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Simulating relativistic beam and plasma systems using an optimal boosted frame.

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Abstract. It was shown recently that it may be computationally advantageous to perform computer simulations in a Lorentz boosted frame for a certain class of systems. However, even if the computer model relies on a covariant set of equations, it was pointed out that algorithmic difficulties related to discretization errors may have to be overcome in order to take full advantage of the potential speedup. In this paper, we summarize the findings, the difficulties and their solutions, and review the applications of the technique that have been performed to date.

1. Introduction

In [1], we have shown that the ratio of longest to shortest space and time scales of a system of two or more components crossing at relativistic velocities is not invariant under a Lorentz transformation. This implies the existence of an "optimum" frame of reference minimizing a measure of the ratio of space and time scales. Since the number of computer operations (e.g., time steps), for simulations based on first-principle formulations, is proportional to the ratio of the longest to shortest time scale of interest, it follows that such simulations will eventually have different computer runtimes, yet equivalent accuracy, depending solely upon the choice of frame of reference. The scaling of theoretical speedup was derived for a generic case of two crossing identical rigid particle beams, and for three particle acceleration related problems: particle beams interacting with electron clouds [2], free electron lasers [3], and laser-plasma accelerators [4]. For all the cases considered, it was found that the ratio of space and time scales varied as γ^2 for a range of γ, the relativistic factor of the frame of reference relative to the optimum frame. For systems involving phenomena (e.g., particle beams, plasma waves, laser light in plasmas) propagating at large γ, theoretical speedup of simulations being performed in an optimum boosted frame could reach several orders of magnitude, as compared to the same simulation being performed in the laboratory frame, for example. As an example, a speed-up of 1,000 was demonstrated on a Particle-In-Cell (PIC) simulation of transverse instability of an ultra-relativistic (γ=500) proton beam interacting with a background of electrons. In the remainder of this paper, we summarize the difficulties and limitations of the method, the solutions that were developed, and review its applications performed to date.

2. Difficulties and limitations

Even if the fundamental electrodynamics and particles equations are written in a covariant form, the numerical algorithms that are derived from them may not retain this property. As an example, we considered in [5] an isolated beam propagating in the laboratory frame at relativistic velocity. When applying the effect of the beam field on itself using the Newton-Lorentz equation of motion, the contribution from the radial electric field is largely canceled by the contribution from the azimuthal magnetic field. However, we showed that the so-called 'Boris particle pusher' [6] (which is widely used in PIC codes), does make an approximation in the calculation of the Lorentz force which leads to an inexact cancellation of the electric component by the magnetic component. The magnitude of the error grows with the beam relativistic factor and in practice, it is unacceptably large for simulations of ultra-relativistic charged beams, where the cancellation needs to be nearly complete. The issue was resolved by changing the form of the Lorentz force term in the Boris pusher, and solving analytically the resulting implicit system of equations (see [5] for details).

For electromagnetic calculations, a limitation may come from numerical dispersion in the electromagnetic solver. The standard Yee solver [7], also widely used in PIC codes, has a relatively high numerical dispersion that is anisotropic and depends on the cell aspect ratio and the ratio of the time step to the cell size in each direction. Short of using a different field solver, this limits the speedup that can be gained by performing the calculation in a boosted frame because the number of cells needs to be kept above a certain minimum level in the longitudinal direction to ensure that the numerical dispersion falls below an acceptable level in that direction. Solvers that produce no numerical dispersion along major axes have been tested in the Scidac codes Osiris [8], Vorpal [9] and Warp [10] with some success, but have yet to be fully validated.

An additional practical complication of numerical simulation in a boosted frame is that inputs and outputs are often specified (or desired) in the laboratory frame. For example, in LWFA simulations, laser and plasma parameters have to be transformed from the laboratory to the new relativistic boosted frame, so that the electromagnetic waves will be Doppler-shifted, and the background plasma, with higher density, is now drifting. Different strategies have been adopted in the three Scidac codes applied to LWFA for laser injection in a Lorentz boosted frame: in Osiris, the laser beam is initialized in the computational box, enlarging the box in the transverse direction and in front of the plasma to accommodate the higher focusing angle and longer wavelength; in Vorpal, the laser is injected from all faces of the computational box; in Warp, the laser is injected at a plane that is fixed in the laboratory frame and drifting in the boosted frame.

The initial phase-space distribution of a particle beam is generally known in the laboratory. For calculations in boosted frames of large γ, deriving the initial beam conditions at a given time can be easy if the initial conditions are simple (e.g., LWFA), or more difficult and/or computationally costly if injecting the beam in a particle accelerator for example, where its longitudinal extent in the boosted frame can cover several lattice periods. In order to circumvent this difficulty, a procedure was implemented in Warp which injects the beam through a transverse plane that is fixed in the laboratory, but drifting in the boosted frame, similarly to the laser injection method. Due to long range space charge forces, it is still necessary to provide a reasonable estimate of the beam distribution near the injection plane; this is accomplished by the use of "frozen" drifting macroparticles.

After the relativistic PIC algorithm evolves the system in the boosted frame, the 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 either as a post-processing script or, more efficiently, at runtime. Nevertheless, 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). As a set of additional diagnostics, we have found it convenient in Warp to record quantities at a number of regularly spaced "stations", immobile in the laboratory frame, at a succession of discrete times, for both detailed time histories and laboratory time-averages.

Details of the input and output procedures can be found in [11] for Warp, in [12] for Osiris and in [13] for Vorpal.

3. Examples of application

3.1. Electron cloud driven instabilities

Several existing and planned future particle accelerators have limitations due to the electron cloud instability that may negatively impact the beam quality and in some cases even lead to severe beam loss. A calculation of electron cloud driven instability [2] for an ultra-relativistic beam was performed with the Warp code framework in (a) standard PIC mode using the new particle pusher in a Lorentz boosted frame; (b) in quasistatic mode [14] using linear maps to push beam particles into the accelerator lattice. The two runs were in good agreement and completed using similar computer resources and runtimes. The speedup factor of the PIC boosted frame calculation compared to a PIC calculation in the laboratory frame was estimated at 500. For many calculations of electron cloud instability, the boosted frame approach may not resolve any additional physics not included in the quasistatic approach. We note, however, that the quasistatic method requires significant special coding for taking into account eventual longitudinal motion of electrons [14], as well as a special parallelization scheme [15] for parallelization along the axis of beam propagation, that are not standard to PIC codes. By contrast, the boosted frame method includes naturally the longitudinal dynamics and requires more modest modifications to an existing standard PIC code or framework (including none for full parallelization).

3.2. Laser wakefield acceleration

Laser driven plasma waves offer orders of magnitude increases in accelerating gradient over standard accelerating structures (which are limited by electrical breakdown), thus holding the promise of much shorter particle accelerators. Yet, computer modeling of the wake formation and beam acceleration requires fully kinetic methods and large computational resources due to the wide range of space and time scales involved [16]. For example, modeling 10 GeV stages for the LOASIS (LBNL) BELLA proposal [17] in one-dimension demanded as many as 5,000 processor hours on a NERSC supercomputer [13]. As discussed in [1], the range of scales can be greatly reduced if one adopts the common assumption that the backward-emitted radiation can be neglected, enabling, for the first time, the full-PIC simulation of the next generation of laser systems [15].

Warp simulations at plasma density $n_e = 10^{19}$ cm^{-3} were performed in 2-1/2D [11] and 3-D [15] using reference frames moving anywhere between $\gamma_f = 1$ (laboratory frame) and 10. These simulations are scaled replicas of 10 GeV stages that would operate at actual densities of 10^{17} cm^{-3} [18, 19] and allow short run times to permit effective benchmarking between the algorithms. Two figures of merit were considered (both evaluated in the laboratory frame): (a) the peak energy of the accelerated electron beam; (b) the average energy history of the electron beams. Agreement within a few percent was observed on the beam peak energy between calculations in all frames, with a speedup of 100 measured between the calculation in the frame at $\gamma = 10$ and the calculation in the laboratory frame. The average beam energy history reveals agreement at the few percent level for the accelerating phase, followed by a growing discrepancy during the decelerating phase. In order to obtain the speedup of 100, a low dispersion electromagnetic solver was used for $\gamma \geq 5$, while the standard Yee solver was used otherwise, for the reasons stated

in the preceding section. Percentage level agreement was obtained during both accelerating and decelerating phases by using the Yee solver for all values of γ, at a cost, but nonetheless achieving a maximum measured speedup of 10. The reasons for the discrepancies at high values of γ between the two electromagnetic solver runs are currently under investigation.

The parallel VORPAL framework has been used to simulate proof-of-principle acceleration of test-particles to 10 GeV energies in one and two spatial dimensions, for plasma channel parameters in which pump depletion and dephasing lengths are equal [20]. The 1D simulations were done both in the laboratory frame and in a Lorentz boosted reference frame [3], showing qualitative agreement in the peak energy of the accelerated particles. The boosted-frame simulations were 1,500x faster, reduced errors in the laser group velocity, and eliminated problems with artificial dark current. The 2D simulations were not feasible in the laboratory frame, but the boosted-frame results [13] showed agreement with the predictions of scaling arguments [18], with an estimated 2,000x speedup.

A set of 3-D benchmarks was performed between OSIRIS boost and OSIRIS and QuickPIC[14] in the laboratory frame, for weakly-nonlinear/nonlinear regimes and self-injected/externally-injected electron beams, with very good qualitative and quantitative agreement. Particular emphasis was given to a 1.5 GeV self-injection stage of LWFA, successfully reproducing the results obtained with laboratory frame simulations presented in [21]. The boosted frame scheme was tested for a broad set of numerical parameters and algorithms, namely different boost speeds with varying resolutions, higher order field solvers [22], particle interpolation schemes [23], and modified Boris pusher [5], showing overall result convergence and consistency. For the particular case of a 1.5 GeV self-injection stage, results recover those in the laboratory frame presented in [21].

3.3. Free electron lasers

In a short wavelength free-electron laser (FEL), a high energy electron beam interacts with a static magnetic undulator. In the optimal boost frame with Lorentz factor γ, the down-shifted FEL radiation and up-shifted undulator have identical wavelengths and the number of required time-steps (presuming the Courant condition applies) decreases by a factor of $2\gamma^2$ for fully electromagnetic simulations. Examples of boosted-frame simulations are compared [25] to results obtained with the eikonal (i.e, SVEA) and wiggler-period averaged code Ginger [24]. It was concluded that if the necessary FEL physics can be studied with an eikonal code, it will run much faster than a full EM code in whatever frame. However, if there are important physical phenomena that cannot be resolved properly by an eikonal code, a boosted-frame electromagnetic code is a very attractive alternative to a brute force full EM calculation in the laboratory frame.

3.4. Coherent synchrotron radiation

Another application for which the Lorentz-boosted frame method might be useful is that of modeling coherent synchrotron radiation (CSR) [26] emitted by high current, high brightness relativistic electron beams. Because full scale electromagnetic simulation of CSR in the laboratory frame is difficult due to the wide range of scales (chicane lengths of order meters, radiation wavelengths of orders microns), in order to make the calculation tractable most CSR simulation codes apply simplifications such as ignoring transverse variation of CSR across the electron beam. We have begun preliminary work of simulating CSR emission with the boosted frame method in Warp, examining the behavior of a high current, short electron beam transiting a simple dipole magnet. Our early results show that upon exit from the undulator the electron beam shows the characteristic energy loss variation with longitudinal position that one expects from previous theoretical analyses of CSR. Further studies are currently underway.

4. Conclusion

The non-invariance of the range of scales of a physical system implies that the computational cost of a certain class of computer simulations depends strongly on the choice of the simulation frame of reference. Some algorithmic difficulties may arise due to the loss of covariance upon discretization of the Maxwell-Vlasov system of equations, and the need to transform input/output data between the laboratory frame and the Lorentz boosted frame. Most such difficulties have been overcome and no "show-stopper" has been identified at this time. First principle simulations in boosted frames have been performed successfully by the Scidac codes Warp, Osiris and Vorpal in application to electron cloud driven instabilities, laser wakefield acceleration and free electron lasers, with speedups ranging between a few and several orders of magnitude. Further testings and studies of advanced numerical techniques are underway to fully validate the method and push the limits toward higher speed-ups. Our recent progress shows that first principle modeling in a Lorentz boosted frame is a viable alternative or complement to using reduced descriptions like the quasistatic [?, 14] or eikonal [24] approximations, or scaled parameters [19], when there is a need to study physics that is not accessible to the other descriptions, or for validation of their simplifications.

5. Acknowledgments

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