



Theoretical and numerical approaches for Vlasov–Maxwell equations

# Modeling of relativistic plasmas with the Particle-In-Cell method

Jean-Luc Vay<sup>a,\*</sup>, Brendan B. Godfrey<sup>b,a</sup><sup>a</sup> Lawrence Berkeley National Laboratory, Berkeley, CA, USA<sup>b</sup> University of Maryland, College Park, MD, USA

## ARTICLE INFO

### Article history:

Received 25 April 2014

Accepted 10 June 2014

Available online 5 August 2014

### Keywords:

Particle-In-Cell

Plasma simulation

Special relativity

Numerical instability

## ABSTRACT

Standard methods employed in relativistic electromagnetic Particle-In-Cell codes are reviewed, as well as novel techniques that were introduced recently. Advances in the analysis and mitigation of the numerical Cherenkov instability are also presented with comparison between analytical theory and numerical experiments. The algorithmic and numerical analytic advances are expanding the range of applicability of the method in the ultra-relativistic regime in particular, where the numerical Cherenkov instability is the strongest without corrective measures.

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## 1. Introduction

Computer simulations of self-consistent electromagnetics and relativistic particle kinetics are critical to the design and understanding of particle accelerators, laser–plasma interaction, fusion or plasma experiments and to the study of space plasmas. For such simulations, the most popular algorithm is the Particle-In-Cell (or PIC) technique, which represents electromagnetic fields on a grid and particles by a sample of macroparticles. In Section 2 of this paper, we review the standard methods employed in relativistic electromagnetic PIC codes, as well as novel techniques that were introduced recently in the code Warp [1,2]. Recent advances in the analysis and mitigation of the numerical Cherenkov instability are presented in Section 3, with comparison between analytical theory and numerical experiments using Warp.

## 2. Particle-In-Cell main steps

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

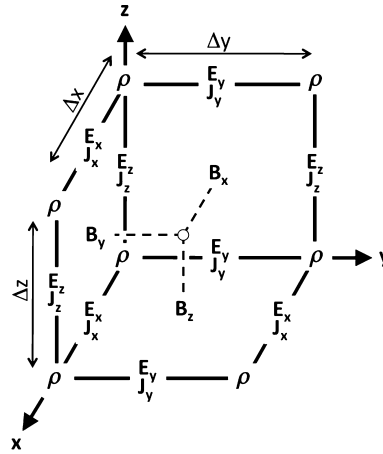
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \quad (1)$$

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

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

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

\* Corresponding author.



**Fig. 1.** Layout of field components on the staggered “Yee” grid. Charge density is defined at the nodes, current densities and electric fields on the edges of the cells and magnetic fields on the faces.

given here in natural units ( $\epsilon_0 = \mu_0 = c = 1$ ), where  $t$  is time,  $\mathbf{E}$  and  $\mathbf{B}$  are the electric and magnetic field components, and  $\rho$  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 given in natural units ( $c = 1$ ). 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.

## 2.1. Field solve

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 this paper, we summarize the widespread second order Finite-Difference Time-Domain (FDTD) algorithm, its extension to non-standard finite-differences 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. [2,4].

### 2.1.1. Finite-Difference Time-Domain (FDTD)

The most popular algorithm for electromagnetic PIC codes is the Finite-Difference Time-Domain (or FDTD) 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 defined respectively as  $D_t G_{i,j,k}^n = (G_{i,j,k}^{n+1/2} - G_{i,j,k}^{n-1/2})/\Delta t$  and  $D_x G_{i,j,k}^n = (G_{i+1/2,j,k}^n - G_{i-1/2,j,k}^n)/\Delta x$ , where  $\Delta t$  and  $\Delta x$  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, as explained below. As shown in Fig. 1, the quantities are given on a staggered (or “Yee”) grid [5], where the electric field components are located between nodes and the magnetic field components are located in the center of the cell faces.

### 2.1.2. Non-Standard Finite-Difference Time-Domain (NSFDTD)

In [6,7], Cole introduced an implementation of the source-free Maxwell’s wave equations for narrow-band applications based on Non-Standard Finite-Differences (NSFD). In [8], Karkkainen et al. adapted it for wideband applications. At the

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