# BOOSTED FRAME PIC SIMULATIONS OF LWFA: TOWARDS THE ENERGY FRONTIER\*

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# Abstract

We address full particle-in-cell simulations of the next generation of Laser Wakefield Accelerators with energy gains  $\gtrsim 10$  GeV. Simulating the long distances involved in these numerical experiments, while still resolving the laser wavelength, is very demanding in terms of computational resources, and is not yet possible to (easily) accomplish with current full physics algorithms. Following the work on simulations of particle beam-plasma interaction scenarios in optimized Lorentz frames by J.-L. Vay [1], the Lorentz transformation for a boosted frame was implemented in OSIRIS [2], leading to a dramatic change in the computational resources required to model LWFA. The critical implementation details will be presented, and the main difficulties discussed. Quantitative comparisons between lab/boost frame results with OSIRIS and QuickPIC [3] were performed, and focus will be make on a 1.5 GeV self-injection configuration. Finally, a discussion on radiation emission is presented, and an analysis technique that uses high resolution particle tracking is introduced.

## **INTRODUCTION**

A new generation of laser systems is now being planned all over the World and will deliver powers above of 10 PW, with a OPCPA configuration (e.g. the upgrade for the future Vulcan 10 PW OPCPA system [4]), pulse durations in the 30 fs range, and pulse energies in the 300 J range. This technology will thus enable the exploration of new scenarios for electron acceleration in Laser Wakefield Accelerators (LWFA) [5]. Phenomenological models and numerical simulations will certainly play a critical role in this process, by providing deeper insights on the physical processes involved and by supporting experimental teams designing the optimal configurations. Nevertheless, the physical parameters associated with this new generation of LWFAs will require strong progress in the numerical codes, and access to very large computing resources. In fact, the optimal acceleration distances will become considerably longer, in the scale of 10s cm - 1 m, depending on the laser intensity and the corresponding LWFA regime. In this framework, reduced codes have been developed with physical simplifications that lower the computational cost of the algorithms. For instance, QuickPIC [3], by using the quasi-static approximation, can be more than a thousand times faster than a full particle in cell (PIC) code for scenarios relevant to plasma wakefield accelerators, and still capture all the relevant physics. An alternative, that uses no physical approximations, has been proposed by J.-L. Vay [1] in the context of particle beam collisions: the simulation of the system in an optimal relativistic frame. This boosted frame scheme, despite several implementation difficulties for LWFA [14], can provide a means to perform the same large scale simulations more rapidly, while keeping all the relevant physics of a standard PIC code.

In this paper, we use the code OSIRIS [2] to introduce the application of boosted frames to LWFA simulations, which will enable the full-PIC simulation of the next generation of systems. First, we describe the advantages of these optimal frames, and discuss the transformation of quantities between frames. Next, we present the results of numerical simulations in the boosted frame, benchmarking with results obtained in the laboratory frame. Finally, a brief discussion on radiation emission by the self-injected electrons is included. Conclusions are presented in the last section.

#### **OPTIMAL FRAMES**

The grid resolution in a PIC simulation is defined by the smallest structure to be resolved, which, in standard LWFA simulations, is the laser wavelength. The plasma structures are usually larger, thus implying an extra computation cost due to the over-resolution of the plasma. This can be avoided by performing the simulation in a relativistic frame moving in the direction of the laser, since the pulse wavelength increases and the plasma contracts. In theory gains are proportional to  $\gamma^2(1 + \beta)^2$  for long plasma columns, where  $\gamma = (1 - \beta^2)^{-1/2}$  is the boost relativistic factor [1].

Quantity initialization is the main step in performing a simulation in a boosted frame. In particular, laser and plasma parameters have to be transformed to the new relativistic frame, so that the electromagnetic waves will be Doppler shifted, and the background plasma, with higher density, is now drifting. After the relativistic PIC algorithm evolves the system in the boosted frame, results must be transformed back to the laboratory frame. To construct a single time shot in the laboratory, a range of boosted time shots is required. This analysis can be done as a postprocessing script or, more efficiently, at runtime. Neverthe-

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Figure 1: Simulation results in the boosted frame for a self-injection configuration with final energy of 1.5GeV obtained with theoretical scalings and confirmed with simulations in the laboratory frame [10]. (a) Electric field in the laser polarization direction after 0.3cm propagation in laboratory; (b) Electron charge density after 0.3cm propagation in laboratory; (c) Longitudinal electric field after 0.3cm propagation; (d) Final longitudinal electron momentum, with energy in laboratory frame units.

less, we emphasize that the transformation of several relevant output quantities for LWFA is straightforward, by using relativistic invariants (e.g., total injected charge), or by simple Lorentz transformation (e.g., maximum particle energy, final laser energy). Finally, specific diagnostics might already contain all space and time information necessary for complete Lorentz transformation (e.g., particle tracking [6]).

#### SIMULATION RESULTS

The boosted frame scheme was implemented in OSIRIS, a three-dimensional fully relativistic, electromagnetic, and massively parallel PIC code, already used to simulate various LWFA scenarios (see, for instance, [7, 8, 9]). A set of benchmarks was performed with OSIRIS and QuickPIC in the laboratory frame, for weaklynonlinear/nonlinear regimes and self-injected/externallyinjected electron beams, with very good qualitative and quantitative agreement. Particular relevance was given to a 1.5 GeV self-injection stage of LWFA, successfully reproducing the results obtained with laboratory frame simulations presented in [10].

### 1.5 GeV Self-injected Electron Beams

Figure 1 presents a summary of the three-dimensional boosted frame simulation (with  $\gamma = 5$ , where  $\gamma$  is the boost

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relativistic factor) of a self-injection configuration. Results show very good agreement with those presented in [10] for the parameter and algorithm scanned performed: different boost speeds with varying resolutions, higher order field solvers [11], particle interpolation schemes [12], and modified Boris pusher [13].

The standard boosted simulation used a moving frame with  $\gamma = 5$ , and required only  $2.4 \times 10^3$  CPU.hours, a gain of  $\sim 20$  times relatively to the laboratory simulation ( $\sim 5 \times 10^4$  CPU.hours). The optimized simulation uses a  $560 \times 140 \times 140 \ \mu\text{m}^3$  window that follows the laser pulse at the speed of light, and is resolved with  $2048 \times 256 \times 256$  grid cells.  $5.4 \times 10^8$  particles with second order shapes were pushed for  $6 \times 10^3$  iterations, corresponding to 0.15 cm of pre-formed plasma in the boosted frame (0.75 cm in the laboratory).

Higher boost velocities will be more advantageous for the simulation of larger LWFA systems. It is important to note that arbitrary high velocities are obviously not possible, since plasma resolution sets an upper limit from contraction. In addition, as the speed increases, additional accuracy is required on the algorithms, and numerical instabilities might arise. This topic will be discussed in a future publication [14].

## Radiation Emission

The self-injected electrons will perform betatron oscillations in the ion channel associated with the blowout region [15, 16], and will therefore radiate. These oscillations occur as the particle is gaining energy from the wakefield, and can be observed in the trajectories depicted in Fig. 2.



Figure 2: Projection of the trajectories of the self-injected particles in the LWFA for the 1.5 GeV configuration. Particles move from the left of the right, and are mostly injected off-axis. Color represents energy.

By post-processing the particles trajectories, estimates for the radiation can be obtained. A detailed discussion of the radiation calculations using particle tracking in OSIRIS will be presented in a future publication [17].

Finally, we note that, as conditions close to the energy frontier are reached, the energy losses associated with the betatron motion of the electrons in the ion channel should be considered. For these scenarios where radiation losses are important, numerical codes should include the radiation damping physics [18], as QuickPIC and OSIRIS already do.

## CONCLUSIONS

We have presented results of LWFA three-dimensional simulations with OSIRIS, performed in an optimized relativistic frame, which moves relatively to the plasma column. This boosted frame enables computational gains of several orders of magnitude, thus allowing for the simulation of the next generation of lasers systems, soon to be available to experimental teams. The simulation in the moving frame requires, however, the quantity Lorentz transformations from and to the laboratory frame, which might constitute an overhead of post-processing, but that can be effectively implemented in the core code. Furthermore, numerical instabilities can arise from the interaction of the laser pulse with a counter-propagating relativistic plasma, particularly for large boost velocities.

Finally, the analysis of the betatron oscillation of the accelerated electrons in the blowout region created by the laser is becoming increasingly relevant, as higher energies are reached and stronger radiation is emitted.

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