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Modeling laser wakefield accelerator experiments with ultrafast particle-in-cell simulations in boosted frames[a)]

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The development of new laser systems at the 10 Petawatt range will push laser wakefield accelerators to novel regimes, for which theoretical scalings predict the possibility to accelerate electron bunches up to tens of GeVs in meter-scale plasmas. Numerical simulations will play a crucial role in testing, probing, and optimizing the physical parameters and the setup of future experiments. Fully kinetic simulations are computationally very demanding, pushing the limits of today's supercomputers. In this paper, the recent developments in the OSIRIS framework [R. A. Fonseca *et al.*, Lect. Notes Comput. Sci. **2331**, 342 (2002)] are described, in particular the boosted frame scheme, which leads to a dramatic change in the computational resources required to model laser wakefield accelerators. Results from one-to-one modeling of the next generation of laser systems are discussed, including the confirmation of electron bunch acceleration to the energy frontier. © *2010 American Institute of Physics*. [doi:10.1063/1.3358139]

I. INTRODUCTION

The propagation of an intense laser pulse in an underdense plasma generates a wakefield that can accelerate electrons with gradients above 1 GeV/cm.[1] Initial laser wakefield acceleration (LWFA) experiments generated a continuous energy spectrum of electron, which accelerated in plasma beatwave structures associated with the propagation of long laser pulses in conditions where Raman-type instabilities are stronger.[2–5] Recent experiments using short pulses with durations below 30 fs, and high powers above 10 TW, demonstrated the possibility to obtain quasimonoenergetic electron bunches, self-injected from the background plasma, with typical energy spreads lower than 10% and final energies up to 1 GeV[6–9] at the centimeter scale. These experiments are characterized by strongly nonlinear plasma waves where plasma electrons are evacuated from the region of the laser, in the so-called "blowout"[10] or "bubble"[11] regimes. The dependence of the laser and plasma parameters on the output beam features was analyzed analytically for these extreme acceleration regimes and, supported by numerical simulations, leads to the establishment of phenomenological models.[10,11] A nonlinear theory for the beam loading of an externally injected electron bunch was also developed.[12] After an initial parameter search with these models, numerical simulations are required to obtain the optimal values for the experiments, and also to fully understand the underlying physics for which there are no current detailed analytical descriptions.

According to simulations and theoretical scalings, the future generation of laser systems is expected to enable output beams in the 10 GeV range. Reaching these tremendous energies may involve the propagation of a moderate intensity laser pulse ($I \simeq 10^{18}-10^{19}$ W/cm^2) through several meters of low density plasma ($n_e \simeq 10^{16}-10^{17}$ cm^{-3}). Since detailed modeling also requires resolving the smallest structures in these scenarios, namely, the laser wavelength, such long distances constitute an important challenge for the LWFA numerical experiments.

In this paper we discuss the modeling of current and future LWFA experiments with one-to-one fully kinetic numerical simulations, focusing on the use of a relativistically moving frame to strongly reduce computational requirements. This paper is organized as follows. In Sec. II, we introduce the main challenges of the fully kinetic modeling of LWFA, in particular the computational requirements for the next generation of laser systems. The main developments of the OSIRIS framework[13] for increased performance, new numerical algorithms, and new physical models are then described. In this context, we introduce in Sec. III the boosted frame scheme for the LWFA, which can reduce computational requirements by 2–3 orders of magnitude. Although physically equivalent to the laboratory frame, the acceleration structures in boosted frames can be remarkably different from their laboratory counterparts. Some apparently counterintuitive features are also discussed and examined, namely, the implications of the space-time transformation in the result analysis. Examples of three-dimensional modeling and design support of recent experiments are mentioned throughout the discussion. Finally, we give an overview of the main results obtained with large OSIRIS boosted frame simulations for the future LWFAs. Concluding remarks and a summary are presented in the final section.

II. CHALLENGES IN PIC MODELING OF LWFA'S

Numerical modeling of LWFA requires resolving the motion of the plasma particles in response to the electric and magnetic fields of the laser pulse. In a particle-in-cell (PIC) code,[14] "superparticles" are used to represent a set of real

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plasma particles that move freely in space. The electric and magnetic fields are stored in a grid and evolved self-consistently with Maxwell's equations. The algorithm integrates the trajectories of the superparticles according to the Lorentz force, calculated by interpolating the field values at the particle positions, and deposits the corresponding currents on the grid.

In a fully kinetic PIC simulation, the laser wavelength, which for state-of-the-art LWFA experiments is usually $\sim 1\ \mu$m, represents the smallest scale to be resolved. This scale contrasts with the centimeter range lengths of the plasma columns used in current experiments. Three-dimensional full-PIC simulations of these configurations are possible,[15,16] although very computationally demanding. Phenomenological theory,[10] however, estimates that the future experiments with the next generation of laser systems will require plasma lengths of several meters to reach the maximum output beam energies. The three-dimensional full-PIC modeling of such an experimental configuration is not reachable with currently available computational capabilities (10^6-10^7 CPU hours are needed). Furthermore, over a million simulation iterations would be required, a challenge on the accuracy of the numerical algorithms.

One possible approach to this challenge is the simplification of Maxwell's equations for a particular physical scenario. For instance, QuickPIC (Ref. 17) is a reduced code especially suited for plasma wakefield and laser wakefield acceleration. QuickPIC takes advantage of the time scale separation for the laser (or particle beam) and plasma evolution to employ the quasistatic approximation, thus reducing the three-dimensional electromagnetic field solver and particle pusher to a sequence of two-dimensional calculations on the transverse directions. These simplifications allow for computational gains of two to four orders of magnitude without hindering accuracy for relevant scenarios. A similar approach was taken to develop the two-dimensional code WAKE.[18] A distinct approach is used in Ref. 19, where Maxwell's equations are solved in cylindrical geometry, using a Fourier expansion along the poloidal direction.

Faster computations may also be obtained with more sophisticated numerical configurations. For example, nonhomogeneous grids can be employed to use distinct grid resolutions for different spatial regions, depending on the refinement required by the local structures.[20]

The physical approximations, however, typically imply limitations on the applicability of the schemes. For instance, the quasistatic approximation is not valid for lasers near depletion and does not model particle self-trapping. Therefore, fully kinetic simulations are usually required for a thorough modeling of LWFA experiments.

A. OSIRIS framework

OSIRIS is a fully relativistic, electromagnetic, and massively parallel PIC code that has been extensively used in LWFA simulations,[6,15,16,21,22] but also in astrophysical scenarios,[23–25] nanoplasma dynamics,[26] and fast ignition.[27,28] The framework includes an advanced visualization infrastructure for fast data display, analysis, and postprocessing.[29]

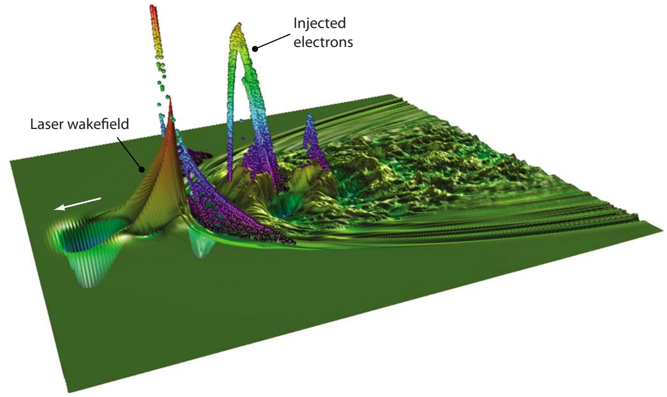

FIG. 1. (Color online) Visualization of a typical accelerating gradient of LWFA from an OSIRIS simulation. The surface represents the longitudinal electric field generated by a laser pulse moving to the left. Accelerated particles are represented by spheres colored by energy (violet/dark: low; red/light: high); the vertical position of the particles represents their energy. In this case, electron injection occurs in all of the first three buckets.

An example of a LWFA visualization is shown in Fig. 1, where accelerated particles are represented together with the accelerating wakefield.

Recent developments of OSIRIS include the optimization of the code scalability for large supercomputers, improvement of the overall computing performance, addition of physical mechanisms which are beyond Maxwell's equations (e.g., multilevel ionization, relativistic collision model[30]), and enhancement of accuracy, stability, and speed of the numerical algorithms.

B. Code scalability and performance

The first step on the way to extreme modeling of LWFA experiments is the optimization of the code performance and scalability to the largest supercomputers currently available, with hundreds of thousands of processors.

In OSIRIS, scalability is ensured with spatial domain decomposition and a local electromagnetic field solver (finite-difference method). Communications are minimized and a dynamic load balancing algorithm was implemented, which consists in adjusting the node boundaries at runtime, according to the distribution of computational load of particles and cells across the simulation box.[29] An efficiency above 80% was obtained for a strong scaling benchmark up to 300 k CPUs.

To increase the overall performance of OSIRIS, tailored routines were developed for the vector units of state-of-the-art processors. In particular, the current deposition and the particle pusher were written with single instruction, multiple data (SIMD) instructions for x86 architectures (streaming SIMD extensions), which enables a more effective use of the CPU. In this case, the code runs in single precision (32 bits) and overall gains of 2–3 times are typically obtained, depending on the particle interpolation level used.

The full description of the current OSIRIS developments will be presented in a separate publication.

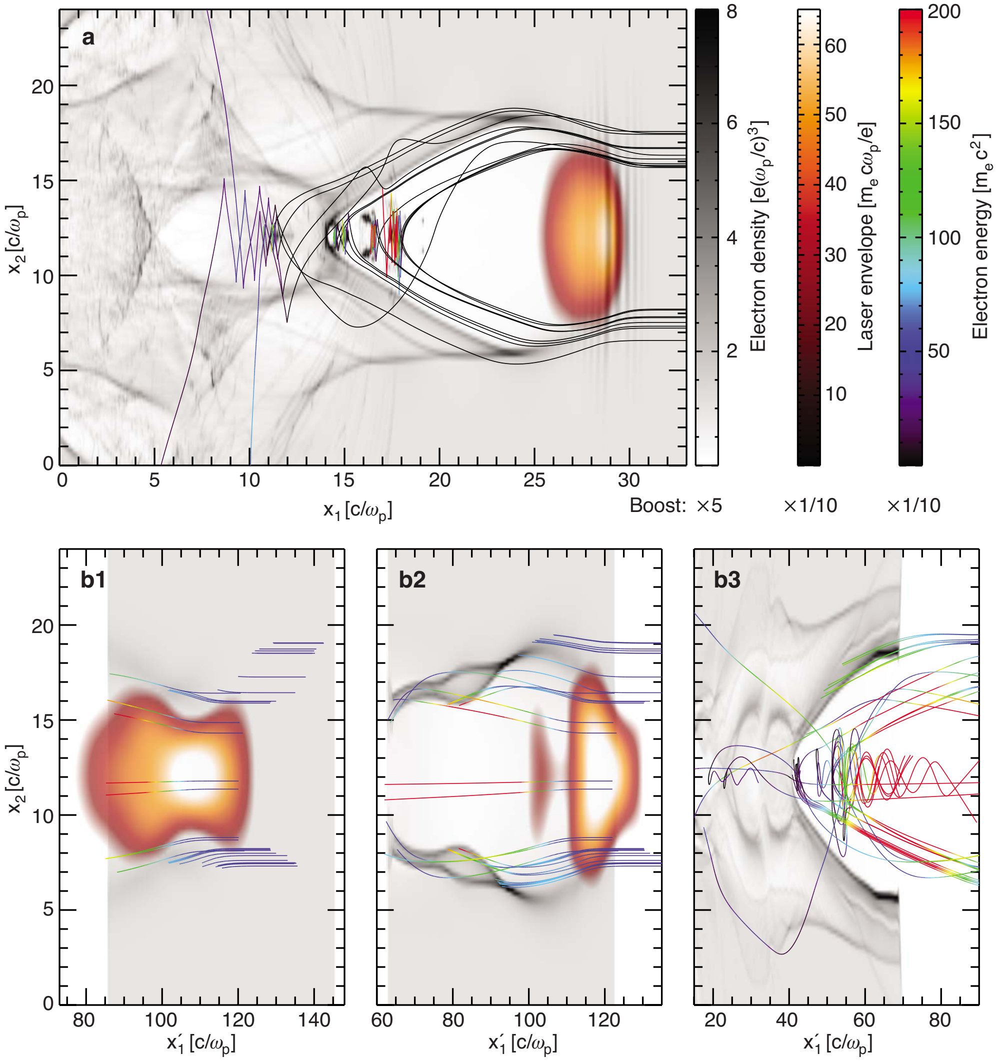

FIG. 2. (Color online) Comparison of spatial and temporal structure shapes in the laboratory frame (frame a) and boosted frame with relativistic factor $\gamma=(1-\beta^2)^{-1/2}=5$ (frames b1–3). The plasma is represented in grayscale (light background) and the laser envelope in orange (dark). A set of particle trajectories is also represented (lighter indicated higher energy). The scales in the boosted frame were set according to the Lorentz transformation of the respective quantity, namely, a compression of the density by γ, a dilatation of the laser pulse by $\gamma(1+\beta)$, and an energy decrease approximated for very relativistic particles $\gamma(1+\beta)$. In the boosted frame the contracted plasma column moves to the left with $\gamma_{\text{plasma}}=5$.

C. Numerical algorithms

Modeling LWFA requires the constant development and implementation of more advanced numerical features to allow for more complex simulation configurations, and more precise modeling for an increasing number of time steps. In this context, open boundary conditions for the electric and magnetic fields were implemented with the perfectly matched layer method.[31,32] The scheme consists in adding an absorbing layer around the computational domain to totally absorb fields propagating towards the boundaries. This is particularly useful for the transverse boundaries of a LWFA simulation box because it ensures the full absorption of the diffracted laser.

It is also possible to alter the computational stencil used to calculate the spatial derivates when solving Maxwell's equations.[33] This allows a better control of the numerical dispersion introduced by the finite difference time domain method, and is relevant to avoid numerical Cherenkov radiation and to more precisely model the propagation of the laser over long distances.[34]

D. Physical mechanisms modeled

In the past few years, LWFA experiments have started to explore alternative electron injection schemes, targeting improved control of the process and higher quality output beams. These schemes typically require modeling additional physical processes in the code.

A first example is the ionization trapping scheme already explored with particle and laser beams.[16,35] To model these experiments with OSIRIS, the existing ionization module[36] was expanded to include additional atom types and to allow the follow up of individual electrons from each ionization level.

Experiments to control the propagation of the self-injection electron bunches with tilted laser wave fronts were also recently performed and modeled with three-dimensional simulations in OSIRIS.[37] The tilted laser wave fronts were implemented in the code by introducing a perpendicular laser wave number chirp across the laser.

In addition, we have developed more advanced diagnostics: full particle tracking[29] and radiation emission from the simulated electrons.[38] This enabled the complete modeling of recent experiments of x-ray synchrotron radiation with LWFA, including the radiation power and spectra estimated from the simulation.[39]

III. ULTRAFAST SIMULATIONS IN BOOSTED FRAMES

An important scheme recently implemented in OSIRIS to reduce the computational requirements of LWFA modeling is the ability to perform simulations in a relativistically moving frame. This concept, introduced in Ref. 40, was successfully applied to a few scenarios, including free electron lasers,[41] collisions of relativistic electron beams,[40] and laser wakefield acceleration.[42–46] The implementation in the OSIRIS framework is described in Refs. 42 and 43 with details on the particularities of laser wakefield simulations. In those scenarios, and when moving from the laboratory frame to a relativistic moving frame (*boosted frame*), the laser pulse is stretched and the plasma contracted, reducing the scale gap between the laser wavelength and the plasma length. These transformations thus allow for larger numerical grid cells and can reduce the number of algorithm iterations by more than three orders of magnitude, with equivalent quantitative outputs. Nevertheless, the scheme is not advantageous if the backward propagating radiation is relevant; in the moving frame, this radiation is upshifted and will therefore require a refined grid in order to be properly resolved. In most LWFA scenarios, however, backward radiation can be neglected, and the boosted frame thus allows for the full-PIC modeling (i.e., including all the essential physics) with large computational gains.

Implementing the boosted frame requires three major steps.[43] First, plasma particles and laser fields have to be initialized in the moving frame. This can be done with standard Lorentz transformations for the particle density and for the electromagnetic fields of a Gaussian pulse. Second, particular sections of the PIC algorithm might require revision for increased precision. For instance, the background plasma is a relativistic flow in this frame, and the relativistically moving particles will create strong currents that may increase the growth rate of numerical instabilities. Finally, diagnostics must be transformed back to the laboratory frame, using the inverse transformations from the initialization.

Result comparison between the boosted and the laboratory frame is illustrated in Fig. 2, showing the impact of the space-time transformation. The wakefield structure stretches similarly to the laser pulse (by a factor of $\gamma[1+\beta]$). Thus, in this case of a short plasma length, a single bubble is longer than the total plasma column in the boosted frame. In fact, due to space-time relativity, the spatial structures at a given moment in the laboratory frame correspond to a time evolution in the moving frame. For instance, in frame b2 the tip of the laser pulse is already in vacuum while no particle injection occurred. Furthermore, the laser has completely exited the plasma in frame b3, but there are electrons still being trapped at the back of the first bucket due to the accelerating field left in the plasma by the laser. The betatron motion of the injected electrons can also be seen in Figs. 2 and 3(b); the frame transformation leads to longer oscillation wavelengths than in the laboratory, but the transverse amplitude is not altered. Finally, we emphasize that the dilatation of all the electromagnetic radiation propagating in the forward (laser) direction, implies that, by leveraging on the smaller computational requirements to employ higher grid resolutions, additional forward radiation wavelengths can be captured in the simulation.

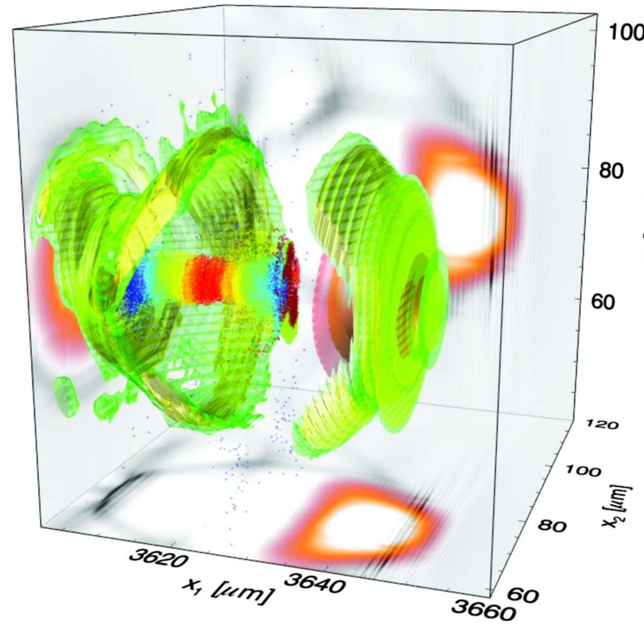

FIG. 3. (Color online) Electron density in the LWFA of the experiment described in Ref. 22 (laboratory frame simulation). Projections in the box walls refer to the plasma electron density (gray/light) and laser envelope (orange/dark). Isosurfaces are shown for the plasma wake (green/yellow—bubble shaped) and laser envelope (orange/light isosurfaces at the front). Electrons injected in the wake are represented by dots colored by energy (blue/light—low; red/dark—high).

Because of the reduced computational requirements, ultrafast modeling of current experiments with plasma lengths at the centimeter scale is now possible with the boosted frame scheme, converting typical week/month scale simulations in the standard laboratory frame to hour/day scale in the moving frame. For example, quick parameter scans were recently performed for self-trapping experiments in Refs. 15 and 22. Figure 3 shows results for the laboratory simulation of self-injection LWFA experiments in Ref. 22, which was complemented with parameter scan with OSIRIS in the boosted frame and QuickPIC in the laboratory frame (J. Vieira, in preparation). By resorting to the boosted frame scheme, the same quantitative results (in particular the monoenergetic peak at 0.8 GeV[22]) were obtained with computational gains up to 20 times, i.e., from 20 days in the laboratory frame to 1 day in the relativistically moving frame.

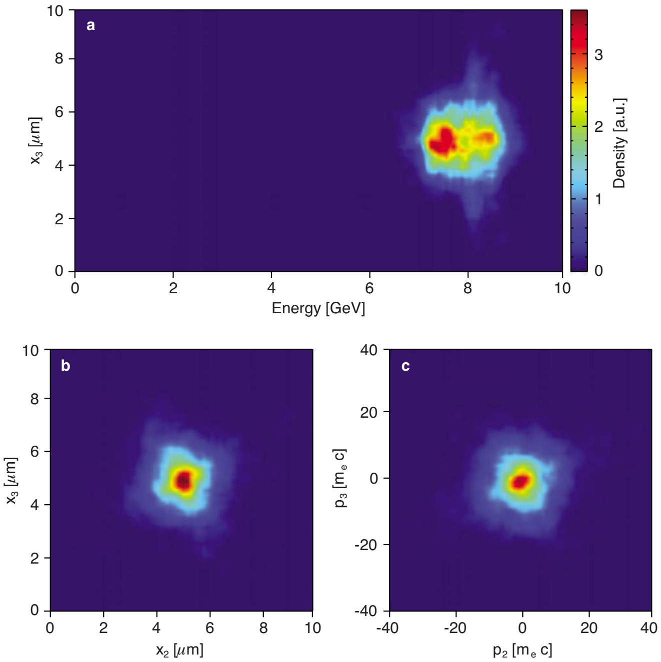

FIG. 4. (Color online) Properties of a self-injected electron beam simulated in a relativistic boosted frame (Ref. 42). The output beam reaches above 8 GeV (frame a) after 27 cm propagation. The transverse position and momenta (frames b and c) show a good quality beam. This analysis emphasizes the relevance of simulating the LWFA in three-dimensions for direct correlation with experiment.

More importantly, the computational savings open the possibility for fully kinetic three-dimensional modeling of the next generation of LWFA with plasma lengths at the meter scale. We have explored three distinct regimes of a 250 J laser with three-dimensional boosted frame simulations in OSIRIS, from a strongly nonlinear scenario at 10 PW, to a weakly nonlinear configuration at 1 PW with propagation distances ranging from 2.5 mm up to 5 m. Results confirm the predictions from the phenomenological models, in particular the possibility to output electrons beams with tens of GeVs.[42] In Fig. 4, the properties of a 8 GeV self-injected electron beam are depicted, including the transverse positions and momenta. The three-dimensional simulation was performed in a boosted frame with $\gamma = 10$, enabling a computational gain of a few hundred times relatively to a standard laboratory simulation.[42] The transverse quantities represented emphasize the relevance of three-dimensional simulations to fully model the dynamics of the system, in particular of the accelerated particles.

IV. CONCLUSIONS

Numerical simulations are an invaluable tool for LWFA research, experimental design, and analysis. The increasing plasma lengths involved in these experiments, in particular the need for meter scale plasma columns for the next generation of laser systems, require larger and longer simulations which may not be possible with supercomputers currently available. Although algorithm simplifications can be made to reduce the computational cost to a practical range, fully kinetic simulations, which include self-injection for instance, are usually required for most scenarios. The simulation of the LWFA in a relativistically moving frame reduces the computational requirements by several orders of magnitude, by closing the gap between the spatial scales of the laser wavelength and of the plasma column. It is thus possible to quickly model current experiments and study the future LWFA's at the meter range. Initial studies already indicate the possibility to accelerate electron beams to the energy frontier.

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