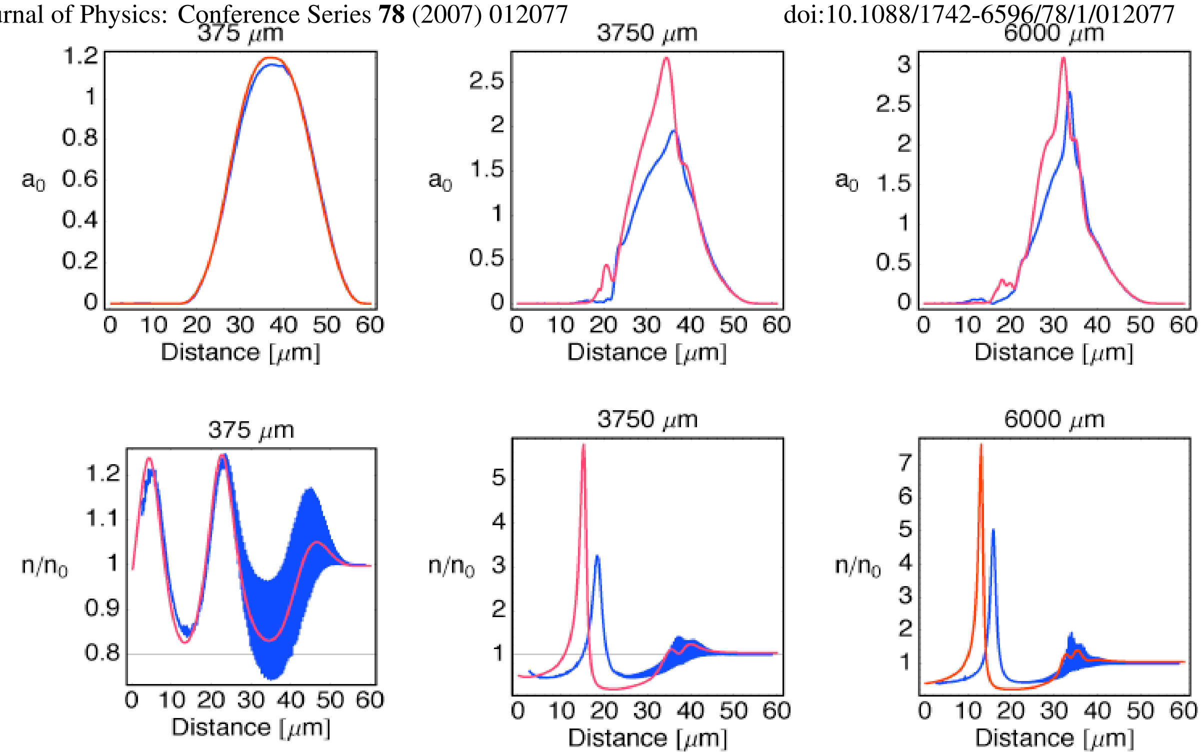

Figure 3: Benchmark results using 2D OSIRIS (red) and QuickPIC (blue) using a 25 TW laser pulse propagating in a plasma channel according to ref. [26]. The top panels show the evolution of on-axis line-outs of the vector potential. The bottom panels show the correspondent evolution of the plasma density.

In recent LWFA experiments, the propagation of 12-40 TW laser pulses in cm scale plasma channels with densities $n_e \sim 10^{18} cm^{-3}$, produced up to 1 GeV quasi-monoenergetic electron beams [28]. Some aspects of the experiment, such as the laser propagation, is ideally suited for a reduced PIC code like QuickPIC. For this purpose, QuickPIC simulations, with similar laser and plasma parameters to those of the experiments of ref. [28] have been performed. The simulations reveal that at the beginning of the propagation, a linear plasma wake, which cannot trap electrons, is created. However, shortly after the beginning of the propagation, the laser self-focuses, creating a non-linear wake where electrons are expelled at the passage of the laser, entering in the so-called blow-out regime [30]. Since full 3D PIC simulations for this problem are very computationally intensive, these results have been benchmarked with 2D simulations. The two models (quasi-static and fully explicit PIC) show good agreement. In Fig. 3, comparisons between the two models (QuickPIC and OSIRIS in this case), for the particular case of a 25 TW laser pulse, are shown.

4. Beyond the 1GeV Barrier—What's next?

4.1. Extrapolation to future experiments in the so-called "blowout" regime

The numerous 3D fully explicit PIC simulations in the blowout regime [6,17], along with a more comprehensive understanding of the structure of the nonlinear relativistic wakes[31,32] have provided the foundation for a theoretical framework for laser wakefield acceleration in the 3D blowout regime. The theory provides a recipe for designing laser wakefield accelerators for a given laser and plasma parameter (as long as the plasma provides guiding for the laser), and provides estimate for the number and energy of the accelerated electrons. This set of scaling laws has verified through a 3D OSIRIS simulation of a 200TW laser propagating in near 1 centimeter of plasma as well as numerous 3D QuickPIC simulations. In many cases, the simulation agree well with the theoretical predictions. The theoretical framework lays out the path for a 100GeV single stage LWFA. The framework, along with the simulation results, have appeared in the June, 2007 issue of *Physical Review Special Topics – Accelerators and Beams* [30].

4.2. Beam-loading for plasma based accelerators in the blow-out regime

However, getting to high energy is only part of the story. In order for plasma-based accelerators to be competitive, the beam quality must be comparable to those in conventional accelerators. Therefore, the feasibility of Laser/Plasma Wakefield Accelerators depends upon the ability to efficiently load a trailing bunch of electrons into the wakefield driven by a laser or an electron beam propagating through a plasma. When accelerating electrons it appears very advantageous to operate in a nonlinear regime -the blowout regime-, where the driver is intense enough to expel all plasma electrons outward. Since the accelerating structure is determined by the three dimensional shape of the wakefield in the blowout regime, an analytical description of beam loading involves the interaction between this shape and the accelerating electrons . In order for the quality of the accelerating beam to be high, the modification of the plasma bubble due to the presence of the beam must be small. A Gaussian beam with longitudinal spot size about 15% of the blowout radius and sufficient charge to absorb almost all of the electromagnetic energy in the bubble is shown, both analytically and through simulations, to maintain low energy spread during the entire acceleration process. The suite of PIC codes described above has been essential in developing a new model for beam loading in this nonlinear regime. In addition, QuickPIC simulations indicate that the beam quality of the trailing beam can remain high over the acceleration distance when it is properly loaded.

4.3. Adapting current codes to petascale platforms

The frontier of the high performance computing is rapidly moving towards a multi-core paradigm. Future Petascale system will have hundreds of thousands of processor cores running at modest frequency, therefore the challenge is to explore the hidden parallelism inside the algorithm to make better use of the available computing resources. The codes OSIRIS and VORPAL have both been structured so that they can run efficiently on a multi-core platform.

In QuickPIC, we have adopted a pipelining algorithm to improve the throughput of the parallel processing. Under the quasi-static approximation, the original QuickPIC algorithm treats the beam-plasma interaction problem by separating the time scales of their evolutions. This allows the reduction of computation from a full update on the plasma particles in the 3D simulation box at each time step to a serials of updates on a 2D transverse plasma slice while the beam passes through it. Such operations are serial but however can be pipelined by dividing them into several pipeline stages. Recently we exploit this parallelism in the quasi-static algorithm and modified QuickPIC to include a pipeline mode. Simulation results shows that this pipeline mode can efficiently scale QuickPIC to 1,024+ processors without sacrificing accuracy. 86% parallel efficiency is achieved on the SEABORG massive parallel computer at NERSC. Future plan is to further extend this scaling to 10,000+ processors with improved efficiency, and apply the same technique for laser drivers.

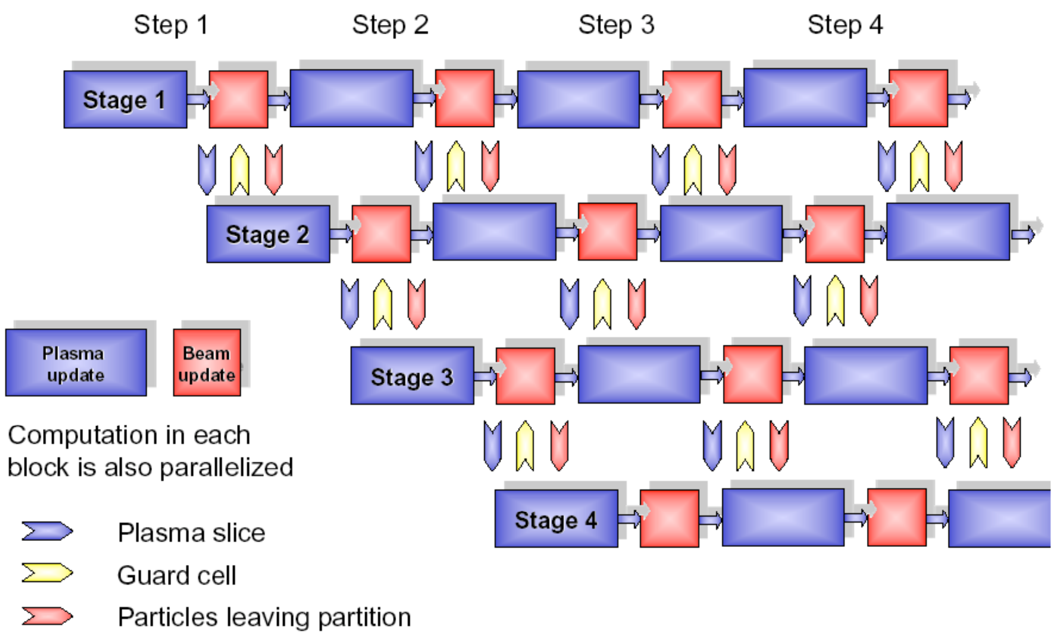

Figure 4: Schematics of the pipelining in QuickPIC.

Although reduced models are very powerful, they have limitations. For example, quasitatic and PGC models cannot be used to simulate particle trapping due to colliding laser pulses, and they fail as the laser pulse becomes significantly depleted, due to strong position-dependent blue-shifting and red-shifting of the spectrum. For this reason, we plan to explore ideas for "merging" or "patching" explicit simulations and reduced models.

5. Conclusions

Three-dimensional PIC simulations of laser wakefield accelerators have shown qualitative as well as quantitative agreements with many recent LWFA experiments from around the world. Much like the invention of chirped pulse amplification (CPA) enabled great advances in the generation of high quality, high energy electron beams using LWFA's in the laboratory, the advances in both hardware and numerical algorithms have allowed similar advances in the numerical study of these systems in a "virtual" laboratory. Although there are many outstanding issues in both the experimental and the computational sides of LWFA research, the future appears bright and many opportunities exist for future research.

6. Acknowledgments

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