HIGH-PERFORMANCE MODELING OF PLASMA-BASED ACCELERATION USING THE FULL PIC METHOD*

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Abstract

Numerical simulations have been critical in the recent rapid developments of plasma-based acceleration concepts. Among the various available numerical techniques, the Particle-In-Cell (PIC) approach is the method of choice for self-consistent simulations from first principles. The fundamentals of the PIC method were established decades ago, but improvements or variations are continuously being proposed. We report on several recent advances in PIC-related algorithms that are of interest for application to plasma-based accelerators, including: (a) detailed analysis of the numerical Cherenkov instability and its remediation for the modeling of plasma accelerators in laboratory and Lorentz boosted frames, (b) analytic pseudo-spectral electromagnetic solvers in Cartesian and cylindrical (with azimuthal modes decomposition) geometries, (c) novel analysis of MaxwellÕs solversÕ stencil variation and truncation, in application to domain decomposition strategies and implementation of Perfectly Matched Layers in high-order and pseudo-spectral solvers.

INTRODUCTION

Laser-driven plasma based electron accelerators (LPAs) have demonstrated the production of high-quality electron beams at energies ranging from 1 MeV [1] to 4 GeV [2] in cm-scale distances, fulfilling the need for compact acceleration. Numerical simulations have been critical in the recent rapid developments of plasma-based acceleration concepts, and among the various available numerical techniques, the electromagnetic Particle-In-Cell (PIC) approach is the method of choice for self-consistent simulations from first principles.

Electromagnetic Particle-In-Cell method

In the electromagnetic Particle-In-Cell method [3], the electromagnetic fields are solved on a grid, usually using Maxwell's equations

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \quad (1)$$

$$\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \mathbf{J} \quad (2)$$

$$\nabla \cdot \mathbf{E} = \rho \quad (3)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (4)$$

given here in natural units, where t is time, $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic field components, and ρ and $\mathbf{J}$ are the charge and current densities. The charged particles are advanced in time using the Newton-Lorentz equations of motion

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}, \quad (5)$$

$$\frac{d(\gamma \mathbf{v})}{dt} = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \quad (6)$$

where m, q, $\mathbf{x}$, $\mathbf{v}$ and $\gamma = 1/\sqrt{1-v^2}$ are respectively the mass, charge, position, velocity and relativistic factor of the particle. The charge and current densities are interpolated on the grid from the particles' positions and velocities, while the electric and magnetic field components are interpolated from the grid to the particles' positions for the velocity update.

Various methods are available for solving Maxwell's equations on a grid, based on finite-differences, finite-volume, finite-element, spectral, or other discretization techniques that apply most commonly on single structured or unstructured meshes and less commonly on multiblock multiresolution grid structures. In the following subsections, we summarize the widespread second order finite-difference time-domain (FDTD) algorithm, as well as the pseudo-spectral analytical time-domain (PSATD) and pseudo-spectral time-domain (PSTD) algorithms. Extension to multiresolution (or mesh refinement) PIC is described in, e.g. [4, 5].

Finite-Difference Time-Domain The most popular algorithm for electromagnetic PIC codes is the Finite-Difference Time-Domain solver

$$D_t \mathbf{B} = -\nabla \times \mathbf{E} \quad (7)$$

$$D_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J} \quad (8)$$

$$[\nabla \cdot \mathbf{E} = \rho] \quad (9)$$

$$[\nabla \cdot \mathbf{B} = 0]. \quad (10)$$

The differential operator is defined as $\nabla = D_x\hat{\mathbf{x}} + D_y\hat{\mathbf{y}} + D_z\hat{\mathbf{z}}$ and the finite difference operators in time and space are

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defined respectively as $D_t G|^n_{i,j,k} = \left(G|^{n+1/2}_{i,j,k} - G|^{n-1/2}_{i,j,k}\right)/\Delta t$ and $D_x G|^n_{i,j,k} = \left(G|^n_{i+1/2,j,k} - G|^n_{i-1/2,j,k}\right)/\Delta x$, where Δt and Δx are respectively the time step and the grid cell size along x, n is the time index and i, j and k are the spatial indices along x, y and z respectively. The difference operators along y and z are obtained by circular permutation. The equations in brackets are given for completeness, as they are often not actually solved, thanks to the usage of a so-called charge conserving algorithm. The quantities are given on a staggered (or "Yee") grid [6], where the electric field components are located between nodes and the magnetic field components are located in the center of the cell faces.

Pseudo Spectral Analytical Time Domain (PSATD) Maxwell's equations in Fourier space are given by

$$\frac{\partial \tilde{\mathbf{E}}}{\partial t} = i\mathbf{k}\times\tilde{\mathbf{B}} - \tilde{\mathbf{J}} \quad (11)$$

$$\frac{\partial \tilde{\mathbf{B}}}{\partial t} = -i\mathbf{k}\times\tilde{\mathbf{E}} \quad (12)$$

$$[i\mathbf{k}\cdot\tilde{\mathbf{E}} = \tilde{\rho}] \quad (13)$$

$$[i\mathbf{k}\cdot\tilde{\mathbf{B}} = 0] \quad (14)$$

where $\tilde{a}$ is the Fourier Transform of the quantity a. As with the real space formulation, provided that the continuity equation $\partial\tilde{\rho}/\partial t + i\mathbf{k}\cdot\tilde{\mathbf{J}} = 0$ and $\mathbf{k}\cdot\mathbf{k}\times\tilde{\mathbf{E}}$ are satisfied, then the last two equations will automatically be satisfied at any time if satisfied initially and do not need to be explicitly integrated.

Decomposing the electric field and current between longitudinal and transverse components $\tilde{\mathbf{E}} = \tilde{\mathbf{E}}_L + \tilde{\mathbf{E}}_T = \hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\tilde{\mathbf{E}}) - \hat{\mathbf{k}}\times\hat{\mathbf{k}}\times\tilde{\mathbf{E}}$ and $\tilde{\mathbf{J}} = \tilde{\mathbf{J}}_L + \tilde{\mathbf{J}}_T = \hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\tilde{\mathbf{J}}) - \hat{\mathbf{k}}\times\hat{\mathbf{k}}\times\tilde{\mathbf{J}}$ gives

$$\frac{\partial \tilde{\mathbf{E}}_T}{\partial t} = i\mathbf{k}\times\tilde{\mathbf{B}} - \tilde{\mathbf{J}}_\mathbf{T} \quad (15)$$

$$\frac{\partial \tilde{\mathbf{E}}_L}{\partial t} = -\tilde{\mathbf{J}}_\mathbf{L} \quad (16)$$

$$\frac{\partial \tilde{\mathbf{B}}}{\partial t} = -i\mathbf{k}\times\tilde{\mathbf{E}} \quad (17)$$

with $\hat{\mathbf{k}} = \mathbf{k}/k$.

If the sources are assumed to be constant over a time interval Δt, the system of equations is solvable analytically and is given by (see [7] for the original formulation and [8] for a more detailed derivation):

$$\tilde{\mathbf{E}}^{n+1}_T = C\tilde{\mathbf{E}}^n_T + iS\hat{\mathbf{k}}\times\tilde{\mathbf{B}}^n - \frac{S}{k}\tilde{\mathbf{J}}^{n+1/2}_T \quad (18)$$

$$\tilde{\mathbf{E}}^{n+1}_L = \tilde{\mathbf{E}}^n_L - \Delta t\tilde{\mathbf{J}}^{n+1/2}_L \quad (19)$$

$$\tilde{\mathbf{B}}^{n+1} = C\tilde{\mathbf{B}}^n - iS\hat{\mathbf{k}}\times\tilde{\mathbf{E}}^n + i\frac{1-C}{k}\hat{\mathbf{k}}\times\tilde{\mathbf{J}}^{n+1/2} \quad (20)$$

with $C = \cos(k\Delta t)$ and $S = \sin(k\Delta t)$.

Combining the transverse and longitudinal components, gives

$$\tilde{\mathbf{E}}^{n+1} = C\tilde{\mathbf{E}}^n + iS\hat{\mathbf{k}}\times\tilde{\mathbf{B}}^n - \frac{S}{k}\tilde{\mathbf{J}}^{n+1/2} + (1-C)\hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\tilde{\mathbf{E}}^n) + \hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\tilde{\mathbf{J}}^{n+1/2})(\frac{S}{k} - \Delta t), \quad (21)$$

$$\tilde{\mathbf{B}}^{n+1} = C\tilde{\mathbf{B}}^n - iS\hat{\mathbf{k}}\times\tilde{\mathbf{E}}^n + i\frac{1-C}{k}\hat{\mathbf{k}}\times\tilde{\mathbf{J}}^{n+1/2}. \quad (22)$$

Considering the fields generated by the source terms without the self-consistent dynamics of the charged particles, this algorithm is free of numerical dispersion and is not subject to a Courant condition. Furthermore, this solution is exact for any time step size subject to the assumption that the current source is constant over that time step.

As shown in [8], by expanding the coefficients S_h and C_h in Taylor series and keeping the leading terms, the PSATD formulation reduces to the better known pseudo-spectral time-domain (PSTD) formulation [9, 10]:

$$\tilde{\mathbf{E}}^{n+1} = \tilde{\mathbf{E}}^n + i\Delta t\mathbf{k}\times\tilde{\mathbf{B}}^{n+1/2} - \Delta t\tilde{\mathbf{J}}^{n+1/2}, \quad (23)$$

$$\tilde{\mathbf{B}}^{n+3/2} = \tilde{\mathbf{B}}^{n+1/2} - i\Delta t\mathbf{k}\times\tilde{\mathbf{E}}^{n+1}. \quad (24)$$

The dispersion relation of the PSTD solver is given by $\sin(\frac{\omega\Delta t}{2}) = \frac{k\Delta t}{2}$. In contrast to the PSATD solver, the PSTD solver is subject to numerical dispersion for a finite time step and to a Courant condition that is given by $c\Delta t \le 2/\pi\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta x^2}}$.

The PSATD and PSTD formulations that were just given apply to the field components located at the nodes of the grid. As noted in [11], they can also be easily recast on a staggered Yee grid by multiplication of the field components by the appropriate coefficients to shift them from the collocated to the staggered locations. The choice between a collocated and a staggered formulation is application-dependent.

Modeling in a Lorentz boosted frame

Modeling the interaction including the laser and the entire plasma in the simulation box is neither practical nor needed, as a window following the beam and the wake (a standard and widespread technique in accelerator physics) is sufficient to capture the physics. However, the large range of scale separations between the plasma column length and the driving laser wavelength still demands tens of millions of time steps for the modeling of a meter long plasma capable of boosting the energy of an electron or positron beam in the range of 10 GeV. The numerical cost can be alleviated by using one or more of: (i) the quasistatic approximation [12], which takes advantage of the separation of time scales in the dynamics of the laser and plasma electrons, (ii) envelope models of the laser, (iii) running the simulation in a Lorentz boosted frame co-propagating in the direction of the laser, rather than in the laboratory frame [13]. We will focus here on the last approach. When using this approach,

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the plasma column is drifting at relativistic velocity relative to the grid, leading to the numerical Cherenkov instability (NCI) [14] that needs to be understood and controled. The next section summarizes the most recent developments in the understanding and mitigation of NCI.

ANALYSIS AND MITIGATION OF THE NUMERICAL CHERENKOV INSTABILITY

The numerical Cherenkov instability [14] is the most serious numerical instability affecting multidimensional PIC simulations of relativistic particle beams and streaming plasmas [15–17]. It arises from coupling between possibly numerically distorted electromagnetic modes and spurious beam modes, the latter due to the mismatch between the Lagrangian treatment of particles and the Eulerian treatment of fields [18]. In recent papers we derived and solved electromagnetic dispersion relations for the numerical Cherenkov instability for both FDTD [19, 20] and PSATD [21, 22] algorithms, developed methods for significantly reducing growth rates, and successfully compared results with those of the Warp simulation code [23].

For either algorithm the dispersion relation can be written in the high energy limit as

$$C_0 + n\sum_{m_z} C_1 \csc\left[\left(\omega - k_z'\right)\frac{\Delta t}{2}\right] + n\sum_{m_z} C_2 \csc^2\left[\left(\omega - k_z'\right)\frac{\Delta t}{2}\right] = 0, \tag{25}$$

with coefficients C_0, C_1, C_2 defined by Eqs. (29) – (31) of [24] for the FDTD algorithm and by Eqs. (40) – (42) of [25] for the PSATD algorithm. Numerical solutions of the complete dispersion relations indicate that Eq. (25) is quantitatively accurate for γ as small as 10 and qualitatively useful for γ as small as 3. At still lower beam energies, the well known electrostatic numerical instability [26, 27] dominates.

Equation (25) involves sums over numerical aliases, $k_z' = k_z + m_z\, 2\pi/\Delta z$, for wave numbers aligned with the direction, z, of beam propagation. In the limit of vanishingly small time-steps and cell-sizes, Eq. (25) simplifies to $C_0 = n$, as expected, with n the beam density divided by γ (*i. e.*, the density of the beam in its rest frame). Thus, all beam resonances in Eq. (25) are numerical artifacts, even $m_z = 0$.

Not surprisingly, the numerical Cherenkov instability is fastest growing at resonances between the spurious beam modes and electromagnetic modes. The resonant instability scales roughly as the cube root of $n\,C_2/\Delta t$, evaluated at $\omega = k_z' v$, and can be destructively fast. The non-resonant instability, on the other hand, scales roughly as the square root of of $n\,C_2$, again evaluated at $\omega = k_z' v$. Although slower growing, it also is troublesome, because it can occur at smaller wave numbers.

Numerical instability growth rates can be unacceptably large if no special measure is taken. They can be reduced by using higher order current and field interpolation, by digital filtering, and by numerical damping of the electromagnetic fields (numerical damping is not explored further in this paper and the reader is refered to [15, 28–30] for more information). Cubic interpolation, for instance, is effective at suppressing higher order modes of the numerical Cherenkov instability and, to a lesser extent, $m_z = 0, -1$ modes. Digital filtering, on the other hand, effectively zeroes fields at large wave numbers, eliminating resonant numerical Cherenkov instabilities there.

A "magic time step" first was observed for the so-called "Galerkin field interpolation" [31] in LPA simulations [15, 17] and subsequently was explained analytically in [24]. It arises from approximate cancellation of the coefficients of E_x and B_y in C_2 for wave numbers near the dominant numerical Cherenkov resonance. The exact location of the "magic time step" depends on details of the field solver. In contrast, a "magic time step" was discovered analytically for the "Uniform field interpolation" [31]. It occurs because C_2 vanishes identically at $v\Delta t/\Delta z = 0.5$ in the high γ limit. One can concoct other, more complicated interpolation schemes with "magic time steps", but the value of doing so seems small. Definitions of the three FDTD interpolation schemes discussed here were provided in Sec. 2.4 and also can be found in [19, 32], and of PSATD variants (a) and (b) of the Esirkepov current conservation algorithm [33] in [25, 34].

The numerical Cherenkov instability can be viewed as the result of numerically induced mismatches between transverse fields as seen by the particles or, more or less equivalently, by mismatches between transverse currents and charge density. Correcting those mismatches, at least as they occur in coefficient C_2 at large γ, can in principle make every value of Δt a "magic time step". A plethora of approaches are provided in [22, 25], from which PSATD options (b1) and (b2) of the second reference are presented here. Option (b1) adjusts the ratio E_x/B_y as seen by the particles so that C_2 vanishes analytically for $v = 1$. The resulting growth rates are significantly reduced, especially for $v\Delta t/\Delta z > 1$. In fact, the residual growth at $v\Delta t/\Delta z > 1$ scales roughly as $1/\gamma$, although higher order numerical modes also play a role.

Implementing these and other schemes in the PSATD algorithm is straightforward, because currents and fields are known in k-space. Analogous schemes can be implemented readily in the FDTD algorithm, if one is willing to transform currents and fields to k-space. But, one would then be better off to use the PSATD algorithm throughout, because it is more accurate and often less unstable. It is, however, possible to set C_2 approximately equal to zero (accurate to six significant figures) by approximating the desired E_x/B_y ratio with a fourth-order rational interpolation function, as described in [32]. Sample simulations indicate that this approach is economical, requires minimal additional digital filtering, and apparently has no adverse effect on physical results at wavelengths long compare to the simulation axial cell size. Although derived for highly relativistic flows, it works reasonably well down to γ of order 3, below which the

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numerical Cherenkov instability ceases to be the dominant numerical effect.

In [35], new field correction factors have been derived that completely eliminate the $m_z = 0$ numerical Cherenkov instability for the generalized PSTD algorithm, including the PSATD algorithm. When combined with a sharp cut-off digital filter at large k, these correction factors reduce peak growth rates to less (often much less) than 0.01 of the beamÕs relativistic plasma frequency. These coefficients are optimal in the sense that they differ from unity only slightly over a broad portion of k-space while eliminating both $m_z = 0$ numerical instability branches. A disadvantage from the implementation perspective is that the coefficients must be computed numerically for each set of simulation parameters.

Software to calculate the rational interpolation coefficients, as well as phase diagrams and resonance curves, are available in Computable Document Format [36] at http://hifweb.lbl.gov/public/BLAST/Godfrey/. The extensive analyses involved in deriving and solving the dispersion relations discussed in this section were performed with *Mathematica* [37].

EXTENSION AND PARALLELIZATION OF PSATD-PIC

A quasi-cylindrical version of the PSATD algorithm

When modeling 3D physical situations, the standard PSATD algorithm typically uses a 3D Cartesian mesh, which can be computationally expensive. However, when the physical situation has close-to-cylindrical symmetry, the calculations can in principle be reduced to a few 2D *quasi-cylindrical*[1] grids, and the resulting simulations can be much faster. This idea has been implemented in FDTD PIC, for instance by [38], and resulted in a speedup of one to two orders of magnitude.

In [39], we extended this idea to the PSTAD algorithm. Instead of the three-dimensional Fourier transform which is used in the standard 3D PSATD, the quasi-cylindrical PSATD algorithm uses the combination of a Hankel transform (radially) and a one-dimensional Fourier transform (longitudinally).

In this Fourier-Hankel formalism, the equations of the Maxwell solver are structurally very similar to (21) and (22), and thus many of the advantages of the standard 3D PSATD carry over to the quasi-cylindrical PSATD. In particular, the quasi-cylindrical algorithm has no Courant condition, and has an ideal dispersion relation in vacuum. In [39], we also benchmarked this algorithm in situations that are relevant to laser-plasma acceleration, and we showed that it avoids a number of numerical artifacts that are otherwise present in FDTD PIC codes.

[1] Here, the term *quasi*-cylindrical refers to the azimuthal decomposition which is generally used (see e.g. [38]), and which can take into account small departures from the purely cylindrical symmetry.

Parallelization and detailed analysis of the effects of stencil spatial variations with arbitrary high-order finite-difference Maxwell solver.

One possible drawback for the use of pseudo-spectral solvers is the difficulty in scaling them to a large number of cores on existing and, even more so on upcoming, supercomputers. To alleviate the problem, we proposed in [8] to take advantage of the finite-speed of light that is an intrinsic property of Maxwell's equations, and use domain decomposition with local FFTs on each subdomain. While initial tests of the method were succesfully conducted, the use of a finite number of guard cells surrounding each subdomain inevitably entails a small approximation when using the PSTD or PSATD algorithm that inevitably leads to a a small error when using pseudo-spectral solvers, which may sometimes result in a growing instability. Using the property that the PSTD and PSATD solvers can be viewed as the limit of FDTD solvers when the stencil order tends to infinity, we presented in [40] a general analytical approach that enables the evaluation of numerical discretization errors of fully three-dimensional arbitrary order finite-difference Maxwell solver, with arbitrary modification of the local stencil in the simulation domain. This model can be used to determine the minimum number of guard cells required to achieve a given numerical accuracy. It is validated against simulations with domain decomposition technique and Perfectly Matched Layers (PMLs), when these are used with a very high-order Maxwell solver, as well as in the infinite order limit of pseudo-spectral solvers. Results confirm that the new analytical approach enables exact predictions in each case. It also confirms that the domain decomposition technique can be used with a very high-order Maxwell solver and a reasonably low number of guard cells with negligible effects on the whole accuracy of the simulation. It also provides a more accurate framework for analyzing the efficiency of PMLs with high-order stencils and pseudo-spectral solvers, confirming earlier results obtained in [41].

CONCLUSION

The Particle-In-Cell (PIC) method continues to be the method of choice for detailed fully kinetic modeling of plasma accelerators. Modeling in a Lorentz boosted frame can provide orders of magnitude speedup, provided that the numerical Cherenkov instability (NCI) is under control. Recent work has led to a full understanding of the instability and to the development of efficient mitigation techniques. The studies have also shown that PIC methods utilizing pseudo-spectral electromagnetic field solvers are inherently more stable to NCI, generating renewed interest into these solvers, that used to be very popular until the replacement of vector supercomputers by massively parallel supercomputers. This has also prompted the development of a novel pseudo-spectral solver with azimuthal Fourier decomposition, and a composition of Fourier and Hankel transforms for fast simulations. The difficulty of scaling pseudo-spectral solvers to many cores is addressed through the use of domain de-

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composition, prompting the development of a novel analytic method for studying the effect of stencil variations.

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