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Short Note

A domain decomposition method for pseudo-spectral electromagnetic simulations of plasmas

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ABSTRACT

Pseudo-spectral electromagnetic solvers (i.e. representing the fields in Fourier space) have extraordinary precision. In particular, Haber et al. presented in 1973 a pseudo-spectral solver that integrates analytically the solution over a finite time step, under the usual assumption that the source is constant over that time step. Yet, pseudo-spectral solvers have not been widely used, due in part to the difficulty for efficient parallelization owing to global communications associated with global FFTs on the entire computational domains.

A method for the parallelization of electromagnetic pseudo-spectral solvers is proposed and tested on single electromagnetic pulses, and on Particle-In-Cell simulations of the wakefield formation in a laser plasma accelerator.

The method takes advantage of the properties of the Discrete Fourier Transform, the linearity of Maxwell's equations and the finite speed of light for limiting the communications of data within guard regions between neighboring computational domains.

Although this requires a small approximation, test results show that no significant error is made on the test cases that have been presented.

The proposed method opens the way to solvers combining the favorable parallel scaling of standard finite-difference methods with the accuracy advantages of pseudo-spectral methods.

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1. Introduction

Particle-In-Cell (PIC) has been the method of choice for the last fifty years for modeling plasmas that include kinetic effects. The most popular electromagnetic formulation uses finite difference discretization of Maxwell's equations in both space and time (FDTD), which produces fast solvers that scale well in parallel, but suffers from various anomalous numerical effects resulting from discretization, field staggering, and numerical dispersion. Aliasing and numerical dispersion lead to an unphysical numerical Cherenkov instability when relativistic particles interact with their gridded self-field [1]. An example is a strong instability that appears in simulations of Laser-Plasma Acceleration (LPA) in Lorentz boosted frames [2,3] or astrophysical shocks [4]. In addition, the staggering of electric and magnetic fields leads to inexact cancelation of relativistic beams' self electric and magnetic components in the calculation of the Lorentz force $\mathbf{E} + \mathbf{v} \times \mathbf{B}$ [5].

Pseudo-spectral methods, which advance the fields in Fourier space [6], offer a number of advantages over standard FDTD solvers. An analytical solution for Maxwell's equations on a grid was given by Haber et al. [7] for a periodic system, leading to a solver that is accurate to machine precision for the modes resolved by the calculation grid, that has no Courant time step limit in vacuum and that has no numerical dispersion. Furthermore, pseudo-spectral methods naturally represent all field values at the nodes of a grid, eliminating staggering errors.

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Due to global communications associated with the use of Fast Fourier Transforms (FFTs) that span the entire domain, pseudo-spectral electromagnetic solvers have not scaled beyond a few thousands of cores. In contrast, the FDTD solvers allow parallelization requiring only local communications between neighboring subdomains, and thus excellent scaling to hundreds of thousand of CPU cores.

In this communication, we report on a domain decomposition method that enables parallelization of pseudo-spectral solvers and requires only local FFTs and communications between neighboring subdomains. This is similar to FDTD decomposition, potentially allowing more accurate pseudo-spectral methods to be scaled to the same level as FDTD. Although this decomposition requires a small approximation, as discussed below, test results show that the error introduced is sufficiently small in practice for the cases that have been tested.

We first present several variations of pseudo-spectral solvers, followed by the new method for domain decomposition, and its application to pseudo-spectral PIC simulations. An example of the application of the method is given on the modeling of the wakefield formation in a laser plasma accelerator [8].

2. Pseudo-spectral electromagnetic solvers

Maxwell's equations in Fourier space are given by

$$\frac{\partial\tilde{\mathbf{E}}}{\partial t} = ic\mathbf{k}\times\tilde{\mathbf{B}} - \tilde{\mathbf{J}}, \tag{1}$$

$$\frac{\partial\tilde{\mathbf{B}}}{\partial t} = -ic\mathbf{k}\times\tilde{\mathbf{E}}, \tag{2}$$

$$i\mathbf{k}\cdot\tilde{\mathbf{E}} = \tilde{\rho}, \tag{3}$$

$$i\mathbf{k}\cdot\tilde{\mathbf{B}} = 0, \tag{4}$$

where $\tilde{a}$ is the Fourier Transform of the quantity a. Provided that the continuity equation $\partial\tilde{\rho}/\partial t + i\mathbf{k}\cdot\tilde{\mathbf{J}} = 0$ is 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

$$\frac{\partial\tilde{\mathbf{E}}_T}{\partial t} = ic\mathbf{k}\times\tilde{\mathbf{B}} - \tilde{\mathbf{J}}_{\mathbf{T}}, \tag{5}$$

$$\frac{\partial\tilde{\mathbf{E}}_L}{\partial t} = -\tilde{\mathbf{J}}_{\mathbf{L}}, \tag{6}$$

$$\frac{\partial\tilde{\mathbf{B}}}{\partial t} = -ic\mathbf{k}\times\tilde{\mathbf{E}}, \tag{7}$$

$$i\mathbf{k}\cdot\tilde{\mathbf{E}} = \tilde{\rho}, \tag{8}$$

$$i\mathbf{k}\cdot\tilde{\mathbf{B}} = 0, \tag{9}$$

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

If the electromagnetic fields within a region are represented by an orthogonal-mode expansion, the fields can be advanced analytically for an interval Δt by adding the contributions of the source terms to each of the modes integrated over that interval [9]. For a discretized system on a regular cartesian grid, if the sources are assumed to be constant over the interval, a Fourier decomposition can be used to analytically advance the transverse components of the fields [7] (a detailed derivation is given in appendix):

$$\tilde{\mathbf{E}}_T^{n+1} = C\tilde{\mathbf{E}}_T^n + iS\hat{\mathbf{k}}\times\tilde{\mathbf{B}}^n - \frac{S}{kc}\tilde{\mathbf{J}}_T^{n+1/2}, \tag{10}$$

$$\tilde{\mathbf{B}}^{n+1} = C\tilde{\mathbf{B}}^n - iS\hat{\mathbf{k}}\times\tilde{\mathbf{E}}^n + i\frac{1-C}{kc}\hat{\mathbf{k}}\times\tilde{\mathbf{J}}^{n+1/2}, \tag{11}$$

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

Integrating the longitudinal component assuming that J_L is constant over one time step, gives

$$\tilde{\mathbf{E}}_L^{n+1} = \tilde{\mathbf{E}}_L^n - \Delta t\tilde{\mathbf{J}}_L^{n+1/2} \tag{12}$$

Combining the transverse and longitudinal components, gives

$$\tilde{\mathbf{E}}^{n+1} = C\tilde{\mathbf{E}}^n + iS\hat{\mathbf{k}}\times\tilde{\mathbf{B}}^n - \frac{S}{kc}\tilde{\mathbf{J}}^{n+1/2} + (1-C)\hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\tilde{\mathbf{E}}^n) + \hat{\mathbf{k}}(\hat{\mathbf{k}}\cdot\tilde{\mathbf{J}}^{n+1/2})\left(\frac{S}{kc} - \Delta t\right), \tag{13}$$

$$\tilde{\mathbf{B}}^{n+1} = C\tilde{\mathbf{B}}^n - iS\hat{\mathbf{k}}\times\tilde{\mathbf{E}}^n + i\frac{1-C}{kc}\hat{\mathbf{k}}\times\tilde{\mathbf{J}}^{n+1/2}. \tag{14}$$

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