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INTEGRATING THE LORENTZ FORCE LAW FOR HIGHLY-RELATIVISTIC PARTICLE-IN-CELL SIMULATIONS*

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Abstract

Integrating the Relativistic Lorentz Force Law for plasma simulations is an area of current research ([1–3]). In particular, recent research indicates that interaction with highly-relativistic laser fields is particularly problematic for current integration techniques [1]. Here is presented a special-purpose integrator yielding improved accuracy for highly-relativistic laser-particle interactions. This integrator has been implemented in the particle-in-cell code VSim [4], and the authors present an accuracy and performance comparison with several particle push methods.

INTRODUCTION

Several current areas of accelerator research involve highly-relativistic radiation interacting with an under-dense plasma, i.e. radiation for which the parameter $a_0 = \frac{eE_{max}}{mc\omega} \gtrsim 1$ for at least one of the species of particles comprising the plasma. Recent work [1], [5] has highlighted that particle-in-cell simulations of such systems using the standard Boris push [6] can exhibit numerical artifacts at standard resolutions. Many simulations of Laser Wakefield Acceleration (LWFA) do not exhibit these artifacts, because particles do not interact with high-a_0 radiation for long times. However, there has been significant recent interest in simulations of the pure Direct Laser Acceleration (DLA) regime [7], where a laser pulse much longer than the plasma wavelength propagates through a plasma, and of hybrid LWFA [8, 9], where beam particles interact significantly with the laser pulse.

Particle-in-cell simulations are both necessary to understand the complex non-linear dynamics of these systems, and very computationally expensive. Thus, algorithms for reducing the computational burden associated with them are desirable. The purpose of this paper is to present a new particle push algorithm for use in particle-in-cell simulations where plasma particles interact with high-a_0 radiation for a substantial portion of the total simulation length.

PLANE-WAVE CASE

The highest-field regions of the simulations of interest resemble a vacuum plane wave plus some perturbations due to interaction with the plasma and the finite spatial extent of the laser pulse. This paper's method exploits that characteristic of these simulations, and hence it will be referred to henceforth as the "luminal push." In the current section we derive the algorithm for the case of a linearly-polarized plane wave travelling in vacuum, polarized along the y axis and propagating along the x axis. We use a leap-frog method, where the coordinates and momenta are alternately held constant. Advancing the coordinates is trivial; the novel part of the method is in integrating the Lorentz Force Law to determine the change in momenta.

In what follows, γ is the Lorentz factor. The quantity $\Gamma = \gamma - \frac{p_x}{mc}$ is a constant of the motion for the particle, and from this can be derived the following set of equations for $u_y = \frac{p_y}{m}$, $u_x = \frac{p_x}{m}$, and γ:

$$\gamma = \frac{c^2(1+\Gamma^2)+u_y^2}{2\Gamma c^2} \quad (1)$$

$$u_x = \frac{c^2(1-\Gamma^2)+u_y^2}{2\Gamma c} \quad (2)$$

$$\frac{du_y}{dt} = \frac{c\Gamma\Omega}{\gamma} \quad (3)$$

where $\Omega = \frac{qB}{m} = \frac{qE}{mc}$, which are constant because x is held constant for this portion of the leap-frog integration. Using the equation for γ yields the following ODE governing the evolution of u_y,

$$\frac{du_y}{dt} = \frac{2c\Gamma^2\Omega}{1+\Gamma^2+\frac{1}{c^2}u_y^2} \quad (4)$$

which can be integrated to yield

$$\frac{1}{6c^2\Gamma}(u^3-u_0^3) + \frac{(1+\Gamma^2)}{2\Gamma}(u-u_0) = c\Gamma\Omega t \quad (5)$$

implicitly defining $u_y(\Delta t)$. The explicit solution to Eq. (5) is

$$u(t) = 2c\sqrt{1+\Gamma^2}\sinh\left(\frac{1}{3}\sinh^{-1}\left(\frac{u_0^3+3c^2(1+\Gamma^2)u_0+6c^3\Gamma^2\Omega t}{2c^3(1+\Gamma^2)^{3/2}}\right)\right) \quad (6)$$

from which u_x and γ can be obtained using Eqs. (1) and (2).

GENERAL FIELDS

General electromagnetic fields can be written as a sum of fields $\vec{E}'$ and $\vec{B}'$ satisfying $\vec{E}'\times\vec{B}' = \vec{E}\times\vec{B}$, $\vec{E}'\cdot\vec{B}' = 0$ and $E'^2 - c^2B'^2 = 0$ and residual fields $\vec{E}''$ and $\vec{B}''$. We will refer to fields satisfying the latter two conditions on $\vec{E}'$ and $\vec{B}'$ as "luminal". The residual fields may or may not be luminal themselves, but we aim to split the fields in such a way that they are small.

In what follows, we derive the choice of $\vec{E}'$ and $\vec{B}'$ that minimizes the energy density of the residual fields. If $\vec{E}$ and $\vec{B}$ are (anti-)parallel, then the Poynting vector vanishes and

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the splitting is trivially complete, so assume that the electric and magnetic fields make an angle $\alpha \neq 0, \pi$ with one another. Then define

$$P^2 = \frac{1}{c}|\vec{E} \times \vec{B}| \quad (7)$$

$$\tan\theta = \frac{\vec{E} \cdot \vec{B}}{c(B^2 + P^2)} \quad (8)$$

$$\vec{B}' = \frac{P}{B}\mathbf{R}_{\vec{E}\times\vec{B}}(\theta)\vec{B} \quad (9)$$

$$\vec{E}' = \frac{\vec{B}' \times (\vec{E} \times \vec{B})}{P^2} \quad (10)$$

$$\vec{B}'' = \vec{B} - \vec{B}' \quad (11)$$

$$\vec{E}'' = \vec{E} - \vec{E}' \quad (12)$$

where $\mathbf{R}_{\vec{E}\times\vec{B}}(\theta)$ is a matrix that rotates about $\vec{E} \times \vec{B}$ by an angle θ.

It should be clear by inspection that the vectors $\vec{E}'$ and $\vec{B}'$ are mutually perpendicular with $\vec{E} \times \vec{B}$ and have magnitudes cP and P, respectively, so they define a luminal field with Poynting Vector equal to $\vec{E} \times \vec{B}$. The energy density of the residual fields $\vec{E}''$ and $\vec{B}''$ is proportional to

$$(E'')^2 + c^2(B'')^2 = |\vec{E} - \vec{E}'|^2 + c^2|\vec{B} - \vec{B}'|^2 \quad (13)$$

$$= E^2 + c^2B^2 + 2c^2P^2 - 2(\vec{E} \cdot \vec{E}' + c^2\vec{B} \cdot \vec{B}') \quad (14)$$

$$(15)$$

and the term

$$(\vec{E}\cdot\vec{E}' + c^2\vec{B}\cdot\vec{B}') = cEP\cos\left(\frac{\pi}{2} - \alpha - \theta\right) + c^2BP\cos\theta \quad (16)$$

is maximized when θ is given as in Equation (8), so that choice of θ minimizes the energy density of the residual field.

This is only one possible splitting of the fields. As long as the residual fields are small, the essential idea of the method is valid. In particular, for a linearly-polarized laser pulse, it may be sufficient to simply use luminal fields with a prescribed polarization, scaled to match the magnitude of the Poynting vector. Furthermore, the square root in Eq. (7) for P^2 and the inverse tangent in Eq. (8) for θ do not need to be calculated to perfect accuracy, so long as $\vec{E}'$ and $\vec{B}'$ are, in fact, mutually perpendicular with magnitudes scaled by c and the residuals are calculated correctly.

To integrate these general fields, we use again a leapfrog approach, first pushing the particle for half a time step using the residual fields and any general-purpose particle pusher, then pushing the particle for a whole time step, using the luminal fields $\vec{E}'$ and $\vec{B}'$ and the methods of the previous section, where that section's x is the axis parallel to the Poynting vector and that section's y is the axis parallel to $\vec{E}'$. Finally we push the particle another half time step, again using any general-purpose particle push algorithm.

NUMERICAL RESULTS

This algorithm was implemented and used to integrate the trajectory of a single particle in a plane wave over 1000 laser periods. The plane wave fields were evaluated analytically at the particle's location each time-step using the Boris integrator, Vay's relativistic integrator [2], and the new luminal integrator. The results are presented in Figs. 1 and 2, from which it is evident that the luminal integrator was much better than the alternatives at correctly computing the longitudinal wavelength Λ and secular drift $\delta\bar{y}$ of the particle's orbit.

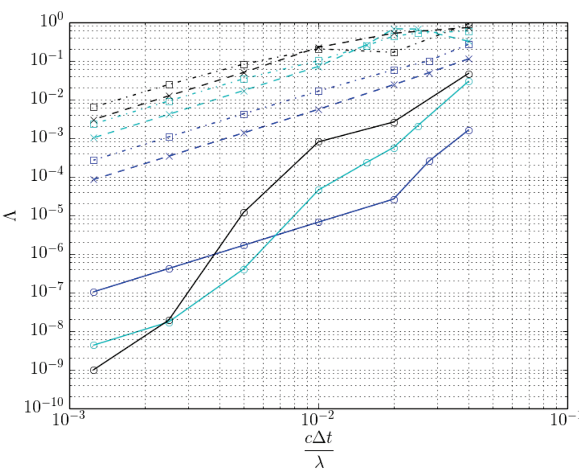

Figure 1: Fractional error in $\bar{\Lambda}$ for particle in plane wave field for 1000 optical cycles, using Boris push (dash-dotted), Vay push (dashed) and Luminal push (solid), for a_0 values of 5 (black), 15 (cyan) and 25 (blue).

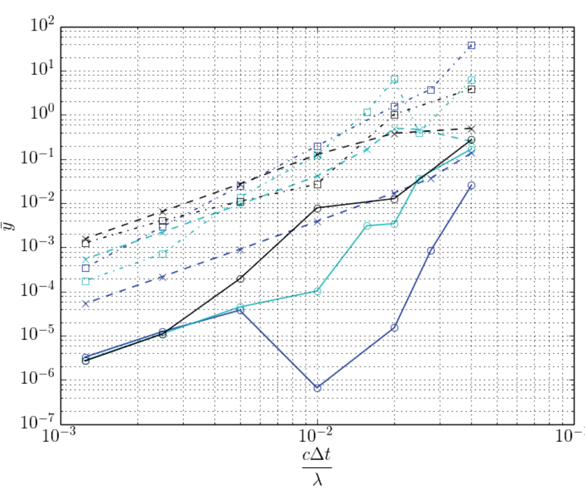

Figure 2: Fractional error in $\delta\bar{y}$ for particle in plane wave field for 1000 optical cycles, using Boris push (dash-dotted), Vay push (dashed) and Luminal push (solid), for a_0 values of 5 (black), 15 (cyan) and 25 (blue).

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CONCLUSION

This paper presents a special-purpose particle push of use in simulations where charged particles interact with high-a_0 radiation. It was demonstrated to have performance superior to alternatives for the case of an analytically-known plane wave field, and an extension to general fields was provided.

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