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REVIEW OF SPECTRAL MAXWELL SOLVERS FOR ELECTROMAGNETIC PARTICLE-IN-CELL: ALGORITHMS AND ADVANTAGES

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Abstract

Electromagnetic Particle-In-Cell codes have been used to simulate both radio-frequency accelerators and plasma-based accelerators. In this context, the Particle-In-Cell algorithm often uses the finite-difference method in order to solve Maxwell's equations. However, while this method is simple to implement and scales well to multiple processors, it is liable to a number of numerical artifacts that can be particularly serious for simulations of accelerators.

An alternative to the finite-difference method is the use of spectral solvers, which are typically less prone to numerical artifacts. The present article reviews recent progress in the use of spectral solvers for simulations of plasma-based accelerators. This includes techniques to scale those solvers to large number of processors, extensions to cylindrical geometry, and adaptations to specific problems such as boosted-frame simulations.

INTRODUCTION

Particle-In-Cell (PIC) codes [1, 2] are widely used in various fields of physics, and in particular in accelerator physics. For many accelerator-related problems, electrostatic PIC codes are usually sufficient to capture the physics at stake. However, some applications do require full electromagnetic PIC codes. This includes for instance accelerators based on laser-plasma interactions [3–7], where e.g. the self-consistent evolution of the laser driver needs to be captured by the PIC algorithm.

For these applications that require an electromagnetic Particle-In-Cell code, the Finite-Difference-Time-Domain (FDTD) method (e.g. [8]) has been the most commonly-used approach for solving Maxwell's equations. However, due to some of the limitations of the FDTD method, other methods are increasingly being used—and this includes spectral solvers.

This paper focuses on spectral solvers for PIC codes and their advantages—with an emphasis on their application to laser-plasma interactions. Note that, for the sake of conciseness, the present paper is restricted to Particle-In-Cell codes that do solve Maxwell's equations on a grid (in which case spectral solvers are sometimes referred to as *pseudo-spectral*), and does not discuss the set of *gridless* spectral electromagnetic algorithms that have been recently developed, in the context of accelerator simulations (e.g. [9–11]).

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SPECTRAL SOLVERS, AND DIFFERENCE WITH FDTD SOLVERS

In order to summarize the principle of the spectral solvers, let us contrast them with the FDTD algorithm. In the standard Yee FDTD algorithm [8], Maxwell's equations

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

$$\frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = \boldsymbol{\nabla}\times\boldsymbol{B} - \mu_0\boldsymbol{j} \quad (2)$$

are discretized in two ways:

- Spatial derivatives are approximated by a finite difference between neighboring points on a staggered grid. For instance,

$$\partial_x E_x|^n_{i,j,k} = \frac{E_x|^n_{i+1/2,j,k} - E_x|^n_{i-1/2,j,k}}{\Delta x}.$$

- Time derivatives are approximated by a finite difference between consecutive time steps. For instance,

$$\partial_t E_x|^{n+1/2}_{i+1/2,j,k} = \frac{E_x|^{n+1}_{i+1/2,j,k} - E_x|^n_{i+1/2,j,k}}{\Delta t}.$$

where we adopted standard notations whereby superscripts represent the index of the time step whereas subscripts represent positions on a staggered grid. As a consequence of the above simple space and time discretizations, the discretized Maxwell equations can easily be rewritten as a set of explicit update equations for the $\boldsymbol{E}$ and $\boldsymbol{B}$ fields.

While the above approximations allow fast execution and efficient parallelization, they also introduce numerical artifacts. One of these numerical artifacts is *spurious numerical dispersion*, i.e. the fact that the phase velocity of simulated electromagnetic waves (in vacuum) differs from the speed of light c, and depends on their wavelength and propagation angle. Spurious numerical dispersion can have a very serious impact in realistic simulations, and can lead to unphysical results. For instance, in the context of laser-plasma interactions, numerical dispersion can lead to spurious early dephasing in laser-driven accelerator [12], unphysical growth of emittance [13], and erroneous angle-frequency correlations in high-harmonics generation [14].

One of the main motivation for spectral solvers is to mitigate numerical dispersion. This is done by overcoming the approximations of FDTD schemes in two ways:

- Spatial derivatives are approximated by a high-order expression involving many grid points. These derivatives are typically evaluated in Fourier space for efficiency. Algorithms that use this feature but retain a

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finite-difference approximation in time are typically referred to as *Pseudo-Spectral Time Domain* algorithms (PSTD) [15, 16].

- Instead of using a finite-difference approximation of the time derivatives, Maxwell's equation can be integrated analytically over one time step, in spectral space. Algorithms that use this additional feature are referred to as *Pseudo-Spectral Analytical Time Domain* algorithms (PSATD) [17, 18].

The above two points are explained in more details in the next paragraphs.

The high-order approximation of the spatial derivative in PSTD and PSATD schemes are of the form

$$\partial_x E_x|^n_{i,j,k} = \sum_{\ell=0}^{p/2-1} c_{\ell,p} \frac{E_x|^n_{i+1/2+\ell,j,k} - E_x|^n_{i-1/2-\ell,j,k}}{\Delta x},$$

where p is the order of the approximation and $c_{\ell,p}$ are coefficients that are given in [19] (For $p = 2$, this reduces to the standard finite-difference expression of the Yee solver). It is common to use large values for p in practice (e.g. $p = 32$ or $p = 64$). Since these large values entail a significant computational cost, these derivatives are often more efficiently evaluated in Fourier space, by using the convolution theorem, i.e.

$$\begin{aligned} \mathcal{F}[\partial_x E_x] &= i[k_x]_p \hat{\mathcal{E}}_x, \\ [k_x]_p &= \sum_{\ell=0}^{p/2-1} c_{\ell,p} \frac{e^{ik_x(\ell+1/2)\Delta x} - e^{-ik_x(\ell+1/2)\Delta x}}{i\Delta x}, \end{aligned}$$

where $\mathcal{F}$ represents the Fourier transform and $\hat{\mathcal{E}}_x \equiv \mathcal{F}[E_x]$. Note that, when p goes to infinity, $[k_x]_p$ goes to k_x, and thus the spatial derivatives are evaluated with full spectral accuracy. However, the case $p = \infty$ is rarely used in practice due to parallelization issues (as explained in the next section).

Using high-order spatial derivatives (i.e. high p) makes the numerical dispersion relation less anisotropic. However, it does not mitigate spurious numerical dispersion altogether, unless the treatment of the time derivative is made more accurate too. One way to achieve this is to retain a finite-difference approximation in time, but use a small time step (much smaller than the Courant-Friedrichs-Lewy limit)—but this comes at a high computational cost. Another possible approach is to integrate Maxwell's equations analytically in spectral space.

When evaluated in spectral space, the spatially-discretized Maxwell equations indeed reduce to a simple set of ordinary differential equations with constant coefficients:

$$\frac{\partial \hat{\boldsymbol{\mathcal{B}}}(\boldsymbol{k},t)}{\partial t} = -i[\boldsymbol{k}]_p \times \hat{\boldsymbol{\mathcal{E}}}(\boldsymbol{k},t) \quad (3)$$

$$\frac{1}{c^2}\frac{\partial \hat{\boldsymbol{\mathcal{E}}}(\boldsymbol{k},t)}{\partial t} = i[\boldsymbol{k}]_p \times \hat{\boldsymbol{\mathcal{B}}}(\boldsymbol{k},t) - \mu_0 \hat{\boldsymbol{\mathcal{J}}}(\boldsymbol{k},t). \quad (4)$$

As such, these equations can be integrated analytically from $t = n\Delta t$ to $t = (n+1)\Delta t$, under the assumption that $\hat{\boldsymbol{\mathcal{J}}}(\boldsymbol{k},t)$ is constant over one time step [17, 18]. By taking $\hat{\boldsymbol{\mathcal{E}}}^n$ and $\hat{\boldsymbol{\mathcal{B}}}^n$ as initial conditions, this analytical integration can yield $\hat{\boldsymbol{\mathcal{E}}}^{n+1}$ and $\hat{\boldsymbol{\mathcal{B}}}^{n+1}$, i.e. the updated fields at the next time step:

$$\begin{aligned} \hat{\boldsymbol{\mathcal{E}}}^{n+1} &= C\hat{\boldsymbol{\mathcal{E}}}^n + iS\frac{[\boldsymbol{k}]_p}{[k]_p} \times \hat{\boldsymbol{\mathcal{B}}}^n - \frac{S}{[k]_p}\hat{\boldsymbol{\mathcal{J}}}^{n+1/2} \\ &\quad +(1-C)\frac{[\boldsymbol{k}]_p([\boldsymbol{k}]_p \cdot \hat{\boldsymbol{\mathcal{E}}}^n)}{[k]_p^2} \\ &\quad +\frac{[\boldsymbol{k}]_p([\boldsymbol{k}]_p \cdot \hat{\boldsymbol{\mathcal{J}}}^{n+1/2})}{[k]_p^2}\left(\frac{S}{[k]_p} - \Delta t\right), \end{aligned} \quad (5)$$

$$\begin{aligned} \hat{\boldsymbol{\mathcal{B}}}^{n+1} &= C\hat{\boldsymbol{\mathcal{B}}}^n - iS\frac{[\boldsymbol{k}]_p \times \hat{\boldsymbol{\mathcal{E}}}^n}{[k_p]} \\ &\quad +i\frac{1-C}{[k]_p^2}[\boldsymbol{k}]_p \times \hat{\boldsymbol{\mathcal{J}}}^{n+1/2}, \end{aligned} \quad (6)$$

where $C = \cos([k]_p c\Delta t)$, $S = \sin([k]_p c\Delta t)$, and $[k]_p = \sqrt{[\boldsymbol{k}]_p^2}$.

In summary, the update of the E and B fields (from time step n to time step $n+1$) in the PSATD scheme consists of three steps:

1. Apply a forward Fourier transform, in order to obtain the fields in spectral space at time step n ($\hat{\boldsymbol{\mathcal{E}}}^n$, $\hat{\boldsymbol{\mathcal{B}}}^n$) from the fields in real space ($\boldsymbol{E}^n$, $\boldsymbol{B}^n$).
2. Apply Eqs. (5)-(6) to obtain the fields in spectral space at time step $n+1$ ($\hat{\boldsymbol{\mathcal{E}}}^{n+1}$, $\hat{\boldsymbol{\mathcal{B}}}^{n+1}$)
3. Apply an inverse Fourier transform, in order to obtain the fields in real space at time step $n+1$ ($\boldsymbol{E}^{n+1}$, $\boldsymbol{B}^{n+1}$) from the fields in spectral space.

Using this scheme and a high spatial order p, spurious numerical dispersion can generally be mitigated to negligible levels.

RECENT DEVELOPMENTS

Parallelization

One of the major issues with spectral solvers has been their scaling across many computing nodes. In principle, the PSTD and PSATD schemes require a global Fourier transform across the whole computational domain. When using a standard domain decomposition technique for parallelization, this Fourier transform can be implemented by a global, distributed Fast Fourier Transform (FFT). However, distributed FFTs do not scale well to many compute nodes, due to the large amount of inter-node communications that they involve.

In the case of Maxwell's equations, one alternative to the global, distributed FFT is to use a local FFT in each subdomain, along with guard cells [18]. In principle, using a local FFT instead of a global one introduces errors. But, because the Maxwell update Eqns. (1)–(2) are a hyperbolic set of equations, the errors remains confined to the guard

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cells (provided that there are enough of them) [18,20]. These errors can thus be eliminated by copying the data from the valid regions of neighboring sub-domains into the guard cells of the local sub-domain, immediately after the Maxwell field update.

The minimal number of guard cells that eliminates these errors can be calculated for any given order p [20]. This number increases with p; and for typical orders (e.g. $p = 32$, $p = 64$), tens of guard cells are required. While this number is large in comparison with FDTD (only one or two guard cells required), its impact on performance can be mitigated by using relatively large sub-domains, with several cores working on the same sub-domain through shared-memory programming paradigms.

By using local FFTs and guard cell exchanges between neighboring sub-domains, a much more favorable scaling can be obtained than with global, distributed FFTs. For instance, it was possible to reach nearly-linear strong scaling on a few hundreds of thousands of cores in [21], whereas global FFTs become prohibitively expensive at this scale.

Cylindrical Geometry

For problems with nearly-cylindrical symmetry, a full 3D Cartesian mesh is not always optimal. In fact, by using an azimuthal expansion and a few 2D r-z grids (one per azimuthal mode), computational costs can be very substantially reduced [22].

PIC codes using the azimuthal expansion were first implemented using the FDTD approach [22–24]. A hybrid PSTD-type algorithm was later implemented by retaining a finite-difference approach in the radial direction while using a spectral approach for the longitudinal derivatives [25]. Finally, a fully spectral (in r and z) PSATD algorithm was derived and implemented [26].

In cylindrical geometry, the PSATD algorithm relies on a Fourier transform along the z direction, and a Hankel transform along the r direction. It turns out that the Fourier-Hankel representation of Maxwell's equations has a similar structure as the 3D Cartesian Fourier representation (Eqs. (3)–(4)). Therefore, the Fourier-Hankel representation of Maxwell's equations can also be integrated analytically over one time step, and, as a result, also mitigates spurious numerical dispersion [26].

SOME ADDITIONAL ADVANTAGES OF SPECTRAL SOLVERS

While, in the previous sections, the spectral solvers were mainly motivated by the mitigation of the spurious numerical dispersion, they do have additional advantages. Two of these advantages are presented in the next subsections.

Accurate Evaluation of the Lorentz Force

A common shortcoming of FDTD PIC codes is the inaccuracy of the calculated Lorentz force in cases where the $\boldsymbol{E}$ and $\boldsymbol{v} \times \boldsymbol{B}$ cancel very closely. This situation arises for instance when a relativistic bunch of electrons co-propagates with a laser: in this case, the term $\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}$ is on the order of $\boldsymbol{E}/\gamma^2$, where γ is the Lorentz factor of the bunch.

This tight cancelation of the $\boldsymbol{E}$ and $\boldsymbol{v} \times \boldsymbol{B}$ terms is difficult to capture in an FDTD PIC code. This is because the fields $\boldsymbol{E}$ and $\boldsymbol{B}$ are staggered in time and space, and are therefore not evaluated exactly in the same way, when interpolated onto the macroparticles. (For instance, $\boldsymbol{B}$ is typically averaged in time, before being interpolated to the macroparticles, whereas $\boldsymbol{E}$ is not.) These slight differences in the evaluation of $\boldsymbol{E}$ and $\boldsymbol{B}$ introduce small numerical errors that can dominate the term $\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}$ in the case where the two terms cancel closely [27].

On the other hand, in the PSATD algorithm, the fields $\boldsymbol{E}$ and $\boldsymbol{B}$ are both defined at the same time (and it is also possible to define them on the same points in space). As a result, the fields are evaluated in a similar way, and can cancel appropriately. This was confirmed for instance in test simulations of an electron co-propagating with a laser [26].

Mitigation of the Numerical Cherenkov Instability

Some types of PIC simulations can become numerically much cheaper when using a different reference frame than that of the laboratory [28]. This is the case for instance in simulations of laser-wakefield acceleration, where the discrepancy between the laser wavelength and the length of the accelerating plasma stage can be greatly reduced in an appropriate Lorentz frame (commonly known as the "boosted frame") [28]. Yet, when using the boosted frame, the bulk of the plasma stage moves relativistically with respect to the grid. In PIC codes, this gives rise to a numerical instability, known as the Numerical Cherenkov Instability (NCI) [29, 30].

Various methods have been used to mitigate the NCI, so as to carry out robust boosted-frame simulations. Some of these methods can be applied to the FDTD or PSTD approach [31–38]. However, the PSATD approach is the only one that is compatible with a particularly robust and elegant mitigation technique: the Galilean technique [39,40].

In the Galilean technique, Maxwell's equations are solved in a Galilean system of coordinates that moves with the bulk of the plasma. It turns out that solving Maxwell's equations with the PSATD scheme in these coordinates suppresses the NCI—without the need for any further numerical correction [39, 40]. Additionaly, this method naturally generalizes to cylindrical coordinates, when using the above mentioned Fourier-Hankel representation.

CONCLUSION

Simulations of accelerators can be numerically challenging when using the electromagnetic PIC algorithm. Spectral solvers can alleviate some of these numerical challenges, by using a more accurate discretization of Maxwell's equations. In addition, recent developments allow to efficiently parallelize these solvers across many nodes, and to port them to cylindrical geometry.

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Yet, it is important to keep in mind that spectral solvers are one possible solution among others, for many of the above challenges. For instance, spurious numerical dispersion can be mitigated to some degree by non-standard finite-difference methods (e.g. [13, 41–43]). Similarly, the inaccuracy in the Lorentz force can be partially mitigated by using higher-order interpolation in time [27]

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