Description of Electromagnetic Spectral Particle-in-Cell Code from the UPIC Framework

Viktor K. Decyk

Department of Physics and Astronomy
University of California, Los Angeles
Los Angeles, California 90095-1547

I. Introduction

This document presents the mathematical foundation of the periodic Particle-in-Cell electromagnetic code in the UCLA Particle-in-Cell Framework. The electromagnetic code includes all the electric and magnetic fields described by Maxwell's equation. This is the most complete of the plasma models, and includes both plasma waves and electromagnetic waves.

II. Electromagnetic Plasma Model

More complex is the electromagnetic model, where the force of interaction is determined by Maxwell's equation. The main interaction loop is as follows:

1. Calculate charge and current density on a mesh from the particles:

$$\rho(\boldsymbol{x}) = \sum_i q_i S(\boldsymbol{x} - \boldsymbol{x}_i) \qquad \boldsymbol{j}(\boldsymbol{x}) = \sum_i q_i \boldsymbol{v}_i S(\boldsymbol{x} - \boldsymbol{x}_i)$$

Note that with this definition of densities, the equation of continuity is automatically satisfied:

$$\nabla \cdot \boldsymbol{j} = \sum_i q_i \boldsymbol{v}_i \cdot \nabla S(\boldsymbol{x} - \boldsymbol{x}_i(t)) = -\frac{\partial \rho}{\partial t}$$

2. Solve Maxwell's equation:

$$\nabla \times \boldsymbol{B} = \frac{4\pi}{c}\boldsymbol{j} + \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t} \qquad \nabla \times \boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \cdot \boldsymbol{B} = 0 \qquad \nabla \cdot \boldsymbol{E} = 4\pi\rho$$

3. Advance particle co-ordinates using the Lorentz Force:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = q_i \int \left[\boldsymbol{E}(\boldsymbol{x}) + \boldsymbol{v}_i \times \boldsymbol{B}(\boldsymbol{x})/c\right] S(\boldsymbol{x}_i - \boldsymbol{x})\, d\boldsymbol{x} \qquad \frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$$

The codes described here are spectral and solve the electric and magnetic fields using Fourier transforms. For the electromagnetic case, the procedure for a gridless system is as follows:

1. Fourier Transform the charge and current densities:

$$\rho(\boldsymbol{k}) = \frac{1}{V}\int \sum_i q_i S(\boldsymbol{x} - \boldsymbol{x}_i(t)) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} d\boldsymbol{x} = \sum_i q_i S(\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i}$$

$$\boldsymbol{j}(\boldsymbol{k}) = \frac{1}{V}\int \sum_i q_i \boldsymbol{v}_i S(\boldsymbol{x} - \boldsymbol{x}_i(t)) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} dx = \sum_i q_i \boldsymbol{v}_i S(\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i}$$

The equation of continuity in Fourier space satisfied:

$$i\boldsymbol{k} \cdot \boldsymbol{j} = i\sum_i q_i \boldsymbol{k} \cdot \boldsymbol{v}_i S(\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i} = -\frac{\partial \rho(\boldsymbol{k})}{\partial t}$$

2. Solve Maxwell's equation in Fourier space:

In a spectral code, one generally separates the electric field **E** into longitudinal and transverse parts $\mathbf{E}_L$ and $\mathbf{E}_T$, which have the property that $\mathbf{k} \times \mathbf{E}_L = 0$ and $\mathbf{k} \bullet \mathbf{E}_T = 0$, and solves them separately. We make use of the equation of continuity to eliminate the longitudinal electric field:

$$\frac{1}{4\pi}\frac{\partial \boldsymbol{E}_L(\boldsymbol{k})}{\partial t} = -\frac{i\boldsymbol{k}}{k^2}\frac{\partial \rho}{\partial t} = -\frac{\boldsymbol{k}}{k^2}(\boldsymbol{k}\bullet\boldsymbol{j})$$

This results in the following sets of equations:

$$\boldsymbol{E}_L(\boldsymbol{k}) = \frac{-i\boldsymbol{k}}{k^2}4\pi\rho(\boldsymbol{k}) \qquad \boldsymbol{j}_T = \boldsymbol{j} - \frac{\boldsymbol{k}(\boldsymbol{k}\bullet\boldsymbol{j})}{k^2}$$

$$\frac{\partial \boldsymbol{E}_T(\boldsymbol{k})}{\partial t} = ic\boldsymbol{k}\times\boldsymbol{B}(\boldsymbol{k}) - 4\pi\boldsymbol{j}_T(\boldsymbol{k}) \qquad \frac{\partial \boldsymbol{B}(\boldsymbol{k})}{\partial t} = -ic\boldsymbol{k}\times\boldsymbol{E}_T(\boldsymbol{k})$$

Note that these equation implies that $\mathbf{j}(\mathbf{k}=0) = 0$. This means that strictly periodic systems have no net current.

3. Fourier Transform the Electric and Magnetic Fields to real space:

$$\boldsymbol{E}_S(\boldsymbol{x}_j) = V\sum_{\boldsymbol{k}=-\infty}^{\infty}\left[\boldsymbol{E}_T(\boldsymbol{k}) + \boldsymbol{E}_L(\boldsymbol{k})\right]S(\boldsymbol{k})e^{i\boldsymbol{k}\bullet\boldsymbol{x}_j} \qquad \boldsymbol{B}_S(\boldsymbol{x}_j) = V\sum_{\boldsymbol{k}=-\infty}^{\infty}\boldsymbol{B}(\boldsymbol{k})S(\boldsymbol{k})e^{i\boldsymbol{k}\bullet\boldsymbol{x}_j}$$

In discretizing time for the field equations, one uses the following scheme: first advance the magnetic field half a step using the old electric field. Then leap-frog the electric field a whole step using the new magnetic field. Finally advance the magnetic field the remaining half step using the new electric field:

$$\boldsymbol{B}(\boldsymbol{k},t-\frac{\Delta t}{2}) = \boldsymbol{B}(\boldsymbol{k},t-\Delta t) - ic\boldsymbol{k}\times\boldsymbol{E}_T(\boldsymbol{k},t-\Delta t)\frac{\Delta t}{2}$$

$$\boldsymbol{E}_T(\boldsymbol{k},t) = \boldsymbol{E}_T(\boldsymbol{k},t-\Delta t) + \left[ic\boldsymbol{k}\times\boldsymbol{B}(\boldsymbol{k},t-\frac{\Delta t}{2}) - 4\pi\boldsymbol{j}_T(k,t-\frac{\Delta t}{2})\right]\Delta t$$

$$\boldsymbol{B}(\boldsymbol{k},t) = \boldsymbol{B}(\boldsymbol{k},t-\frac{\Delta t}{2}) - ic\boldsymbol{k}\times\boldsymbol{E}_T(\boldsymbol{k},t)\frac{\Delta t}{2}$$

The time step must be short enough to resolve light waves. This is known as the Courant condition:

$$c\Delta t \lesssim \Delta$$

The discrete equations of motion for the particles are as follows:

$$\boldsymbol{v}_i(t+\frac{\Delta t}{2}) = \boldsymbol{v}_i(t-\frac{\Delta t}{2}) + \frac{q_i}{m_i}\left[\boldsymbol{E}_S(\boldsymbol{x}_i(t)) + (\frac{\boldsymbol{v}_i(t+\frac{\Delta t}{2}) + \boldsymbol{v}_i(t-\frac{\Delta t}{2})}{2})\times\boldsymbol{B}_S(x_i(t))/c\right]\Delta t$$

$$\boldsymbol{x}_i(t+\triangle t) = \boldsymbol{x}_i(t) + \boldsymbol{v}_i(t+\frac{\Delta t}{2})\triangle t$$

The first equation is an implicit equation where the new velocity appears on both side of the equation. The solution is known as the Boris Mover. It consists of an acceleration a half time step using only the electric field:

$$\boldsymbol{v}_i(t) = \boldsymbol{v}_i(t-\frac{\Delta t}{2}) + \frac{q_i}{m_i}\boldsymbol{E}_S(\boldsymbol{x}_i(t))\frac{\Delta t}{2}$$

Followed by a rotation about the magnetic field:

$$\boldsymbol{v}_i^R(t) = \left\{\boldsymbol{v}_i(t)\left[1-(\frac{\Omega_i\Delta t}{2})^2\right] + \boldsymbol{v}_i(t)\times\boldsymbol{\Omega}_i\Delta t + \frac{(\Delta t)^2}{2}\left[\boldsymbol{v}_i(t)\cdot\boldsymbol{\Omega}_i\right]\boldsymbol{\Omega}_i\right\}/\left[1+(\frac{\Omega_i\Delta t}{2})^2\right]$$

where the cyclotron frequency is defined to be:

$$\boldsymbol{\Omega}_i = \frac{q_i\boldsymbol{B}_S(x_i(t))}{m_i c}$$

Finally, there is another acceleration a half time step using only the electric field:

$$\boldsymbol{v}_i(t+\frac{\Delta t}{2}) = \boldsymbol{v}_i^R(t) + \frac{q_i}{m_i}\boldsymbol{E}_S(\boldsymbol{x}_i(t))\frac{\Delta t}{2}$$

The use of the grid in the spectral electromagnetic code is analogous to its use in the electrostatic code. The charge density and longitudinal electric field are the same while the current is given by:

$$\boldsymbol{j}(\boldsymbol{r}) = \sum_i q_i\boldsymbol{v}_i\sum_{s'}W(\boldsymbol{r}-\boldsymbol{x}_i)\delta_{r,s'}$$

The interpolated electric and magnetic fields are given by:

$$\boldsymbol{E}_S(\boldsymbol{x}_i) = \sum_{\boldsymbol{r}}\left[\boldsymbol{E}_T(r)+\boldsymbol{E}_L(r)\right]W(\boldsymbol{x}_i-\boldsymbol{r})\Delta \quad \boldsymbol{B}_S(\boldsymbol{x}_i) = \sum_{\boldsymbol{r}}\boldsymbol{B}(r)W(\boldsymbol{x}_i-\boldsymbol{r})\Delta$$

III. Energy and Momentum Flux

For the electromagnetic model, the energy flux is well known to be given by the Poynting vector **S**:

$$\nabla \bullet \boldsymbol{S} + \frac{\partial}{\partial t}\left[\frac{\boldsymbol{E} \bullet \boldsymbol{E}}{8\pi} + \frac{\boldsymbol{B} \bullet \boldsymbol{B}}{8\pi}\right] = -\boldsymbol{j} \bullet \boldsymbol{E}$$

where

$$\boldsymbol{S} = \frac{c}{4\pi}\boldsymbol{E} \times \boldsymbol{B}$$

This equation describes the conservation of energy: the time rate of change of electromagnetic field energy plus the outflow of the energy is equal to the negative of the work done on the particles. This equation is not unique and other energy flux equations can also be derived: only differences in energy and flux are significant. It is less well known that analogous energy flux equations can be derived for the electrostatic and Darwin models.

In addition to the energy flux, the momentum flux equation is also useful. For the electromagnetic case, the equation is well known:

$$\nabla \bullet \overleftrightarrow{\mathbf{T}} - \frac{1}{c^2}\frac{\partial \boldsymbol{S}}{\partial t} = \rho \boldsymbol{E} + \boldsymbol{j} \times \boldsymbol{B}/c$$

where

$$\overleftrightarrow{\mathbf{T}} = \frac{1}{4\pi}\left[\boldsymbol{EE} + \boldsymbol{BB} - \frac{1}{2}(\boldsymbol{E} \bullet \boldsymbol{E} + \boldsymbol{B} \bullet \boldsymbol{B})\overleftrightarrow{\mathbf{I}}\right]$$

is the Maxwell Stress Tensor. The quantity $\mathbf{S}/c^2$ is the momentum in the electromagnetic field.

These energy and momentum flux equations are not unique, and alternative forms are possible and useful.

IV. Units

These codes use dimensionless grid units, which means that distance is normalized to some distance δ. Generally, this distance δ is the smallest distance which needs to be resolved in the code, such as a Debye length. Time is normalized to some frequency ω_0. Generally this frequency is the highest frequency that needs to be resolved in the code, such as the plasma frequency. Charge is normalized to the absolute value of the charge of an electron e. Mass is normalized to the mass of an electron m_e. Other variables are normalized from some combination of these.

In summary, dimensionless position, time, velocity, charge, and mass are given by:

$$\widetilde{x} = x/\delta \qquad \widetilde{t} = \omega_0 t \qquad \widetilde{\boldsymbol{v}} = \boldsymbol{v}/\delta\omega_0 \qquad \widetilde{q} = q/e \qquad \widetilde{m_e} = m/m_e$$

Dimensionless charge and current densities are given by:

$$\widetilde{\rho} = \rho\delta^3/e \qquad \widetilde{j} = j\delta^3/e\delta\omega_0$$

Dimensionless electric field, potential, magnetic field, and vector potential are given by:

$$\widetilde{\boldsymbol{E}} = e\boldsymbol{E}/m_e\omega_0^2\delta \qquad \widetilde{\phi} = e\phi/m_e\omega_0^2\delta^2 \qquad \widetilde{\boldsymbol{B}} = e\boldsymbol{B}/m_e c\omega_0 \qquad \widetilde{\boldsymbol{A}} = e\boldsymbol{A}/m_e c\delta\omega_0$$

Dimensionless energy is given by:

$$\widetilde{W} = W/m_e\omega_0^2\delta^2$$

Dimensionless Energy density flux (Poynting vector) is given by:

$$\widetilde{\boldsymbol{S}} = \boldsymbol{S}/m_e\omega_0^3$$

The dimensionless particle equations of motion are:

$$\widetilde{m_i}\frac{d\widetilde{\boldsymbol{v}_i}}{d\widetilde{t}} = \widetilde{q_i}\left[\widetilde{\boldsymbol{E}} + \widetilde{\boldsymbol{v}_i} \times \widetilde{\boldsymbol{B}}\right] \qquad \frac{d\widetilde{\boldsymbol{x}_i}}{d\widetilde{t}} = \widetilde{\boldsymbol{v}_i}$$

The dimensionless Maxwell's equations are:

$$\widetilde{c}^2\,\widetilde{\nabla} \times \widetilde{\boldsymbol{B}} = A_f\widetilde{\boldsymbol{j}} + \frac{\partial\widetilde{\boldsymbol{E}}}{\partial\widetilde{t}} \qquad \widetilde{\nabla} \times \widetilde{\boldsymbol{E}} = -\frac{\partial\widetilde{\boldsymbol{B}}}{\partial\widetilde{t}}$$

$$\widetilde{\nabla} \bullet \widetilde{\boldsymbol{E}} = A_f\widetilde{\rho}$$

The dimensionless energy flux equation is:

$$\widetilde{\nabla} \bullet \boldsymbol{S} + \frac{1}{A_f}\left[\frac{\widetilde{\boldsymbol{E}} \bullet \widetilde{\boldsymbol{E}}}{2} + \widetilde{c}^2\,\frac{\widetilde{\boldsymbol{B}} \bullet \widetilde{\boldsymbol{B}}}{2}\right] = -\widetilde{\boldsymbol{j}} \bullet \widetilde{\boldsymbol{E}}$$

where

$$A_f = \frac{4\pi e^2}{m_e \omega_0^2 \delta^3}$$

defines the relation between the sources and the fields. Whatever time and space scales are chosen, these equations have the same form. Only the constant A_f changes.

In these codes, the normalization length is chosen to be the grid spacing,

$$\delta = L_x / N_x = L_y / N_y = L_z / N_z$$

and the normalization frequency to be the plasma frequency ω_{pe}. In that case, one can show that:

$$A_f = \frac{1}{n_o \delta^3} = \frac{N_x N_y N_z}{N_p}$$

where Np is the number of particles. The grid spacing is then related to some other dimensionless physical parameter, typically the Debye length. Thus:

$$\lambda_{De} / \delta = \frac{v_{the}}{\delta \omega_{pe}} = \widetilde{v}_{the}$$

where the dimensionless thermal velocity is an input to the code. Note that if the grid space is equal to Debye length, then A_f is identical to the plasma parameter g which appears as an small expansion parameter in plasma theory.

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