X-Dispersionless Maxwell solver for plasma-based particle acceleration

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A semi-implicit finite difference time domain (FDTD) numerical Maxwell solver is presented for full electromagnetic Particle-in-Cell (PIC) codes for the simulations of plasma-based acceleration. The solver projects the volumetric Yee lattice into planes transverse to a selected axis (the particle acceleration direction) that makes the scheme quasi-one-dimensional. The scheme removes the numerical dispersion of electromagnetic waves running parallel the selected axis. The fields locations in the transverse plane are selected so that the scheme is Lorentz-invariant for relativistic transformations along the selected axis. This completely removes the problem of numerical Cerenkov instability (NCI). The fields positions build rhombi in plane (RIP) patterns. The RIP scheme uses a compact local stencil that makes it perfectly suitable for massively parallel processing via domain decomposition along all three dimensions. No global/local spectral methods are involved.
I. INTRODUCTION

Plasma-based particle acceleration is a rapidly developing route towards future compact accelerators [1][3]. The reason is that plasma supports fields orders of magnitude higher than conventional accelerators [5][6]. Thus, particle acceleration can be accomplished on much shorter distances as compared with the solid-state accelerating structures. However, the plasma is a highly nonlinear medium and requires accurate and computationally efficient numerical modeling to understand and tune the acceleration process. The main working horse for plasma simulations are Particle-in-Cell codes [7][11]. These provide the most appropriate description of plasma as an ensemble of particles pushed according to the relativistic equations of motion using self-consistent electromagnetic fields, which are maintained on a spatial grid [12].

From a numerical point of view, plasma-based acceleration represents a classic multi-scale problem. Here, we have the long scale of acceleration distance that can range from centimeters [14] to several meters [14][15], and the short scale of plasma wavelength that ranges from a few micrometers to near millimeter scales. In addition, if the plasma wave is created by a laser pulse, there is additionally the laser wavelength scale in the sub-micron range. This natural scale disparity makes the simulations of plasma-based acceleration so computationally demanding.

Presently, two types of PIC codes are used to simulate the plasma-based accelerator structures: (i) universal full electromagnetic PIC codes [7][11], which solve the unabridged set of Maxwell equations and (ii) quasi-static PIC codes [8][16][17], which analytically separate the short scale of plasma wavelength and the long propagation distance scale. The quasi-static PIC codes are proven to be both accurate and very computationally efficient when simulating beam-driven plasma-based wake field acceleration (PBWFA). Unfortunately, the quasi-static approximation for the Maxwell equations eliminates any radiation. Thus, the laser pulse driver has to be described in an envelope approximation [18]. Further, the quasi-static codes fail at simulating sharp plasma boundaries and self-trapping of particles from background plasma.

For this reason, we here consider full electromagnetic (EM) PIC codes which are usually applied for Laser Wake Field Acceleration (LWFA) in plasmas. The full EM PIC correctly describes the laser evolution even in highly nonlinear regimes. The full EM PIC codes are computationally very expensive because they do not separate the different scales. A significant scale adjustment can be made if one makes a Lorentz transformation of the system into a reference frame moving in the direction of acceleration with a relativistic speed. This leads to the Lorentz contraction of the propagation distance with the relativistic factor $\gamma = 1/\sqrt{1 - V^2/c^2}$, where $V$ is the relative velocity of the reference frame. Simultaneously, the driver - and its wavelength - become longer at nearly the same factor. This so-called "Lorentz-boost" [19] evens the scale disparity and potentially gives a large computational speed up.

However, in "Lorentz-boosted" PIC simulations, the background plasma - both electrons and ions - is moving backward at a relativistic velocity. This moving plasma is a source of free energy that can be easily transformed into high amplitude noise fields. The major numerical mechanism for this parasitic conversion is the Cerenkov resonance [20]. The problem of existing FDTD Maxwell solvers is that they employ the Yee lattice [21]; individual components of the electromagnetic fields are located at staggered positions in space. The resulting numerical scheme includes a Courant stability restriction on the time step which leads to numerical dispersion. This results in electromagnetic waves with phase velocities below the vacuum speed of light. Thus, the relativistic particles may stay in resonance with the waves and radiate. This non-physical Cerenkov radiation plagues the Lorentz-boosted PIC simulations [22]. Moreover, even normal PIC simulations in the laboratory frame suffer from the numerical Cerenkov effect [23][24]. Any high density bunch of relativistic particles - e.g. the accelerated witness bunch - emits Cerenkov radiation as well. This affects the bunch energy and emittance [25].

In principle, the Yee scheme can be modified - or extended - by using additional neighbouring cells with the goal to tune the numerical dispersion so that the Cerenkov resonance is avoided in the zero order [26][27]. This reuces the Cerenkov instability, but does not eliminate it. One of the reasons is that the Yee lattice itself is not Lorentz-invariant. The individual field components are located all at different positions staggered in space. In the boosted frame, the fields are Lorentz-transformed and find themselves at the wrong positions. For example, when the boosted frame moves in the $X-$direction, the pairs $E_y, B_z$ and $E_z, B_y$ transform one into another. Yet, they are located at different positions within the Yee lattice cell.

The different positions of the field pairs $E_y, B_z$ and $E_z, B_y$ on the Yee lattice also cause another problem relevant to the high energy physics. When we want to simulate high current relativistic beams [28], this spatial staggering may lead to a beam numerical self-interaction. A real beam of ultra-relativistic, $\gamma \gg 1$, particles has a small physical self-interaction due to the difference of these fields with the transverse force $q(E_\perp + \beta_\parallel e\parallel \times B_\perp)$. Here $e\parallel$ is the unit vector in the propagation direction and $1 - \beta_\parallel = 1 - v_\parallel/c \approx 1/2\gamma^2$ is the relative difference of the particles longitudinal velocity $v_\parallel$ from the speed of light $c$. For 50 GeV electrons with $\gamma \approx 10^5$, this real difference is as small as $1 - \beta_\parallel \approx 5 \cdot \gamma^{-11}$. The transverse self-fields $E_\perp$ and $B_\perp$ of the ultra-relativistic bunch are also nearly equal with the same miniscule relative difference. However, the Yee lattice defines these fields at different positions in space. These fields must be interpolated to the individual particle positions. This interpolation leads to errors and
differences between the transvers fields acting on the particle. As a consequence, the bunch self-action due to the numerical errors is many orders of magnitude larger than the real one. This results not only in the bunch numerical self-focusing/defocusing and emittance growth, but also in significant numerical bremsstrahlung and stopping - when these effects are included in the PIC code.

We conclude, the Yee lattice is not optimal for simulating high energy applications.

II. PSEUDO-SPECTRAL METHODS AND ALIASING

Recently, pseudo-spectral methods originally proposed by Haber et al. [29], shortly discussed in [12] and used by O. Buneman in his TRISTAN code [30] have seen a remarkable revival [10]. The seeming advantage of the spectral methods is that they are dispersionless and provide an “infinite order” of approximation, even calling the method after Haber “a pseudo-spectral analytical time-domain (PSATD) algorithm” [31].

Indeed, following Sommerfeld [32] we can write the Maxwell equations in the Fourier space as

$$\partial F \over \partial t = i \mathbf{c} \times \mathbf{F} - \mathbf{J}$$ (1)

where $\mathbf{J} = FFT[\mathbf{J}]$ is the Fourier image of the real current while $\mathbf{F} = FFT[\mathbf{F}]$ is the Fourier image of the complex electromagnetic field $\mathbf{F} = \mathbf{E} + i \mathbf{B}$. It is straightforward to show that the numerical scheme advancing the fields from the time step $n$ to $n+1$ in the form

$$\mathbf{F}^{n+1} = C_k \hat{\mathbf{F}}^n + i S_k \times \hat{\mathbf{F}}^n - \hat{\mathbf{C}}_k \hat{\mathbf{J}}^{n+1/2} + i \hat{\mathbf{S}}_k \times \hat{\mathbf{J}}^{n+1/2}$$

$$+ (\hat{C}_k - 1) (e_k \cdot \hat{\mathbf{J}}^{n+1/2}) e_k + (1 - C_k) (e_k \cdot \hat{\mathbf{F}}^n) e_k$$ (2)

is dispersionless in vacuum and provides second order approximation for the plasma currents. Here, $C_k = \cos(\mathbf{c} \tau)$, $\hat{C}_k = \cos(\mathbf{c} \tau / 2)$, $S_k = e_k \sin(\mathbf{c} \tau)$, $\hat{S}_k = e_k \sin(\mathbf{c} \tau / 2)$, $\tau$ is the time step, $k = |\mathbf{k}|$, $e_k = \mathbf{k} / k$.

Unfortunately, Eq. (2) only gives acceptable results on an infinite grid. The reason is that Eq. (2) is not linear, although the Fourier transform is a linear operator. The non-linearities appear in the Eq. (2) in various ways. First of all, Eq. (2) is not linear in $k$. Consequently, it is subject to aliasing [34]. Let us take the seemingly harmless product $C_k \hat{\mathbf{F}}^n$. In configuration space on a finite grid with $M$ cells (for simplicity, we take a 1D example), it corresponds to the convolution

$$FFT^{-1} \left[ C_k \hat{\mathbf{F}}^n \right] = \sum_{m=1}^{M} FFT^{-1} \left[ C_k \right]_{m} \mathbf{F}^{n}_{l-m}$$ (3)

For indices in the range $l - m < 0$, the convolution (3) overrun the finite grid boundary and automatically takes field values $\mathbf{F}^{n}_{M+l-m}$ from the very other side of the grid. This makes little physical sense and is generally called “aliasing” of the pseudo-spectral methods [35]. All other products of two functions depending on $k$, such as $S_k$, $\hat{C}_k$ and $\hat{S}_k$ in (2) result in unphysical aliasing as well. This makes the pseudo-spectral schemes unphysical unless some “de-aliasing” procedure removes these effects.

The aliasing of the $k$-products in (2) can be removed in a relatively straightforward way: the arrays of images in the configuration space must be “padded” by zeroes so that the aliased convolution does not touch non-zero values from the other side [36]. This de-alising procedure works well for equations with quadratic nonlinearities even though it may be expensive in multi-dimensional simulations.

The pseudo-spectral PIC codes, however, contain another nonlinearity that is not quadratic at all and is a much more severe source of aliasing. The current $\mathbf{J}$ has a highly nonlinear dependence on the fields, and thus its Fourier image $\hat{\mathbf{J}}[\mathbf{F}]$ used in (2) is fully aliased. This can be readily seen even in the hydrodynamic version of the current

$$\mathbf{J} = q n \mathbf{p} / m \gamma,$$ (4)

where $n(\mathbf{r})$ is the particle density. For low-amplitude linear oscillations, the local momentum can be interpreted as $\mathbf{p} = \mathbf{e} \mathbf{E} / q \omega$. For simplicity, we here assume a harmonic field $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0(\mathbf{r}) \exp(-i \omega t)$. Transforming (4) to the Fourier space, we have
\[ \tilde{J} = \frac{1}{im\omega} FFT [n(r)E(r)/\gamma(E)] \]

For the simplest non-relativistic (\( \gamma = 1 \)) hydrodynamic case, the Fourier image of the product \( n(r)E(r)/\gamma(E) \) corresponds to a convolution in the Fourier space

\[ \tilde{J} = \frac{1}{im\omega} \sum_{k=-K/2}^{K/2} \tilde{n}_k E_{K/2-k} \]

where \( K \) is the number of modes. This convolution aliases spectra of the particle density \( \tilde{n}_k \) and the field \( E_{K/2-k} \). The simplest non-relativistic hydrodynamic case corresponds to the quadratic nonlinearity and could be corrected by padding. However, the density deposition in full PIC codes cannot be described by this oversimplified approximation. In addition, the relativistic \( \gamma \)-factor of particles \( \gamma = \sqrt{1 + p^2/m^2c^2} \) depends on the fields in a highly nonlinear way. Moreover, for the particle push, the fields have to be interpolated to the particle positions using the macroparticle shape distributions. Thus, the current \( J \) depends on the fields in a non-quadratic non-local non-linear way. The calculation of \( J \) does not correspond to a simple convolution in the Fourier-space. This leads to a heavy aliasing of the pseudo-spectral currents \( \tilde{J} \) that cannot be removed in any easy way.

The physical signatures of this aliasing will manifest in different ways depending on the particular physics of the problem leading to global artefacts sometimes clearly seen on the grid. One of these signatures is the persistence of Cerenkov instability in pseudo-spectral codes despite the absence of numerical dispersion [37]. The particles interact with waves from the upper numerical Brillouin zone then. In an effort to remove the Cerenkov instability in pseudo-spectral codes, filtering currents of the most unstable modes is often applied [38]. This artificial filtering, however, may lead to additional unphysical effects in the pseudo-spectral simulations. Another approach is elimination of numerical Cerenkov instability in flowing-plasma particle-in-cell simulations by using Galilean coordinates [39]. This approach removes relative motion between the numerical grid and the streaming plasma: the grid cells flow together with the plasma. Unfortunately, this trick works only in one direction and does not help removing numerical Cerenkov emission of the high current bunch being accelerated in the opposite direction.

Further, the FFT-based solvers are intrinsically global. This means, they need information about fields in the full simulation domain to update the local field at a particular point in space. This contradicts the causality principle of the special relativity: only fields within \( ct \) distance from the space point may cause the local fields to change. The propagator [2] explicitly separates the fields and currents into the propagating transverse fields and non-propagating longitudinal fields. According to the Helmholtz theorem [40], this separation is unique, when the boundary conditions are well defined. Yet, the local field knows nothing about the distant boundaries dynamics at the time step. The global nature of the FFT solvers also means that any local error (including the boundary conditions and aliasing) spreads immediately over all the simulation domain.

We conclude that pseudo-spectral methods are far from ideal candidates for PIC simulations and that a better FDTD method is required. In this work, a new FDTD solver is presented that does not employ spectral transformations and yet has the unique property of having no numerical dispersion along one selected spatial axis. The solver uses Lorentz-invariant field locations for transformations along this selected axis, and so particles moving in this direction do not generate non-physical Cerenkov radiation.

III. THE GENERAL QUASI-1D MAXWELL SOLVER

We here develop a FDTD 3D Maxwell solver that has no dispersion for plane waves propagating in vacuum in one selected direction. In plasma-based acceleration this is usually the direction of particle acceleration: the driving laser optical axis. The solver should retain its dispersionless properties not only in vacuum, but also inside dense plasmas, i.e., the optimal time step/grid step relation should not be compromised by the presence of plasma. The solver must not use spectral transformations and should have a compact local stencil. This is the pre-requisite for efficient parallelization via domain decomposition. In short, we develop an efficient Maxwell solver for quasi-1D problems.

We select the \( X \)-direction for dispersionless propagation. For electromagnetic waves propagating in \( X \), we have the Maxwell equations
Here, the vector \( \Gamma = G + J \) combines the vacuum diffraction operator \( G \) for \( E \) and the medium response (currents) \( J \), while \( \Phi \) is the vacuum diffraction operator for \( B \).

We use a semi-implicit trapezoidal scheme for the discretization of the transverse fields on a 3D grid. We write here explicitly the \( i \)-index along the \( X \)-axis only as the scheme can be easily generalized for arbitrary transverse geometries (e.g. Cartesian, or cylindrical, etc.):

\[
\frac{E_{y(i+1)}^{n+1} + E_{y(i)}^{n} - E_{y(i+1)}^{n}}{2c\tau} = -\frac{B_{z(i+1)}^{n+1} + B_{z(i)}^{n} - B_{z(i+1)}^{n}}{2h_x} - \frac{\Gamma_{y(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{y(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{y(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{y(i+1/2)}^{n+1/2}}{2h_x}
\]

\[
\frac{E_{z(i+1)}^{n+1} + E_{z(i)}^{n} - E_{z(i+1)}^{n}}{2c\tau} = -\frac{B_{y(i+1)}^{n+1} + B_{y(i)}^{n} - B_{y(i+1)}^{n}}{2h_x} - \frac{\Gamma_{z(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{z(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{z(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{z(i+1/2)}^{n+1/2}}{2h_x}
\]

\[
\frac{E_{x(i)}^{n+1} - E_{x(i)}^{n}}{c\tau} = \frac{\Gamma_{x(i)}^{n+1/2}}{2h_x}
\]

\[
\frac{B_{y(i+1)}^{n+1} + B_{y(i)}^{n} - B_{y(i+1)}^{n}}{2c\tau} = -\frac{E_{z(i+1)}^{n+1} + E_{z(i)}^{n} - E_{z(i+1)}^{n}}{2h_x} - \frac{\Gamma_{z(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{z(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{z(i+1/2)}^{n+1/2}}{2h_x}
\]

\[
\frac{B_{z(i+1)}^{n+1} + B_{z(i)}^{n} - B_{z(i+1)}^{n}}{2c\tau} = -\frac{E_{y(i+1)}^{n+1} + E_{y(i)}^{n} - E_{y(i+1)}^{n}}{2h_x} - \frac{\Gamma_{y(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{y(i+1/2)}^{n+1/2}}{2h_x} + \frac{\Gamma_{y(i+1/2)}^{n+1/2}}{2h_x}
\]

\[
\frac{B_{x(i)}^{n+1} - B_{x(i)}^{n}}{c\tau} = \frac{\Gamma_{x(i)}^{n+1}}{2h_x}
\]

Here, \( \tau \) is the time step and \( h_x \) is the spatial grid step in the \( X \)-direction.

These equations (13)-(18) build a system of coupled linear equations relating the updated fields at the time step \( n + 1 \) with already known fields at the time steps \( n \) and \( n + 1/2 \). Although this implicit system of linear equations can generally be solved using a fast matrix inversion method (the system has a sparse matrix), we will be interested in the special case \( c\tau = h_x = \Delta \). In this particular case, the inversion is straightforward.

First, we add Eqs. (13)+(17) and (14)+(16) to obtain transport components
\[ T_{y(i)}^{+(n+1)} = E_{y(i)}^{n+1} + B_{z(i)}^{n+1} = E_{y(i-1)}^{n} + B_{z(i-1)}^{n} \]
\[ + \Delta \left( \Gamma_{y(i-1/2)}^{n+1/2} + \Phi_{z(i-1/2)}^{n+1/2} \right) \]
\[ T_{z(i)}^{+(n+1)} = E_{z(i)}^{n+1} + B_{y(i)}^{n+1} = E_{z(i+1)}^{n} + B_{y(i+1)}^{n} \]
\[ + \Delta \left( \Gamma_{z(i+1/2)}^{n+1/2} + \Phi_{y(i+1/2)}^{n+1/2} \right) \]

or simply

\[ T_{y(i)}^{+(n+1)} = T_{y(i)}^{+(n)} + \Delta \left( \Gamma_{y(i-1/2)}^{n+1/2} + \Phi_{z(i-1/2)}^{n+1/2} \right) \]
\[ T_{z(i)}^{+(n+1)} = T_{z(i)}^{+(n)} + \Delta \left( \Gamma_{z(i+1/2)}^{n+1/2} + \Phi_{y(i+1/2)}^{n+1/2} \right) \]

Then, we subtract the same Eqs. \([13]-[17]\) and \([14]-[16]\) to obtain

\[ T_{y(i)}^{-(n+1)} = E_{y(i)}^{n+1} - B_{z(i)}^{n+1} = E_{y(i+1)}^{n} - B_{z(i+1)}^{n} \]
\[ + \Delta \left( \Gamma_{y(i+1/2)}^{n+1/2} - \Phi_{z(i+1/2)}^{n+1/2} \right) \]
\[ T_{z(i)}^{-(n+1)} = E_{z(i)}^{n+1} - B_{y(i)}^{n+1} = E_{z(i-1)}^{n} - B_{y(i-1)}^{n} \]
\[ + \Delta \left( \Gamma_{z(i-1/2)}^{n+1/2} - \Phi_{y(i-1/2)}^{n+1/2} \right) \]

or

\[ T_{y(i)}^{-(n+1)} = T_{y(i)}^{-(n)} + \Delta \left( \Gamma_{y(i+1/2)}^{n+1/2} - \Phi_{z(i+1/2)}^{n+1/2} \right) \]
\[ T_{z(i)}^{-(n+1)} = T_{z(i)}^{-(n)} + \Delta \left( \Gamma_{z(i-1/2)}^{n+1/2} - \Phi_{y(i-1/2)}^{n+1/2} \right) \]

These are the marching equations. The transport components \(T_{y,z}^{+,-}\) must be shifted one cell in the corresponding direction and the diffraction/refraction terms be correctly added.

For the fields, we get

\[ E_{y(i)}^{n+1} = \frac{1}{2} \left( E_{y(i-1)}^{n} + E_{y(i+1)}^{n} \right) - \frac{1}{2} \left( B_{z(i+1)}^{n} - B_{z(i-1)}^{n} \right) \]
\[ + \frac{\Delta}{2} \left( \Gamma_{y(i-1/2)}^{n+1/2} + \Phi_{z(i-1/2)}^{n+1/2} + \Gamma_{y(i+1/2)}^{n+1/2} - \Phi_{z(i+1/2)}^{n+1/2} \right) \]
\[ E_{z(i)}^{n+1} = \frac{1}{2} \left( E_{z(i-1)}^{n} + E_{z(i+1)}^{n} \right) + \frac{1}{2} \left( B_{y(i+1)}^{n} - B_{y(i-1)}^{n} \right) \]
\[ + \frac{\Delta}{2} \left( \Gamma_{z(i-1/2)}^{n+1/2} - \Phi_{y(i-1/2)}^{n+1/2} + \Gamma_{z(i+1/2)}^{n+1/2} + \Phi_{y(i+1/2)}^{n+1/2} \right) \]

\[ B_{y(i)}^{n+1} = \frac{1}{2} \left( B_{y(i-1)}^{n} + B_{y(i+1)}^{n} \right) + \frac{1}{2} \left( E_{z(i+1)}^{n} - E_{z(i-1)}^{n} \right) \]
\[ + \frac{\Delta}{2} \left( -\Gamma_{z(i-1/2)}^{n+1/2} + \Phi_{y(i-1/2)}^{n+1/2} + \Gamma_{z(i+1/2)}^{n+1/2} + \Phi_{y(i+1/2)}^{n+1/2} \right) \]
\[ B_{z(i)}^{n+1} = \frac{1}{2} \left( B_{z(i-1)}^{n} + B_{z(i+1)}^{n} \right) - \frac{1}{2} \left( E_{y(i+1)}^{n} - E_{y(i-1)}^{n} \right) \]
\[ + \frac{\Delta}{2} \left( \Gamma_{y(i-1/2)}^{n+1/2} + \Phi_{z(i-1/2)}^{n+1/2} - \Gamma_{y(i+1/2)}^{n+1/2} + \Phi_{z(i+1/2)}^{n+1/2} \right) \]

or simply
IV. THE THREE-DIMENSIONAL RIP MAXWELL SOLVER IN CARTESIAN COORDINATES

Let us now look at the diffraction/refraction terms. For simplicity, we use Cartesian coordinates.

We project the Yee lattice onto the \((Y,Z)\) plane. The grid becomes planar and has the form of Rhombi-in-Plane (RIP), as shown in Fig. 1. The pairs of transverse fields are now combined at positions according to the transport properties \((19)-(20)\). The pair \(E_y, B_z\) is located at the rhombi vertices \((i,j+1/2,k)\). The pair \(E_z, B_y\) is located at the rhombi vertices \((i,j,k+1/2)\). The longitudinal field \(E_x\) we place at point \((i,j,k)\) which is the center of the full integer rhombus. The longitudinal field \(B_x\) we place at the center of the half integer rhombus \((i,j+1/2,k+1/2)\). The grid is shown in Fig.1.

Then, the diffraction/refraction terms at the half time step will be:

\[
E_y^{(n+1)} = \frac{T_y^{+(n+1)} + T_y^{-(n+1)}}{2} \\
E_z^{(n+1)} = \frac{T_z^{+(n+1)} + T_z^{-(n+1)}}{2} \\
B_y^{(n+1)} = \frac{T_y^{+(n+1)} - T_y^{-(n+1)}}{2} \\
B_z^{(n+1)} = \frac{T_z^{+(n+1)} - T_z^{-(n+1)}}{2}
\]
\[
\Gamma_{y(i+1/2,j+1/2,k)}^{n+1/2} = \left( \frac{\partial B_x}{\partial z} - j_y \right)_{x(i+1/2,j+1/2,k)}^{n+1/2} + \frac{1}{2} \left( j_y^{n+1/2} + j_y^{n+1/2} \right) + \frac{B_x^{n+1/2}}{2h_z} \]

\[
\Gamma_{z(i+1/2,j,k+1/2)}^{n+1/2} = \left( \frac{\partial B_x}{\partial y} - j_y \right)_{x(i+1/2,j,k+1/2)}^{n+1/2} + \frac{1}{2} \left( j_y^{n+1/2} + j_y^{n+1/2} \right) - \frac{B_x^{n+1/2}}{2h_y} \]

\[
\Gamma_{z(i,j,k)}^{n+1/2} = \left( \frac{\partial B_x}{\partial y} - j_y \right)_{x(i,j,k)}^{n+1/2} + \frac{1}{2} \left( j_y^{n+1/2} + j_y^{n+1/2} \right) - \frac{B_x^{n+1/2}}{2h_y} \]

\[
\Phi_{y(i+1/2,j,k+1/2)}^{n+1/2} = \frac{1}{2} \left( \frac{\partial B_x}{\partial y} - j_y \right)_{x(i+1/2,j,k+1/2)}^{n+1/2} + \frac{1}{2} \left( j_y^{n+1/2} + j_y^{n+1/2} \right) - \frac{B_x^{n+1/2}}{2h_y} \]

Similar formulas are obtained for the fields at the half-time steps. After straightforward manipulations, we get the simple marching equations

\[
T_{y(i+1/2)}^{+(n+1/2)} = T_{y(i-1/2)}^{+(n-1/2)} + \Delta \left( G_y^{n+1/2} + F_y^{n+1/2} \right) \]

\[
T_{z(i+1/2)}^{+(n+1/2)} = T_{z(i+1/2)}^{+(n-1/2)} + \Delta \left( G_z^{n+1/2} + F_z^{n+1/2} \right) \]

\[
T_{y(i-1/2)}^{-(n+1/2)} = T_{y(i+1/2)}^{-(n-1/2)} + \Delta \left( G_y^{n+1/2} - F_y^{n+1/2} \right) \]

\[
T_{z(i-1/2)}^{-(n+1/2)} = T_{z(i+1/2)}^{-(n-1/2)} + \Delta \left( G_z^{n+1/2} - F_z^{n+1/2} \right) \]

with the diffraction/refraction terms

\[
\Gamma_{y(i+1/2,j+1/2,k)}^{n+1/2} = \left( \frac{\partial B_x}{\partial z} - j_y \right)_{x(i+1/2,j+1/2,k)}^{n+1/2} + \frac{1}{2} \left( j_y^{n+1/2} + j_y^{n+1/2} \right) + \frac{B_x^{n+1/2}}{2h_z} \]

\[
\Gamma_{z(i+1/2,j,k+1/2)}^{n+1/2} = \left( \frac{\partial B_x}{\partial y} - j_y \right)_{x(i+1/2,j+1/2,k+1/2)}^{n+1/2} + \frac{1}{2} \left( j_y^{n+1/2} + j_y^{n+1/2} \right) - \frac{B_x^{n+1/2}}{2h_y} \]

\[
\Gamma_{z(i,j,k)}^{n+1/2} = \left( \frac{\partial B_x}{\partial y} - j_y \right)_{x(i,j,k)}^{n+1/2} + \frac{1}{2} \left( j_y^{n+1/2} + j_y^{n+1/2} \right) - \frac{B_x^{n+1/2}}{2h_y} \]
The fields at the half-time steps are required to calculate the diffraction terms only. Without diffraction, the need to maintain the additional set of fields at half-time steps vanishes and the RIP scheme becomes identical to the standard 1D PIC scheme [12], which is the workhorse of 1D plasma simulations due to its excellent stability and accuracy.
Figure 2. Intensity of fluctuating fields in the “streaming plasma” simulations. The Yee scheme is fully subject to the numerical Cerenkov instability and reaches saturation within a few plasma periods. The FFT-based solver avoids the first order numerical Cerenkov resonance and is subject to second order aliasing resonance. The RIP simulation of streaming plasma shows several orders of magnitude lower noise fields. The noise field growth rate is very low here. Mention that the FFT solver \cite{2} is identical to the RIP solver for waves running along the $X$-axis. Yet, the FFT solver is subject to NCI because of aliasing. The stationary plasma case shows no instability at all in the RIP simulation.

VI. DISPERSION AND STABILITY OF THE RIP SCHEME

We apply the plane-wave analysis to the marching equations (15), (18) and (27)-(30) with the refraction/diffraction terms (35)-(40) assuming $\mathbf{F} = \tilde{\mathbf{F}} \exp(-i\omega t + i\mathbf{k}\mathbf{r})$. For simplicity, we assume uniform plasma frequency $\omega^2 = 4\pi n e^2 / \gamma$ and the linear current response to the electric field $\frac{\Delta}{2c} \sin \frac{\omega \Delta}{2c} \mathbf{J} = iq^2 n \mathbf{E}$. For the case of interest, $c\tau = h_x = \Delta$, these equations become

\begin{align}
\frac{2}{\Delta} \sin \frac{\omega \Delta}{2c} \cos \frac{k_z \Delta}{2} \tilde{E}_y &= - \frac{2}{\Delta} \sin \frac{k_x \Delta}{2} \cos \frac{\omega \Delta}{2c} \tilde{B}_z \\
&+ \frac{2}{h_z} \sin \frac{k_x h_z}{2} \cos \frac{k_x \Delta}{2} \tilde{B}_x + \frac{\Delta}{2c} \sin \frac{\omega \Delta}{2c} \tilde{E}_y
\end{align}

\begin{align}
\frac{2}{\Delta} \sin \frac{\omega \Delta}{2c} \cos \frac{k_z \Delta}{2} \tilde{E}_z &= \frac{2}{\Delta} \sin \frac{k_x \Delta}{2} \cos \frac{\omega \Delta}{2c} \tilde{B}_y \\
&- \frac{2}{h_y} \sin \frac{k_y h_y}{2} \cos \frac{k_x \Delta}{2} \tilde{B}_x + \frac{\Delta}{2c} \sin \frac{\omega \Delta}{2c} \tilde{E}_y
\end{align}

\begin{align}
\frac{2}{\Delta} \sin \frac{\omega \Delta}{2c} \tilde{E}_x &= \frac{2}{h_y} \sin \frac{k_y h_y}{2} \tilde{B}_z - \frac{2}{h_z} \sin \frac{k_z h_z}{2} \tilde{B}_y \\
&+ \frac{\Delta}{2c} \sin \frac{\omega \Delta}{2c} \tilde{E}_x
\end{align}
\[
\frac{2}{\Delta} \sin \frac{\omega \Delta}{2c} \cos \frac{k_x \Delta}{2} \tilde{B}_y = \frac{2}{\Delta} \sin \frac{k_x \Delta}{2} \cos \frac{\omega \Delta}{2c} \tilde{E}_z 
\]
(57)

\[
\frac{2}{\Delta} \sin \frac{\omega \Delta}{2c} \cos \frac{k_x \Delta}{2} \tilde{B}_z = -\frac{2}{\Delta} \sin \frac{k_x \Delta}{2} \cos \frac{\omega \Delta}{2c} \tilde{E}_y 
\]
(58)

\[
\frac{2}{\Delta} \sin \frac{\omega \Delta}{2c} \tilde{B}_z = \frac{2}{k_y h_y} \sin \frac{k_y h_y}{2} \tilde{E}_y - \frac{2}{k_z h_z} \sin \frac{k_z h_z}{2} \tilde{E}_y 
\]
(59)

The dispersion relation in vacuum (\(\omega_p = 0\)) is rather simple:

\[
\left( \frac{1}{h_y^2} \sin^2 \frac{k_y h_y}{2} + \frac{1}{h_z^2} \sin^2 \frac{k_z h_z}{2} \right) + \frac{1}{\Delta^2} \sin^2 \frac{\Delta k_x}{2} \left( 1 - \Delta^2 \left( \frac{1}{h_y^2} \sin^2 \frac{k_y h_y}{2} + \frac{1}{h_z^2} \sin^2 \frac{k_z h_z}{2} \right) \right) = \frac{1}{\Delta^2} \sin^2 \frac{\Delta \omega}{2c} 
\]
(60)

The stability condition in vacuum is

\[
\Delta^2 \left( \frac{1}{h_y^2} + \frac{1}{h_z^2} \right) < 1 
\]
(61)

In the presence of plasmas, it is modified to

\[
\frac{1}{\Delta^2} > \frac{1}{h_y^2} + \frac{1}{h_z^2} + \frac{e^2 \omega_p^2}{4} 
\]
(62)

The RIP scheme combines dispersionless properties of the standard 1D solver along the \(X\)--axis with the Yee dispersion for waves running in the transverse direction. Indeed, setting \(k_y = k_z = 0\) in the dispersion relation (60), we immediately obtain \(\omega = ck_x\) and the phase velocity

\[
V_{ph} = \frac{\omega}{k_x} = c 
\]
(63)

for plane waves propagating in the \(X\)--direction.

Conversely, setting \(k_x = 0\), we obtain the usual 2D Yee dispersion relation for waves propagating in the transverse direction

\[
\frac{1}{h_y^2} \sin^2 \frac{k_y h_y}{2} + \frac{1}{h_z^2} \sin^2 \frac{k_z h_z}{2} = \frac{1}{\Delta^2} \sin^2 \frac{\Delta \omega}{2c} 
\]
(64)

with all its known advantages and drawbacks.

**VII. NUMERICAL TESTS OF THE RIP MAXWEL SOLVER**

**A. Numerical Cerenkov instability test**

As a first test, we take the numerical Cerenkov instability. We compare the standard Yee solver, the FFT-based solver \([2, 3]\) and the RIP solver, all implemented on the VLPL platform \([8]\). No artificial filtering of fields or currents is used. The initial configuration is a spherical plasma of Gaussian density profile \(n = n_0 \exp \left( -r^2/\sigma^2 \right)\) consisting of electrons and protons moving in the \(X\)--direction with the average momentum \(< p_0 > /m_\alpha c = (p_{0x}, 0, 0)\), where \(\alpha\) denotes the particle type \((\alpha = e, p)\), with \(m_p/m_e = 1846\). To seed the instability, the electrons have a small initial temperature \(< (p_0 - < p_0 >)^2 > = \sigma_p^2\). In relativistically normalized units, we simulation parameters are: the peak
plasma density is $n_0 = 1$ with the corresponding non-relativistic plasma frequency $\omega_p = \sqrt{4\pi n_0 e^2/m_e}$. The initial particle momenta $p_{x,0} = -10$ and $\sigma_{p_x} = 10^{-4}$. The grid steps were $h_x = h_z = 1.88 \ell/\omega_p$ and $h_y = c\tau = \Delta = 0.63 \ell/\omega_p$. As a diagnostics for the comparison, we selected the growth of the maximum local field intensity $I = E^2 + B^2$ on the grid. The results are shown in Fig.2.

We see that the fluctuating fields in simulations using the Yee scheme grow to the non-linear saturation within a few plasma oscillations. This is because the Yee solver is exposed to the first order Cerenkov resonance. The FFT-based solver is dispersionless and avoids the first order Cerenkov resonance. Still, the second order aliasing of the spectral FFT solver leads to the numerical Cerenkov instability, though at a lower growth rate as compared with the standard Yee solver.

In contrast, the RIP solver is free from NCI. The noise in the RIP scheme remains many orders of magnitude lower over a long simulation time of $t = 100 \cdot 2\pi/\omega_p$. The very slow growth of the noise fields here has nothing to do with the Cerenkov resonance, but is the unavoidable “numerical heating” always present in PIC codes.

Finally, we do another simulation with a stationary plasma, $p_0 = /m_e c = (0,0,0)$, while keeping all other parameters the same. We observe here no numerical heating at all. Intensity of fluctuating noise fields remains constant over many hundreds of plasma periods here. The higher absolute level of the noise for the streaming plasma is the natural consequence of the larger initial noise current source in this case. Fig.2 demonstrates clearly that the RIP scheme is free from Cerenkov instability for plasmas drifting along the selected axis.

We stress here that the FFT-based method (2) is identical to the RIP solver for waves running in the $X$-direction. Yet, we observe a quite different behaviour with respect to the numerical Cerenkov instability. This is because of the aliasing errors in the FFT method (2).

We mention here that the numerical Cerenkov instability of uniformly streaming plasma can be alleviated by using
Figure 4. Quasilinear wake field generation by a short proton bunch. (a) electron density; (b) longitudinal electric field $eE_x/mc\omega$; (c) transverse electric field $eE_y/mc\omega$.

a co-moving grid as proposed by Lehe et al. [39]. The method exploits a Galilean transformation to a grid in which the background plasma does not stream through the cell boundaries. Yet, the dense bunch of accelerated particles moves in the opposite direction at twice the light speed relative to this grid and is fully exposed to the Čerenkov resonance.

B. Laser-driven plasma bubble

As the second numerical test, we select laser-plasma particle acceleration in the bubble regime [44]. A circularly polarized laser pulse with initial vector potential $A = \Re \left[a(\xi, r_\perp)(e_y + i e_z) \exp(i k\xi)\right]$ is used. Here, $\xi = x - ct$ and the envelope shape has been selected as a spherical Gaussian $a(\xi, r_\perp) = a_0 \exp(-\xi^2/\sigma^2_\parallel - r^2_\perp/\sigma^2_\perp)$ with the amplitude $a_0 = 5$, length $\sigma_\parallel = 5\lambda$ and radius $\sigma_\perp = 5\lambda$, where the laser wavelength $\lambda = 2\pi/k$. The plasma consisting of electrons and protons has an initial density $n = 0.01 n_c$, where $n_c = m_e\omega^2/4\pi e^2$ is the critical density. At the plasma boundary, the density increases linearly from $n = 0$ to $n = 0.01 n_c$ over a length $L = 38\lambda$. The simulation results after an acceleration distance of $L_a = 300\lambda$ are shown in Fig.3. The simulation box has the size $40\lambda \times 40\lambda \times 40\lambda$. The grid steps are $h_x = 0.05\lambda$, $h_y = 0.25\lambda$, $h_z = 0.25\lambda$ and the time step is $\tau = 0.045\lambda/c$ in the Yee simulation, and $\tau = h_x/c$ in the RIP simulation.

We see that the trapped electron bunch of the bubble has a fine longitudinal structure in the Yee simulation. At the same time, the bubble accelerating field $E_x$ is rippled with the short-wavelength radiation emitted by the relativistic electrons due to the numerical Čerenkov resonance. This numerical emission is clearly seen in Fig.3(c) as the bow-like short wavelength radiation emanating from the dense electron bunch. The RIP simulation shows a rather smooth electron bunch and no signatures of numerical Čerenkov emission. The $E_z$-field of the relativistic electron bunch has a clean quasi-static form: it is not bow-shaped, but perpendicular to the bunch. Further, a small additional numerical dephasing can be observed at the leading edge of the bubble.

To check the RIP scheme convergence, we did an additional simulation with rough resolution. We doubled the longitudinal grid step and the time step to $h_x = c\tau = 0.1\lambda$, so that we have only 10 cells per laser wavelength. The results are shown in the last row in Fig.3. One observes little difference from the higher resolution simulation, shown in the middle row in Fig.3. This attests excellent convergence properties of the RIP scheme.
C. Quasi-linear wake

Finally, we check how well the RIP scheme describes long term evolution of a quasi-linear wake in plasma. We take a spherical Gaussian proton bunch $n_p = n_0 \exp \left( -\xi^2/\sigma_||^2 - r^2_\perp/\sigma_\perp^2 \right)$ with the peak bunch density $n_p = 0.2 \, n$ and the radii $\sigma_|| = \sigma_\perp = c/\omega_p$, where $\omega_p = \sqrt{4\pi ne^2/m_e}$ is the background plasma frequency. The grid steps are $h_x = c\tau = 0.125 \, k_p^{-1}$, $h_y = h_z = 0.2 \, k_p^{-1}$, where $k_p = \omega_p/c$ is the plasma wave number. The background plasma is represented by 8 macroparticles per cell and the proton bunch has a single macroparticle per cell. The protons have energy of 400 GeV. The resulting wake field is shown in Fig. 4.

The electron density perturbation is significant and reaches $\delta n/n \approx 0.5$. No numerical Cerenkov emission by the relativistic proton driver is observed. The wake phase front curvature changes sign from negative at the position of the proton bunch driver to positive far behind it. This curvature change is well known and is due to the relativistic effects \[45\]. We see that the RIP scheme is robust and nicely describes long quasi-linear wakes.

VIII. DISCUSSION

The new RIP scheme is a compact stencil FDTD Maxwell solver that removes the numerical dipersion in one selected direction. For the waves propagating in the transverse direction, it corresponds to the Yee solver. The RIP scheme is local and does not use any global spectral method. This allows for efficient parallelization via domain decomposition in all three dimensions. The computational costs of the RIP solver is comparable with that if the Yee solver. The RIP solver can be used for simulations of quasi-1D physics problems like laser wake field acceleration.

APPENDIX

We derive the second order relativistic particle pusher in constant fields. Because the Lorentz-force acting on the particle depends on the particle velocity, a simple leap-frog scheme does not work here. Boris \[41\] suggested an operator-split method. It works very well for non-relativistic particles: the particle momentum is pushed half-step along the $E$–field, then is rotated full step in the $B$–field using the trapezoidal formula and finally is pushed second half-step along the $E$–field. For relativistic particle motion, however, it is unclear which $\gamma$–factor has to be taken to calculate the velocity $v$ in the $v \times B$ rotation. Vey \[42\] modified the Boris pusher making it Lorentz-invariant. Still, the both schemes of Boris and Vey rely on operator splitting.

Our approach is different. We do not split the Lorentz force operator. Instead, we apply the trapezoidal integrator me to the full Lorentz force:

\[ \frac{p - p^0}{\tau} = qE + \frac{q}{2} \frac{p + p^0}{\gamma^0} \times B \]  \hspace{1cm} (65)

Here, $p^0$ is the known particle momentum before the push and $\gamma^0 = \sqrt{1 + p^0}$. We are looking for the updated particle momentum $p$ and $\gamma = \sqrt{1 + p}$.

We can cast (65) in the form

\[ p = a + \frac{p \times b}{\gamma^0} \]  \hspace{1cm} (66)

where

\[ a = p^0 + q\gamma E + \frac{q\gamma}{2} \frac{p^0}{\gamma^0} \times B \]  \hspace{1cm} (67)

and

\[ b = \frac{q\gamma}{2} B \]  \hspace{1cm} (68)

We rewrite (66) as

\[ \gamma p = \gamma a + p \times b \]  \hspace{1cm} (69)
Scalar multiplication of (69) with \( p \) gives

\[ p^2 = a \cdot p \]  \hspace{1cm} (70)

Scalar multiplication of (69) with \( b \) gives

\[ b \cdot p = a \cdot b \]  \hspace{1cm} (71)

Scalar multiplication (69) with \( a \) gives

\[ \gamma a \cdot p - \gamma a^2 = a \cdot (p \times b) = p \cdot (b \times a) = b \cdot (a \times p) \]  \hspace{1cm} (72)

Vector multiplication \( a \) with (69) gives

\[ \gamma a \times p = p (a \cdot b) - b (a \cdot p) \]  \hspace{1cm} (73)

From (70) and (72) we get

\[ \gamma (p^2 - a^2) = \frac{b}{\gamma} [p (a \cdot b) - b (a \cdot p)] = \frac{[(a \cdot b)^2 - b^2 p^2]}{\gamma} \]  \hspace{1cm} (74)

or

\[ \gamma^2 (\gamma^2 - 1 - a^2) = (a \cdot b)^2 - b^2 (\gamma^2 - 1) \]  \hspace{1cm} (75)

This leads to the quadratic equation

\[ \gamma^4 + \gamma^2 (b^2 - 1 - a^2) - b^2 - (a \cdot b)^2 = 0 \]  \hspace{1cm} (76)

with the solution

\[ \gamma^2 = \frac{1 + a^2 - b^2}{2} + \sqrt{\left(\frac{1 + a^2 - b^2}{2}\right)^2 + b^2 + (a \cdot b)^2} \]  \hspace{1cm} (77)

This defines the updated \( \gamma \).

Now we have to find \( p \). For this, we vector multiply \( b \) with (69):

\[ \gamma (b \times p - b \times a) = p \cdot b - b (p \cdot b) = pb^2 - b (a \cdot b) \]  \hspace{1cm} (78)

Using (69), we find

\[ \gamma^2 a - \gamma^2 p - \gamma b \times a = pb^2 - b (a \cdot b) \]  \hspace{1cm} (79)

Solving for \( p \), we find

\[ p = \frac{\gamma^2 a + \gamma a \times b + b (a \cdot b)}{\gamma^2 + b^2} \]  \hspace{1cm} (80)

Together with (77) this is the solution of the particle pusher.
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