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

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I. Introduction

This document presents the mathematical foundation of the periodic Particle-in-Cell Darwin code in the UCLA Particle-in-Cell Framework. The Darwin code 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. 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:

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

whereas the Darwin subset has:

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

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:

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

$$\frac{\partial \boldsymbol{j}(\boldsymbol{x})}{\partial t} = \sum_i q_i \left[\frac{d\boldsymbol{v}_i}{dt} S(\boldsymbol{x} - \boldsymbol{x}_i) - \boldsymbol{v}_i \nabla \cdot \boldsymbol{v}_i S(\boldsymbol{x} - \boldsymbol{x}_i) \right]$$

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

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

and then differentiate:

$$\frac{\partial \boldsymbol{j}(x)}{\partial t} = \boldsymbol{a} - \nabla \bullet \overleftrightarrow{\mathbf{M}}$$

2. Solve Maxwell's equation:

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

$$\nabla \times \boldsymbol{E}_L = 0 \qquad \nabla \bullet \boldsymbol{E}_T = 0$$

$$\nabla \times \boldsymbol{B} = \frac{4\pi}{c}\boldsymbol{j}_T = \frac{4\pi}{c}\boldsymbol{j} + \frac{1}{c}\frac{\partial \boldsymbol{E}_L}{\partial t} \qquad \nabla^2 \boldsymbol{E}_T = \frac{1}{c}\nabla \times \frac{\partial \boldsymbol{B}}{\partial t} = \frac{4\pi}{c^2}\frac{\partial \boldsymbol{j}_T}{\partial t}$$

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

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

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

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

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

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

$$\frac{\partial \boldsymbol{j}(\boldsymbol{k})}{\partial t} = \sum_i q_i \left[\frac{d\boldsymbol{v}_i}{dt} - i(\boldsymbol{k}\bullet\boldsymbol{v}_i)\boldsymbol{v}_i\right] S(\boldsymbol{k})\, e^{-i\boldsymbol{k}\bullet\boldsymbol{x}_i}$$

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

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

$$\frac{\partial \boldsymbol{j}_T(\boldsymbol{k})}{\partial t} = \frac{\partial \boldsymbol{j}(\boldsymbol{k})}{\partial t} - \frac{\boldsymbol{k}}{k^2}\left(\boldsymbol{k}\bullet\frac{\partial \boldsymbol{j}(\boldsymbol{k})}{\partial t}\right) \qquad \boldsymbol{E}_T(\boldsymbol{k}) = -\frac{4\pi}{k^2c^2}\frac{\partial \boldsymbol{j}_T(\boldsymbol{k})}{\partial t}$$

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

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

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 $\mathbf{E}_T$:

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

is unstable when

$$kc < \omega_{pe}$$

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

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

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:

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

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. Because of the leapfrog scheme, the positions are already known at time t, but the velocities are retarded by half a time step.

The time-centered velocities and derivatives are obtained by updating the particle velocities from the particle equations of motion and taking the averages and differences:

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

One does not actually update the new velocities in memory. Instead, one deposits the current and the current derivative. The iteration starts by first calculating $\mathbf{E}_L(t)$ from $\mathbf{x}(t)$, $\mathbf{B}$ from $\mathbf{x}(t)$ and $\mathbf{v}(t-dt/2)$ and using the previous value $\mathbf{E}_T(t-dt)$. Then advance the 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 in memory. Finally, solve for improved $\mathbf{E}_T(t)$ and $\mathbf{B}(t)$. Repeat as needed.

This iteration scheme works well and converges in about 1 or 2 iterations so long as the plasma density does not vary too much, specifically if

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

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:

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

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

The discrete equations of motion for the particles are the same as for the electromagnetic code:

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

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

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:

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

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 Darwin code is analogous to its use in the electrostatic and electromagnetic codes.

III. Energy and Momentum Flux

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

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

where

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

This can be verified by taking the divergence of **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,

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

where

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

along with the electrostatic result,

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

where

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

to obtain:

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

where the alternative energy flux vector is:

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

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

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

But the field momentum vector is:

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

and the stress tensor is:

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

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.

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:

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

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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