

Description of Spectral Particle-in-Cell Codes from the UPIC Framework

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I. Introduction

This document presents the mathematical foundation of the periodic Particle-in-Cell codes in the UCLA Particle-in-Cell Framework. There are 3 main kinds of codes described here. The first is an electrostatic code which uses only the Coulomb force of interaction between particles. This is the most fundamental of plasma models and is useful when inductive electric and magnetic fields are not important. The second is the electromagnetic code, which 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. The third is the Darwin model. It is an example of a radiationless, or near-field, electromagnetic model. It includes the induced electric and magnetic fields described by Faraday's and Ampere's laws, but excludes retardation effects and therefore light waves. It is primarily useful when the thermal velocity of particles is much smaller than the speed of light and light waves are not important. It is more complex than the electromagnetic code, but the time step can be much larger.

II. Electrostatic Plasma Model

The simplest model is the electrostatic model, where the force of interaction is determined by solving only the Poisson equation in Maxwell's equation. The main interaction loop is as follows:

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

$$\rho(\mathbf{x}) = \sum_i q_i S(\mathbf{x} - \mathbf{x}_i)$$

2. Solve Poisson's equation:

$$\nabla \cdot \mathbf{E} = 4\pi\rho$$

3. Advance particle co-ordinates using Newton's Law:

$$m_i \frac{d\mathbf{v}_i}{dt} = q_i \int \mathbf{E}(\mathbf{x}) S(\mathbf{x}_i - \mathbf{x}) d\mathbf{x} \quad \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

The function $S(\mathbf{x})$ is the particle shape function. For point particles, this would be a delta function, but in computer modeling extended shapes are commonly used. The codes described here are spectral and solve the electric field using Fourier transforms. For the electrostatic case and periodic boundary conditions, a procedure for a gridless system is as follows:

1. Fourier Transform the charge density:

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

2. Solve Poisson's equation in Fourier space:

$$\mathbf{E}(\mathbf{k}) = \frac{-i\mathbf{k}}{k^2} 4\pi\rho(\mathbf{k})$$

Note that this equation implies that $\rho(\mathbf{k}=0) = 0$. This means that strictly periodic systems are charge neutral.

3. Fourier Transform the Smoothed Electric Field to real space:

$$\mathbf{E}_s(\mathbf{x}_i) = V \sum_{\mathbf{k}=-\infty}^{\infty} \mathbf{E}(\mathbf{k}) S(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}_i}$$

For delta function particles shapes, $S(\mathbf{k}) = 1/V$. When solving these equations on the computer, we generally use discrete space and time co-ordinates. In discretizing time, the explicit leap-frog integration scheme is commonly used, because it is second order accurate. In this scheme, the particle co-ordinates are known at staggered times.

The discrete equations of motion are as follows:

$$\mathbf{v}_i(t + \Delta t/2) = \mathbf{v}_i(t - \Delta t/2) + \frac{q_i}{m_i} \mathbf{E}_s(\mathbf{x}_i(t)) \Delta t$$

$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \mathbf{v}_i(t + \Delta t/2) \Delta t$$

Although it is possible to use the gridless spectral field solver shown above in a very accurate particle code, this is quite slow. More commonly, charge density is accumulated on a grid from the particle co-ordinates according to some interpolation scheme. The fields are then calculated at the grid points, then interpolated to obtain the force at the particle's position. If we have (Nx,Ny,Nz) grid points for a system of size (Lx,Ly,Lz), then the grid spacings are:

$$\Delta_x = L_x/N_x \quad \Delta_y = L_y/N_y \quad \Delta_z = L_z/N_z$$

and the charge deposit is then defined to be:

$$\rho(\mathbf{r}) = \sum_i q_i \sum_{s'} W(\mathbf{r} - \mathbf{x}_i) \delta_{\mathbf{r},s'}$$

where \mathbf{r}, \mathbf{s}' are defined at integer values n, m, l , as follows:

$$\mathbf{r} = (n\Delta_x, m\Delta_y, l\Delta_z) \quad \mathbf{s}' = (n', m', l')$$

and the vector delta function is the product of three Kronecker delta functions:

$$\delta_{\mathbf{r},s'} = \delta_{n,n'} \delta_{m,m'} \delta_{l,l'}$$

This is analogous to the gridless case we had before:

$$\rho(\mathbf{x}) = \sum_i q_i S(\mathbf{x} - \mathbf{x}_i)$$

The important feature is that the interpolation function W be smooth and have limited support, that is, it is zero outside a small range. The interpolation function is usually the product of three interpolation functions in each co-ordinate. For example, the most common interpolation function is linear, given by:

$$W_x(x) = \begin{cases} (\Delta_x + x)/\Delta_x^2, & -\Delta_x < x \leq 0 \\ (\Delta_x - x)/\Delta_x^2, & 0 \leq x < \Delta_x \end{cases}$$

and similarly for the other co-ordinates. However, quadratic and cubic B-spline functions are sometimes used.

The Discrete Fourier Transform can now be used to obtain the Fourier transform of the density:

$$\rho(\mathbf{k}') = \frac{1}{N} \sum_{\mathbf{r}} \rho(\mathbf{r}) e^{-i\mathbf{k}' \cdot \mathbf{r}} = \frac{1}{N} \sum_{\mathbf{r}} \sum_i q_i W(\mathbf{r} - \mathbf{x}_i) e^{-i\mathbf{k}' \cdot \mathbf{r}}$$

where $N = N_x N_y N_z$, and we define \mathbf{k}' as follows:

$$\mathbf{k}' = \left(\frac{2\pi n'}{L_x}, \frac{2\pi m'}{L_y}, \frac{2\pi l'}{L_z} \right)$$

This is analogous to the gridless case we had before:

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

The major complication of using a grid is that non-physical grid forces can arise that were absent before. These arise from aliasing, which occurs when the continuous particle co-ordinates \mathbf{x}_i have spatial variations less than the grid spacing. Such variations cannot be resolved, but get mapped onto longer wavelengths.

To see explicitly how this occurs, we can write the interpolation function as an infinite Fourier series, as follows:

$$W(\mathbf{x}) = \sum_{\mathbf{k}=-\infty}^{\infty} W(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} \quad W(\mathbf{k}) = \frac{1}{V} \int W(\mathbf{x}) e^{-i\mathbf{k} \cdot \mathbf{x}} d\mathbf{x}$$

this leads to:

$$\rho(\mathbf{k}') = \frac{1}{N} \sum_i q_i \sum_{\mathbf{k}=-\infty}^{\infty} W(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x}_i} \sum_{\mathbf{r}} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}}$$

The last sum over \mathbf{r} is a geometric series which can be summed explicitly to give:

$$\sum_{\mathbf{r}} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} = N \sum_{\mathbf{k}_N=-\infty}^{\infty} \delta_{\mathbf{k}, \mathbf{k}' + \mathbf{k}_N}$$

where \mathbf{k}_N represents wavelengths which cannot be resolved:

$$\mathbf{k}_N = \left(\frac{2\pi n''}{\Delta_x}, \frac{2\pi m''}{\Delta_y}, \frac{2\pi l''}{\Delta_z} \right)$$

As a result, one can write the Fourier transform of the density as follows:

$$\rho(\mathbf{k}') = \sum_i q_i \left[W(\mathbf{k}') + \sum_{\mathbf{k}_N \neq 0} W(\mathbf{k}' + \mathbf{k}_N) e^{-i\mathbf{k}_N \cdot \mathbf{x}_i} \right] e^{-i\mathbf{k}' \cdot \mathbf{x}_i}$$

Compare this with the gridless case we had before:

$$\rho(\mathbf{k}) = \sum_i q_i S(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x}_i}$$

One can see that $W(\mathbf{k}')$ acts like a particle shape factor, similar to the function $S(\mathbf{k})$ in the gridless case. The terms involving non-zero values of \mathbf{k}_N are the non-physical aliased terms. The electric field is solved at the gridpoints as in the gridless case, except for the use of the Discrete Fourier Transform.

$$E(\mathbf{k}') = \frac{-i\mathbf{k}'}{k'^2} 4\pi\rho(\mathbf{k}')$$

$$E(\mathbf{r}) = \sum_{\mathbf{k}'} E(\mathbf{k}') e^{i\mathbf{k}' \cdot \mathbf{r}}$$

Obtaining the electric field at the particle's location involves another interpolation.

$$E_s(\mathbf{x}_i) = \sum_{\mathbf{r}} E(\mathbf{r}) W(\mathbf{x}_i - \mathbf{r}) \Delta$$

where

$$\Delta = \Delta_x \Delta_y \Delta_z$$

Proceeding as before, one can show that:

$$E_s(\mathbf{x}_i) = V \sum_{\mathbf{k}'} E(\mathbf{k}') \left[W(\mathbf{k}') + \sum_{\mathbf{k}_N \neq 0} W(\mathbf{k}' + \mathbf{k}_N) e^{i\mathbf{k}_N \cdot \mathbf{x}_i} \right] e^{i\mathbf{k}' \cdot \mathbf{x}_i}$$

This is analogous to the gridless case:

$$E_s(\mathbf{x}_i) = V \sum_{\mathbf{k}=-\infty}^{\infty} E(\mathbf{k}) S(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}_i}$$

Note that with a grid, the force accelerating a particle no longer depends merely on the separation of particles, but also on the distance of each particle from the grid. In other words, the particles are not only interacting with each other, but also with a periodic structure formed by the grid itself. This non-conservative force usually leads to self-heating, sometimes to instability. The aliasing can be minimized in one of two ways. One is to use a higher order interpolation function whose Fourier series is as small as possible for $\mathbf{k} > \mathbf{k}_N$. This is more expensive in computer time. Alternatively, one can use an additional shape function $S(\mathbf{x})$ in addition to the interpolation function. Both these methods effectively make the particles “fatter,” and it is hard to maintain density variations that are smaller than the particle size. One can also regard them as filter functions.

The most common interpolation functions in use are the B-splines. They have a Fourier transforms for each component i given by:

$$W_n(k_i) = \frac{1}{L_i} \left[\frac{\sin(k_i \Delta / 2)}{k_i \Delta / 2} \right]^{n+1}$$

These functions have maxima near $\mathbf{k} = (p+1/2)\mathbf{k}_N$, where p is an integer > 1 . The worst aliasing occurs for $p = 1$, which maps density variations at $\mathbf{k} = 3\mathbf{k}_N/2$ to $\mathbf{k} = \mathbf{k}_N/2$.

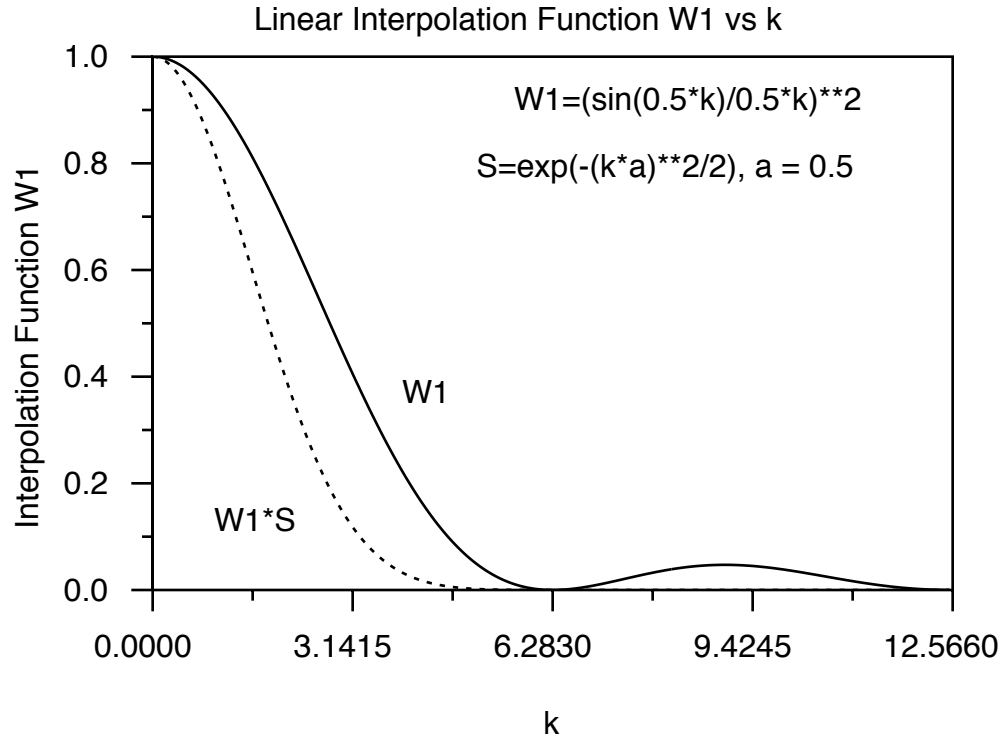


Figure 1. Fourier transform of first order interpolation function W1 with and without a gaussian smoothing function S. Modes with $k > 2\pi$ mapped to modes with $k < 2\pi$.

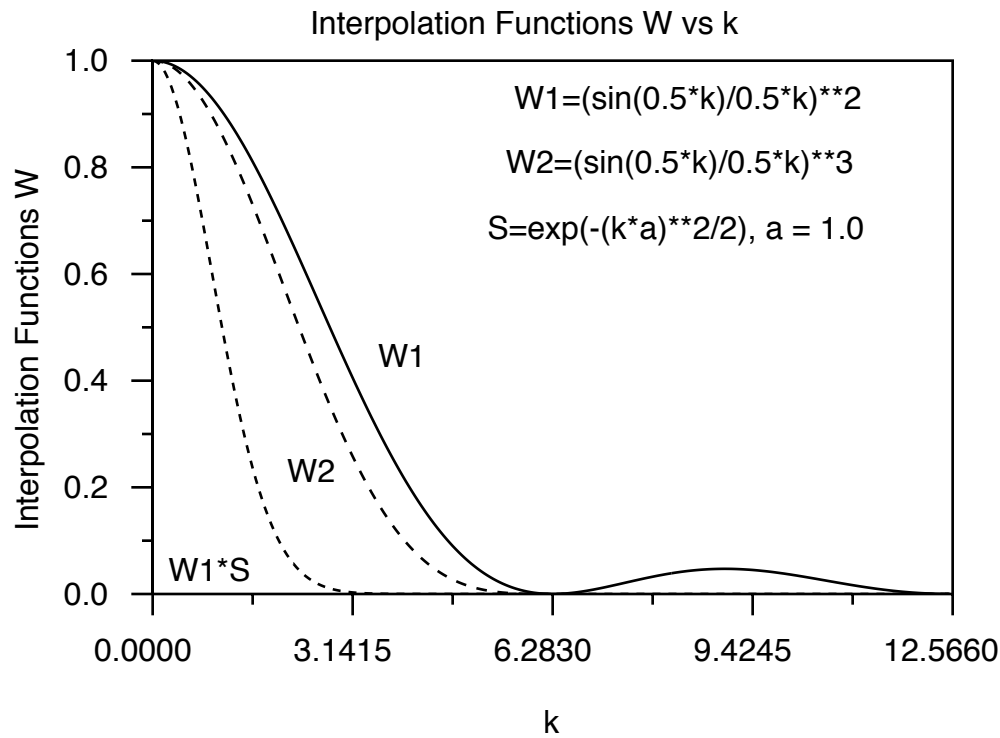


Figure 2. Fourier transforms of first and second order interpolation functions W1 and W2, and W1 with gaussian smoothing S.

A particle shape (or filter) function $S(\mathbf{k})$ which is small in the vicinity of $\mathbf{k}=\mathbf{k}_N/2$ will suppress the aliasing. Of course, one is also suppressing some physical modes, so this scheme is limiting the resolution of the model. The lesson here is that when using grids, one must suppress, one way or another, information which cannot be resolved. Higher order interpolations have better resolution, but are more costly. In Fourier space, a common filter function is:

$$S(k_i) = e^{-(k_i a_i)^2 / 2} / L_i$$

where \mathbf{a} is the particle size, which corresponds to a gaussian particle in space.

If filtering is used to suppress aliasing, then the effective particle shape is given by:

$$S_{eff}(\mathbf{k}) = V \cdot \prod_i W(k_i) S(k_i)$$

In real space this corresponds to a convolution of the interpolation function with the filter function. For non-spectral codes, such filtering is typically done in real space. When filtering is used, spectral electrostatic codes can conserve energy to parts per million over thousands of time steps, and conserve momentum to round-off error.

Even when aliasing is suppressed, grid effects are still present, primarily due to the use of “fat” particles rather than point particles. The easiest way to understand this, is to note that in Fourier space one replaces $q_i \Rightarrow q_i S_{eff}(\mathbf{k})$, both in the charge deposit and in the force calculation. In plasma theory, charge enters only in the calculation of the plasma frequency, so that if aliasing is negligible:

$$\omega_{pe}^2 \Rightarrow \omega_{pe}^2 (V \cdot S_{eff}(\mathbf{k}))^2$$

Where the plasma frequency now depends on \mathbf{k} , and may not be isotropic. For linear interpolation, gaussian smoothing with $a/\Delta > 0.5$, and an isotropic grid, one has:

$$\omega_{pe}^2 \Rightarrow \omega_{pe}^2 e^{-k^2(a^2 + \Delta^2/6)} \approx \omega_{pe}^2 [1 - k^2(a^2 + \Delta^2/6)]$$

Thus to see how the grid affects the plasma, one can replace the plasma frequency which appears in plasma theory with the above expression. Whether this k dependence of the plasma frequency is important or not depends on the plasma parameters and waves under study. For example, the dispersion relation for plasma waves:

$$\omega^2 = \omega_{pe}^2 + 3k^2 v_{the}^2$$

becomes:

$$\omega^2 = \omega_{pe}^2 + \left[3 - \frac{a^2 + \Delta^2/6}{\lambda_{DE}^2} \right] k^2 v_{the}^2$$

Whether this is important or not depends on the size of the grid relative to the Debye length.

III. 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:

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

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

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

2. Solve Maxwell's equation:

$$\begin{aligned} \nabla \times \mathbf{B} &= \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} & \nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{B} &= 0 & \nabla \cdot \mathbf{E} &= 4\pi\rho \end{aligned}$$

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

$$m_i \frac{d\mathbf{v}_i}{dt} = q_i \int [\mathbf{E}(\mathbf{x}) + \mathbf{v}_i \times \mathbf{B}(\mathbf{x})/c] S(\mathbf{x}_i - \mathbf{x}) d\mathbf{x} \quad \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

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:

$$\begin{aligned} \rho(\mathbf{k}) &= \frac{1}{V} \int \sum_i q_i S(\mathbf{x} - \mathbf{x}_i(t)) e^{-ik \cdot \mathbf{x}} d\mathbf{x} = \sum_i q_i S(\mathbf{k}) e^{-ik \cdot \mathbf{x}_i} \\ \mathbf{j}(\mathbf{k}) &= \frac{1}{V} \int \sum_i q_i \mathbf{v}_i S(\mathbf{x} - \mathbf{x}_i(t)) e^{-ik \cdot \mathbf{x}} d\mathbf{x} = \sum_i q_i \mathbf{v}_i S(\mathbf{k}) e^{-ik \cdot \mathbf{x}_i} \end{aligned}$$

The equation of continuity in Fourier space satisfied:

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

2. Solve Maxwell's equation in Fourier space:

In a spectral code, one generally separates the electric field \mathbf{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 $\mathbf{k} \cdot \mathbf{E}_T = 0$, and solves them separately. We make use of the equation of continuity to eliminate the longitudinal electric field:

$$\frac{1}{4\pi} \frac{\partial E_L(\mathbf{k})}{\partial t} = -\frac{i\mathbf{k}}{k^2} \frac{\partial \rho}{\partial t} = -\frac{\mathbf{k}}{k^2} (\mathbf{k} \cdot \mathbf{j})$$

This results in the following sets of equations:

$$\begin{aligned} E_L(\mathbf{k}) &= \frac{-i\mathbf{k}}{k^2} 4\pi\rho(\mathbf{k}) & \mathbf{j}_T &= \mathbf{j} - \frac{\mathbf{k}(\mathbf{k} \cdot \mathbf{j})}{k^2} \\ \frac{\partial E_T(\mathbf{k})}{\partial t} &= i\mathbf{k} \times \mathbf{B}(\mathbf{k}) - 4\pi\mathbf{j}_T(\mathbf{k}) & \frac{\partial \mathbf{B}(\mathbf{k})}{\partial t} &= -i\mathbf{k} \times \mathbf{E}_T(\mathbf{k}) \end{aligned}$$

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:

$$E_s(\mathbf{x}_j) = V \sum_{\mathbf{k}=-\infty}^{\infty} [E_T(\mathbf{k}) + E_L(\mathbf{k})] S(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}_j} \quad B_s(\mathbf{x}_j) = V \sum_{\mathbf{k}=-\infty}^{\infty} \mathbf{B}(\mathbf{k}) S(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}_j}$$

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:

$$\begin{aligned} \mathbf{B}(\mathbf{k}, t - \frac{\Delta t}{2}) &= \mathbf{B}(\mathbf{k}, t - \Delta t) - i\mathbf{k} \times \mathbf{E}_T(\mathbf{k}, t - \Delta t) \frac{\Delta t}{2} \\ E_T(\mathbf{k}, t) &= E_T(\mathbf{k}, t - \Delta t) + \left[i\mathbf{k} \times \mathbf{B}(\mathbf{k}, t - \frac{\Delta t}{2}) - 4\pi\mathbf{j}_T(\mathbf{k}, t - \frac{\Delta t}{2}) \right] \Delta t \\ \mathbf{B}(\mathbf{k}, t) &= \mathbf{B}(\mathbf{k}, t - \frac{\Delta t}{2}) - i\mathbf{k} \times \mathbf{E}_T(\mathbf{k}, t) \frac{\Delta t}{2} \end{aligned}$$

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:

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

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

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:

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

Followed by a rotation about the magnetic field:

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

where the cyclotron frequency is defined to be:

$$\boldsymbol{\Omega}_i = \frac{q_i \mathbf{B}_s(\mathbf{x}_i(t))}{m_i c}$$

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

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

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:

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

The interpolated electric and magnetic fields are given by:

$$\mathbf{E}_s(\mathbf{x}_i) = \sum_r [\mathbf{E}_T(r) + \mathbf{E}_L(r)] W(\mathbf{x}_i - \mathbf{r}) \Delta \quad \mathbf{B}_s(\mathbf{x}_i) = \sum_r \mathbf{B}(r) W(\mathbf{x}_i - \mathbf{r}) \Delta$$

IV. Darwin Plasma Model

Most complex is the Darwin (radiationless electromagnetic) model, where the force of interaction is determined by the Darwin subset of Maxwell's equation. The difference between the two is in the expression for Ampere's law. Maxwell's equation has:

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

whereas the Darwin subset has:

$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{E}_L}{\partial t}$$

This small difference is significant because it turns the equations from hyperbolic form to elliptic form and eliminates light waves.

The main interaction loop is as follows:

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

$$\begin{aligned} \rho(\mathbf{x}) &= \sum_i q_i S(\mathbf{x} - \mathbf{x}_i) & \mathbf{j}(\mathbf{x}, t) &= \sum_i q_i \mathbf{v}_i(t) S(\mathbf{x} - \mathbf{x}_i(t)) \\ \frac{\partial \mathbf{j}(\mathbf{x})}{\partial t} &= \sum_i q_i \left[\frac{d\mathbf{v}_i}{dt} S(\mathbf{x} - \mathbf{x}_i) - \mathbf{v}_i \nabla \cdot \mathbf{v}_i S(\mathbf{x} - \mathbf{x}_i) \right] \end{aligned}$$

In the code, we actually deposit two quantities separately, an acceleration density and a velocity flux:

$$\mathbf{a}(\mathbf{x}) = \sum_i q_i \frac{d\mathbf{v}_i}{dt} S(\mathbf{x} - \mathbf{x}_i) \quad \vec{\mathbf{M}}(\mathbf{x}) = \sum_i q_i \mathbf{v}_i \mathbf{v}_i S(\mathbf{x} - \mathbf{x}_i)$$

and then differentiate:

$$\frac{\partial \mathbf{j}(\mathbf{x})}{\partial t} = \mathbf{a} - \nabla \cdot \vec{\mathbf{M}}$$

2. Solve Maxwell's equation:

As in the electromagnetic code, we separate the electric field \mathbf{E} into longitudinal and transverse parts, $\mathbf{E} = \mathbf{E}_L + \mathbf{E}_\perp$ and solve them separately:

$$\begin{aligned}\nabla \times \mathbf{E}_L &= 0 & \nabla \cdot \mathbf{E}_T &= 0 \\ \nabla \times \mathbf{B} &= \frac{4\pi}{c} \mathbf{j}_T = \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{E}_L}{\partial t} & \nabla^2 \mathbf{E}_T &= \frac{1}{c} \nabla \times \frac{\partial \mathbf{B}}{\partial t} = \frac{4\pi}{c^2} \frac{\partial \mathbf{j}_T}{\partial t}\end{aligned}$$

$$\nabla \cdot \mathbf{B} = 0 \quad \nabla \cdot \mathbf{E}_L = 4\pi\rho$$

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

$$m_i \frac{d\mathbf{v}_i}{dt} = q_i \int [\mathbf{E}(\mathbf{x}) + \mathbf{v}_i \times \mathbf{B}(\mathbf{x})/c] S(\mathbf{x}_i - \mathbf{x}) d\mathbf{x} \quad \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

For the Darwin case, the procedure for solving these equations for a gridless system is as follows:

1. Fourier Transform the charge, current, and derivative of current densities

$$\begin{aligned}\rho(\mathbf{k}) &= \frac{1}{V} \int \sum_i q_i S(\mathbf{x} - \mathbf{x}_i(t)) e^{-i\mathbf{k} \cdot \mathbf{x}} d\mathbf{x} = \sum_i q_i S(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x}_i} \\ \mathbf{j}(\mathbf{k}) &= \frac{1}{V} \int \sum_i q_i \mathbf{v}_i S(\mathbf{x} - \mathbf{x}_i(t)) e^{-i\mathbf{k} \cdot \mathbf{x}} d\mathbf{x} = \sum_i q_i \mathbf{v}_i S(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x}_i} \\ \frac{\partial \mathbf{j}(\mathbf{k})}{\partial t} &= \sum_i q_i \left[\frac{d\mathbf{v}_i}{dt} - i(\mathbf{k} \cdot \mathbf{v}_i) \mathbf{v}_i \right] S(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x}_i}\end{aligned}$$

2. Solve the Darwin subset of Maxwell's equation in Fourier space:

$$\begin{aligned}\mathbf{E}_L(\mathbf{k}) &= \frac{-i\mathbf{k}}{k^2} 4\pi\rho(\mathbf{k}) & \mathbf{B}(\mathbf{k}) &= -\frac{4\pi}{c} \frac{i\mathbf{k} \times \mathbf{j}(\mathbf{k})}{k^2} \\ \frac{\partial \mathbf{j}_T(\mathbf{k})}{\partial t} &= \frac{\partial \mathbf{j}(\mathbf{k})}{\partial t} - \frac{\mathbf{k}}{k^2} (\mathbf{k} \cdot \frac{\partial \mathbf{j}(\mathbf{k})}{\partial t}) & \mathbf{E}_T(\mathbf{k}) &= -\frac{4\pi}{k^2 c^2} \frac{\partial \mathbf{j}_T(\mathbf{k})}{\partial t}\end{aligned}$$

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

$$\mathbf{E}_s(\mathbf{x}_j) = V \sum_{\mathbf{k}=-\infty}^{\infty} [\mathbf{E}_T(\mathbf{k}) + \mathbf{E}_L(\mathbf{k})] S(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}_j} \quad \mathbf{B}_s(\mathbf{x}_j) = V \sum_{\mathbf{k}=-\infty}^{\infty} \mathbf{B}(\mathbf{k}) S(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}_j}$$

Discretizing time for these field equations is much more complex than for the electromagnetic model, since one cannot use the leap-frog algorithm for \mathbf{E}_T . In fact, \mathbf{E}_T depends on the acceleration $d\mathbf{v}_j/dt$ of all the particles, but the acceleration of a particle depends on \mathbf{E}_T , so we have a very large system of coupled equations!

A simple iterative scheme where one uses old values of $d\mathbf{v}_j/dt$ on the right hand side to find new values of \mathbf{E}_T :

$$\mathbf{E}_T(\mathbf{x}_j) = - \sum_{k=-\infty}^{\infty} \left[\frac{4\pi}{k^2 c^2} \right] \left[\frac{\partial \mathbf{j}_T^o(t)}{\partial t} \right] e^{ik \cdot \mathbf{x}_j}$$

is unstable when

$$kc < \omega_{pe}$$

To stabilize the iteration, one can modify the equation by subtracting a constant from both sides:

$$\nabla^2 \mathbf{E}_T^n - \frac{\omega_{p0}^2}{c^2} \mathbf{E}_T^n = \frac{4\pi}{c^2} \frac{\partial \mathbf{j}_T}{\partial t} - \frac{\omega_{p0}^2}{c^2} \mathbf{E}_T^o$$

where the shift constant is the average plasma frequency:

$$\omega_{p0}^2 = \frac{4\pi}{V} \sum_i \frac{q_i^2}{m_i}$$

and the superscripts n and o refer to new and old values of the iteration. The solution to this new equation is:

$$\mathbf{E}_T^n(\mathbf{x}_j) = - \sum_{k=-\infty}^{\infty} \left[\frac{4\pi}{k^2 c^2 + \omega_{p0}^2} \right] \left[\frac{\partial \mathbf{j}_T(t)}{\partial t} - \frac{\omega_{p0}^2}{4\pi} \mathbf{E}_T^o \right] e^{ik \cdot \mathbf{x}_j}$$

Note when the solution has converged, this equation reduces to the original one.

Solving this equation requires knowledge of the velocities and accelerations of the particles at time t. This is obtained from the leap-frog scheme follows:

$$\mathbf{v}_j(t) = \left[\frac{\mathbf{v}_j(t + \Delta t/2) + \mathbf{v}_j(t - \Delta t/2)}{2} \right] \quad \frac{d\mathbf{v}_j(t)}{dt} = \left[\frac{\mathbf{v}_j(t + \Delta t/2) - \mathbf{v}_j(t - \Delta t/2)}{\Delta t} \right]$$

The iteration starts by first calculating $\mathbf{E}_L(t)$ from $\mathbf{x}(t)$, and setting

$$\mathbf{v}_j(t + \Delta t/2) = \mathbf{v}_j(t - \Delta t/2)$$

This is equivalent to assuming the forces are small and that changes in the currents are dominated by convection. Next solve for initial $\mathbf{E}_T(t)$ and $\mathbf{B}(t)$. The iteration loop then has two parts. First, advance particles, calculate $d\mathbf{v}_j(t)/dt$ and $\mathbf{v}_j(t)$, and deposit $d\mathbf{j}(t)/dt$ and $\mathbf{j}(t)$. Do not update particles. Second, solve for improved $\mathbf{E}_T(t)$ and $\mathbf{B}(t)$. Repeat.

When converged, use the electromagnetic Boris Mover to update the particles.

This iteration scheme works well and converges in about 2 iterations so long as the plasma density does not vary too much, specifically if

$$\max(\omega_p^2(\mathbf{x})) < 1.5\omega_{p0}^2$$

Beyond that, the number of iterations needed increases, and eventually the algorithm becomes unstable again. It can be stabilized by modifying the shift constant as follows:

$$\omega_{po}^2 = \frac{1}{2}[\max(\omega_p^2(\mathbf{x})) + \min(\omega_p^2(\mathbf{x}))]$$

As the density variation becomes more extreme, the number of iterations increases, but it seems to remain stable.

V. Radiative and Darwin Electromagnetic Fields

The transverse parts of Maxwell's equations are:

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

where

$$\mathbf{E} = \mathbf{E}_L + \mathbf{E}_T$$

The transverse parts of the Darwin subset can be written:

$$\nabla \times \mathbf{B}_D = \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{E}_L}{\partial t} \quad \nabla \times \mathbf{E}_D = -\frac{1}{c} \frac{\partial \mathbf{B}_D}{\partial t}$$

The subscript D has been added to indicate that the Darwin fields are different than the Maxwell fields. Let us separate the transverse Maxwell fields into two parts, the Darwin part defined by the above equations and a Radiative part, given the subscript R.

$$\mathbf{B} = \mathbf{B}_D + \mathbf{B}_R \quad \mathbf{E}_T = \mathbf{E}_D + \mathbf{E}_R$$

Subtracting the Darwin equations from the Maxwell equations, gives us an equation for the Radiative parts:

$$\nabla \times \mathbf{B}_R = \frac{1}{c} \frac{\partial \mathbf{E}_T}{\partial t} \quad \nabla \times \mathbf{E}_R = -\frac{1}{c} \frac{\partial \mathbf{B}_R}{\partial t}$$

This separation allows us to see more clearly that the Darwin part of the electromagnetic field is driven by the plasma current, whereas the Radiative part is driven by the displacement current. The field \mathbf{E}_D in the electromagnetic and Darwin models are not exactly the same, however. In the electromagnetic case, the current \mathbf{j} includes a response to the field \mathbf{E}_R , which is missing in the Darwin current.

Nevertheless, separating the total electric field into three parts, $\mathbf{E} = \mathbf{E}_L + \mathbf{E}_D + \mathbf{E}_R$ is a very useful diagnostic in illuminating physical processes in plasmas.

A similar separation can be done in terms of the vector potential \mathbf{A} . In the Coulomb Gauge, where

$$\mathbf{A} = \mathbf{A}_D + \mathbf{A}_R \quad \nabla \cdot \mathbf{A}_D = 0 \quad \nabla \cdot \mathbf{A}_R = 0$$

The full set of Maxwell's equation for the vector potential can be written:

$$\nabla^2 \mathbf{A} = -\frac{4\pi}{c} \mathbf{j}_T - \frac{1}{c} \frac{\partial \mathbf{E}_T}{\partial t} \quad \mathbf{j}_T = \mathbf{j} + \frac{1}{4\pi} \frac{\partial \mathbf{E}_L}{\partial t}$$

The Darwin subset can be written:

$$\nabla^2 \mathbf{A}_D = -\frac{4\pi}{c} \mathbf{j}_T$$

Subtracting the two gives the equation for radiative part of the vector potential:

$$\nabla^2 \mathbf{A}_R = -\frac{1}{c} \frac{\partial \mathbf{E}_T}{\partial t} = \frac{4\pi}{c} \mathbf{j}_T - \nabla \times \mathbf{B}$$

The Radiative and Darwin fields can then be derived:

$$\mathbf{B}_D = \nabla \times \mathbf{A}_D \quad \mathbf{B}_R = \nabla \times \mathbf{A}_R$$

and

$$\mathbf{E}_D = -\frac{1}{c} \frac{\partial \mathbf{A}_D}{\partial t} \quad \mathbf{E}_R = -\frac{1}{c} \frac{\partial \mathbf{A}_R}{\partial t}$$

These decompositions are used primarily as filters for diagnostics. For example, one can see the light wave more clearly when \mathbf{A}_R is analyzed, than when \mathbf{A} itself is analyzed.

VI. Energy and Momentum Flux

For the electromagnetic model, the energy flux is well known to be given by the Poynting vector \mathbf{S} :

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

where

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

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.

For the electrostatic model, an energy flux equation is given by:

$$\nabla \cdot \mathbf{S} + \frac{\partial}{\partial t} \left[\frac{\mathbf{E}_L \cdot \mathbf{E}_L}{8\pi} \right] = -\mathbf{j} \cdot \mathbf{E}_L$$

where

$$\mathbf{S} = \left[\mathbf{j} - \frac{1}{4\pi} \nabla \frac{\partial \phi}{\partial t} \right] \phi$$

and

$$\mathbf{E}_L = -\nabla \phi$$

This equation can be easily shown by making use of the equation of continuity and the identity:

$$\nabla \cdot (f\mathbf{V}) = \mathbf{V} \cdot \nabla f + f(\nabla \cdot \mathbf{V})$$

An alternate form of this equation can be derived by using the result,

$$\nabla \cdot \left[\frac{\phi \nabla \phi}{8\pi} \right] = \frac{\mathbf{E}_L \cdot \mathbf{E}_L}{8\pi} - \frac{1}{2} \rho \phi$$

to obtain:

$$\nabla \cdot \mathbf{S}' + \frac{\partial}{\partial t} \left[\frac{1}{2} \rho \phi \right] = -\mathbf{j} \cdot \mathbf{E}_L$$

where the alternative energy flux vector is

$$\mathbf{S}' = \mathbf{j} \phi + \frac{1}{8\pi} \left[\frac{\partial \phi}{\partial t} \nabla \phi - \phi \nabla \frac{\partial \phi}{\partial t} \right]$$

The electrostatic energy in the form $\rho \phi / 2$ is useful for isolated systems.

For the Darwin model, an energy flux equation is given by:

$$\nabla \cdot \mathbf{S} + \frac{\partial}{\partial t} \left[\frac{\mathbf{E}_L \cdot \mathbf{E}_L}{8\pi} + \frac{\mathbf{B} \cdot \mathbf{B}}{8\pi} \right] = -\mathbf{j} \cdot (\mathbf{E}_L + \mathbf{E}_T)$$

where

$$\mathbf{S} = \frac{c}{4\pi} \left[(\mathbf{E}_L + \mathbf{E}_T) \times \mathbf{B} - \frac{1}{c} \mathbf{E}_T \frac{\partial \phi}{\partial t} \right]$$

This can be verified by taking the divergence of \mathbf{S} , and making use of the Darwin equations. In the Darwin model, the main point to notice is that the transverse electric field \mathbf{E}_T does not enter into the definition of the field energy.

An alternate form for the Darwin case can be derived by using the result,

$$\nabla \cdot \left[\frac{\mathbf{A} \times \mathbf{B}}{8\pi} \right] = \frac{\mathbf{B} \cdot \mathbf{B}}{8\pi} - \frac{1}{2c} \mathbf{j}_T \cdot \mathbf{A}$$

where

$$\mathbf{B} = \nabla \times \mathbf{A}$$

along with the previous alternate form for electrostatics to obtain:

$$\nabla \cdot \mathbf{S}' + \frac{\partial}{\partial t} \left[\frac{1}{2} \rho \phi + \frac{1}{2c} \mathbf{j}_T \cdot \mathbf{A} \right] = -\mathbf{j} \cdot (\mathbf{E}_L + \mathbf{E}_T)$$

where the alternative energy flux vector is:

$$\mathbf{S}' = \mathbf{S} + \frac{1}{8\pi} \frac{\partial}{\partial t} [\phi \nabla \phi + \mathbf{A} \times \mathbf{B}]$$

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

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

where

$$\hat{\mathbf{T}} = \frac{1}{4\pi} \left[\mathbf{E}\mathbf{E} + \mathbf{B}\mathbf{B} - \frac{1}{2}(\mathbf{E} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{B}) \hat{\mathbf{I}} \right]$$

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

In the electrostatic case, there is no momentum in the longitudinal field and the magnetic field vanishes, so the momentum flux equation reduces to:

$$\nabla \cdot \hat{\mathbf{T}} = \rho \mathbf{E}$$

where

$$\hat{\mathbf{T}} = \frac{1}{4\pi} \left[\mathbf{E}\mathbf{E} - \frac{1}{2}(\mathbf{E} \cdot \mathbf{E}) \hat{\mathbf{I}} \right]$$

In the Darwin case, the momentum flux equation is formally the same as in the electromagnetic case:

$$\nabla \cdot \hat{\mathbf{T}} - \frac{1}{c^2} \frac{\partial \mathbf{S}}{\partial t} = \rho(\mathbf{E}_L + \mathbf{E}_T) + \mathbf{j} \times \mathbf{B}/c$$

But the field momentum vector is:

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

and the stress tensor is:

$$\hat{\mathbf{T}} = \frac{1}{4\pi} \left[\mathbf{E}_L \mathbf{E}_L + \mathbf{E}_L \mathbf{E}_T + \mathbf{E}_T \mathbf{E}_L + \mathbf{B}\mathbf{B} - \frac{1}{2}(\mathbf{E}_L \cdot \mathbf{E}_L + 2\mathbf{E}_L \cdot \mathbf{E}_T + \mathbf{B} \cdot \mathbf{B}) \hat{\mathbf{I}} \right]$$

Note that the Darwin model does have momentum in the electromagnetic field, even though there is no radiation. The transverse electric field \mathbf{E}_T does not contribute to this momentum, just as it does not contribute to the Darwin field energy. Note also that, unlike the electromagnetic case, the “Poynting” vector for energy is not the same as the “Poynting” vector for momentum.

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

VII. 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:

$$\widetilde{x} = x/\delta \quad \widetilde{t} = \omega_0 t \quad \widetilde{\mathbf{v}} = \mathbf{v}/\delta\omega_0 \quad \widetilde{q} = q/e \quad \widetilde{m}_e = m/m_e$$

Dimensionless charge and current densities are given by:

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

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

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

Dimensionless energy is given by:

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

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

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

The dimensionless particle equations of motion are:

$$\widetilde{m}_i \frac{d\widetilde{\mathbf{v}}_i}{d\widetilde{t}} = \widetilde{q}_i [\widetilde{\mathbf{E}} + \widetilde{\mathbf{v}}_i \times \widetilde{\mathbf{B}}] \quad \frac{d\widetilde{\mathbf{x}}_i}{d\widetilde{t}} = \widetilde{\mathbf{v}}_i$$

The dimensionless Maxwell's equations are:

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

$$\widetilde{\nabla} \cdot \widetilde{\mathbf{E}} = A_f \widetilde{\rho}$$

The dimensionless energy flux equation is:

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

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

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

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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