Inspiration from ISSS9: Gentle introduction to PIC

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Introducing the ISSS9

http://www.isss9.uvsq.fr/

Introducing the ISSS9

ISSS in general

• Series of international summer schools, lectures given by renowned experts in the field
• History since 1982 (ISSS1 in Kyoto)
• Held each 2-3 years
• The next one preliminary scheduled for 2011 in Canada
• Relativelly easy to get support!!!

ISSS9 summary

• Four days of intensive learning (theoretical morning course, practical 'hands-on' afternoon) sessions
• Four days of regular workshop: talks oriented to applications of space plasma simulations to real problems; ussually tutorial approach.
• About 80 students, 20 teachers and assistants from various countries

Tutorials:

• Particle in cell (PIC) simulations
• Delta-F simulations
• Vlasov simulations
• Test particles simulations
• Hybrid simulations
• Magnetohydrodynamic (MHD) simulations

All lecture notes and sample codes you can get at

http://www.isss9.uvsq.fr/

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

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Particle-in-Cell Codes

PIC codes integrate the trajectories of many particles interacting self-consistently via electromagnetic fields. PIC codes are possible whenever there is some differential equation which describes fields in terms of particle sources.

PIC codes are used in almost all areas of plasma physics, such as fusion energy research, plasma accelerators, space physics, ion propulsion, plasma processing, and many other areas.

What distinguishes PIC codes from molecular dynamics that a grid is used as a scaffolding to calculate fields rather than direct binary interactions => reduces calculation to order N rather than N^2.

Particle-in-Cell Codes

PIC codes differ in what kind of forces are included in the plasma description. We will include 3 here, but others are possible.

We will concentrate on Spectral codes, although finite-difference, and finite-element methods are also used.

The topics to be covered are:
- Electrostatic Plasma Model
- Electromagnetic Plasma Model
- Darwin Plasma Model
- Radiative and Darwin Electromagnetic Fields
- Energy and Momentum Flux

Electrostatic Codes

Simplest plasma model is electrostatic:

1. Calculate charge density on a mesh from particles:

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

2. Solve Poisson's equation:

$$\nabla \bullet \boldsymbol{E} = 4\pi\rho$$

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

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

Note:

- S(x) is a particle shape function, for example a delta function

Electrostatic Codes

Periodic analytic solution (gridless):

1. Fourier transform the charge density:

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

2. Solve Poisson's equation in Fourier space:

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

3. Fourier transform Smoothed Electric Field to real space:

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

Notes:

- For delta functions, S(k) = 1/V
- Periodic systems are charge neutral
- Gridless solutions are very accurate, but slow

Electrostatic Codes

Time-Difference equations of motion: second order leap-frog scheme

$$\frac{d\boldsymbol{v}_i}{dt} = \frac{q_i}{m_i}\boldsymbol{E}_s \approx \frac{\boldsymbol{v}_i(t+\Delta t/2) - \boldsymbol{v}_i(t-\Delta t/2)}{\Delta t} = \frac{q_i}{m_i}\boldsymbol{E}_s(t)$$

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i \approx \frac{\boldsymbol{x}_i(t+\Delta t) - \boldsymbol{x}_i(t)}{\Delta t} = \boldsymbol{v}_i(t+\Delta t/2)$$

Solution is explicit time advance:

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

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

Note:

- Time step should resolve plasma frequency

Electrostatic Codes

Define grid:

$$\Delta_x = L_x / N_x \qquad \Delta_z = L_z / N_z \qquad \Delta_z = L_z / N_z$$

Deposit charge on discrete grid:

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

where we define:

$$\boldsymbol{r} = (n\Delta_x, m\Delta_y, l\Delta_z) \qquad \boldsymbol{s}' = (n', m', l') \qquad \delta_{\boldsymbol{r},\boldsymbol{s}'} = \delta_{n,n'}\delta_{m,m'}\delta_{l,l'}$$

analogous to gridless case:

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

Interpolation function W(x) should be smooth with limited support

- B-splines typically used

Tri-Linear interpolation most common: $W(r)=W_x(x)*W_y(y)*W_z(z)$

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

Electrostatic Codes

Discrete Fourier Transform (DFT) of charge density:

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

where discrete wavenumbers are defined:

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

analogous to gridless case:

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

Electrostatic Codes

Major complication of grid is non-physical forces (aliasing). Arises when particle co-ordinates have spatial variations less than grid space: they get mapped to longer wavelengths.

Express interpolation as infinite Fourier series:

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

this leads to:

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

The sum is geometric series:

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

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

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

Electrostatic Codes

One can express the Fourier transform of grid density:

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

Compare to gridless result:

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

One can see W(k′) acts like a particle shape function. Terms involving $\mathbf{k}_\mathrm{N}$ are non-physical aliased terms.

Solution of electric field is same as gridless case, except for use of DFT:

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

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

Electrostatic Codes

Obtaining electric field at particle location involves interpolation:

$$\boldsymbol{E}_S(\boldsymbol{x}_i) = \sum_{\boldsymbol{r}} \boldsymbol{E}(r) W(\boldsymbol{x}_i - \boldsymbol{r}) \Delta \qquad \Delta = \Delta_x \Delta_y \Delta_z$$

Proceeding as before:

$$\boldsymbol{E}_S(\boldsymbol{x}_i) = V \sum_{\boldsymbol{k}'} \boldsymbol{E}(\boldsymbol{k}') \Big[W(\boldsymbol{k}') + \sum_{k_N \neq 0} W(\boldsymbol{k}' + \boldsymbol{k}_N) e^{i\boldsymbol{k}_N \cdot \boldsymbol{x}_i} \Big] e^{i\boldsymbol{k}' \cdot \boldsymbol{x}_i}$$

This is analogous to the gridless case:

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

Note:

- Forces now depend not only on separation of particles, but also on separation of particle from grid
- Non-conservative forces usually leads to self-heating

Electrostatic Codes

Aliasing is controlled by behavior of Fourier transform of interpolation function for **k** > **k**$_N$. Fourier transform of B-splines:

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

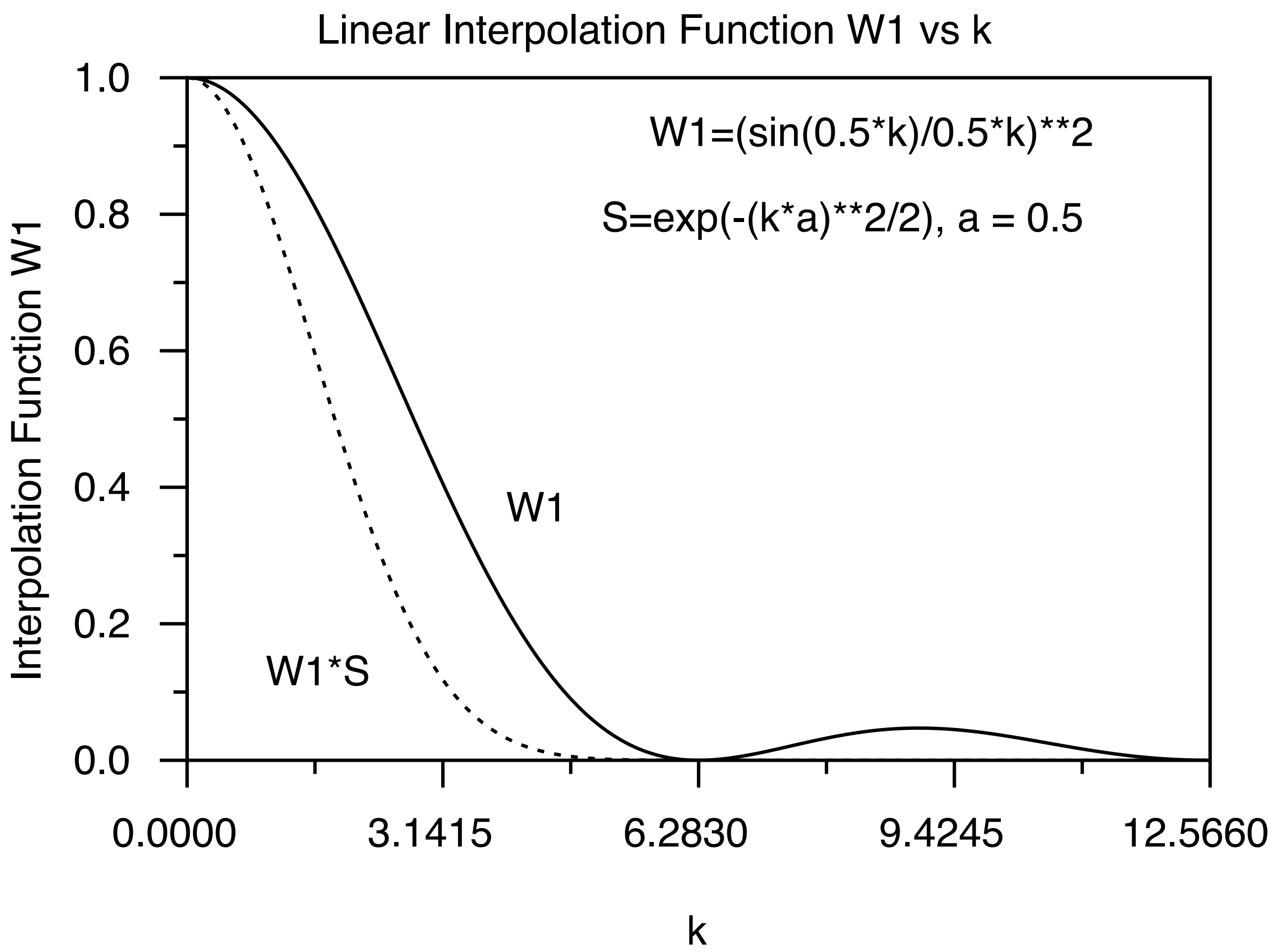
These functions have maximum near **k** = (p+1/2) **k**$_N$, for p > 1. Worst alias occurs for p =1, which maps densities at **k** = 3 **k**$_N$/2 to **k** = **k**$_N$/2.

A simple improvement is to use a particle shape (filter) function S(**k**) along with the interpolation function. If S(**k**) is small in the vicinity of **k** = **k**$_N$/2, one can suppress the largest aliased terms. One is also suppressing physical modes, so this limits the resolution of model.

A common filter function is:

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

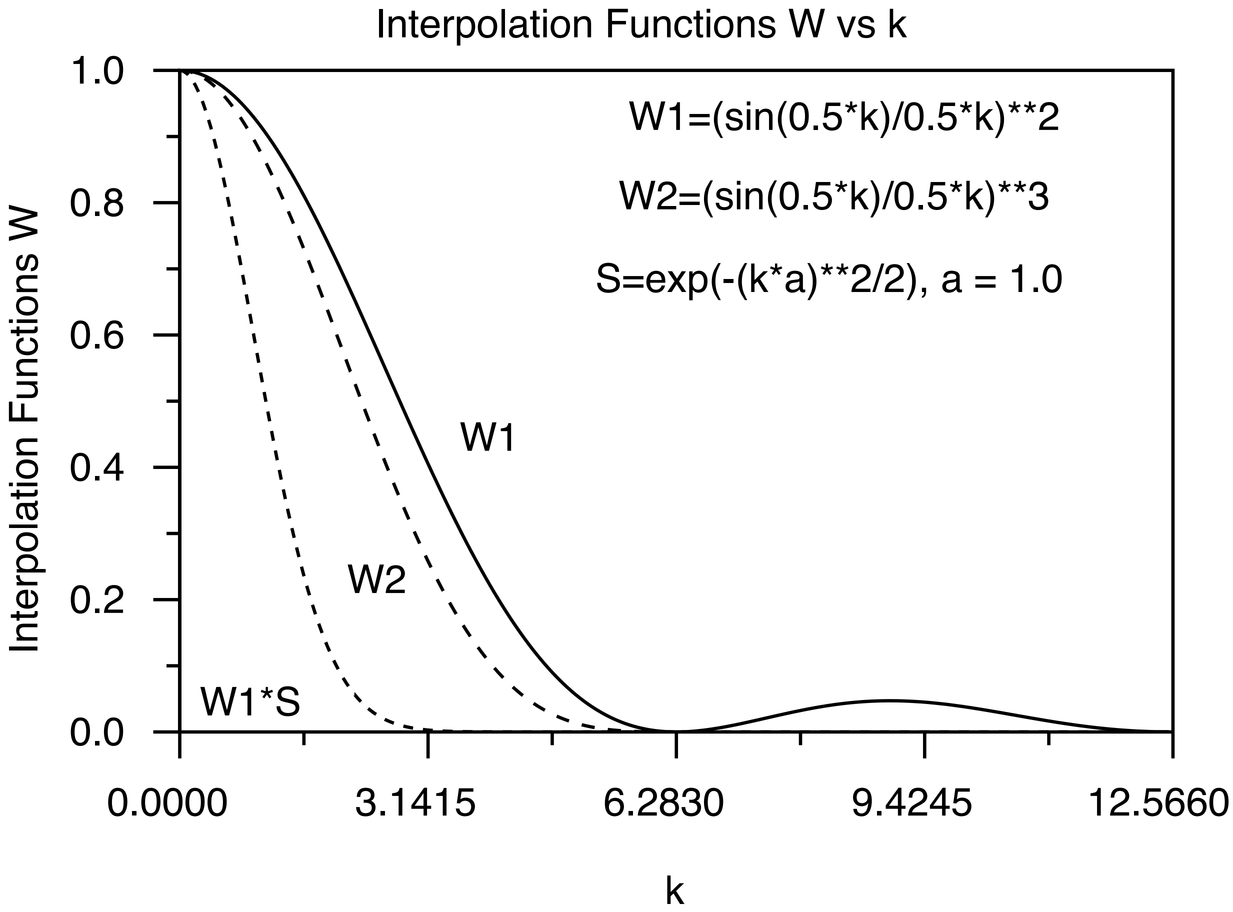
Electrostatic Codes



Fourier transform of first order interpolation function W1 with and without gaussian smoothing with a = 0.5.

- Modes with $k>2\pi$ mapped to modes with $k < 2\pi$.

Electrostatic Codes



Fourier transform of first and second order interpolation functions W1 and W2, and W1 with gaussian smoothing with a = 1.0.

Electrostatic Codes

If filter is used to suppress aliasing, the effective particle shape is:

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

In real space this corresponds to a convolution of the interpolation function with the filter function, which makes particles "fatter".

Even when aliasing is suppressed, grid effects are still present. To see this, replace q_i with $q_i S_{eff}(\mathbf{k})$ in plasma theory, which modifies the plasma frequency:

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

For linear interpolation, isotropic grid, and gaussian smoothing:

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

This may or may not be important. For plasma waves:

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

Electromagnetic Codes

More complex plasma model is electromagnetic:

1. Calculate charge and current densities on a mesh from 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 equation of continuity is satisfied by this definition:

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

2. Solve Maxwell's equation:

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

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

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

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

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$$

Electromagnetic Codes

Periodic analytic solution (gridless):

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 is satisfied in Fourier space:

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

Electromagnetic Codes

Periodic analytic solution (gridless):

2. Solve Maxwell's equation in Fourier space:

Separate **E** field into longitudinal and transverse parts, where $\mathbf{k} \times \mathbf{E}_L = 0$ and $\mathbf{k} \bullet \mathbf{E}_T = 0$. Eliminate longitudinal field in Ampere's law with equation of continuity:

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

This results in the following equations:

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

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

Note:

- Periodic systems are current neutral

Electromagnetic Codes

Periodic analytic solution (gridless):

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

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

$$\boldsymbol{B}_S(\boldsymbol{x}_j) = V \sum_{\boldsymbol{k}=-\infty}^{\infty} \boldsymbol{B}(\boldsymbol{k}) S(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{x}_j}$$

Electromagnetic Codes

Time-Difference field equations:
first advance magnetic field a half step with old **E** field:

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

then leap-frog electric field a whole step with new **B** field:

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

Finally, advance magnetic field a half step with new **E** field:

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

Note:

- Time step should resolve light waves: $c\Delta t \lesssim \Delta$

Electromagnetic Codes

Discrete equations of motion for particles are:

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

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

Solution is the Boris Mover:

first accelerate a half step with **E** field only:

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

Then rotate a whole step with **B** field only:

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

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

Finally, accelerate a half step again with **E** field only:

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

Darwin Codes

Most complex plasma model is Darwin:
Electromagnetic Ampere's law:

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

Darwin Ampere's law:

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

This small difference changes the character of the equations from hyperbolic to elliptic: No light waves.

Darwin Codes

1. Calculate charge, current, and derivative of current densities:

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

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

Actually, we deposit acceleration density and velocity flux:

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

Then differentiate:

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

Darwin Codes

2. Solve Darwin subset of Maxwell's equation

Separate **E** field into longitudinal and transverse parts, $\mathbf{E} = \mathbf{E}_L + \mathbf{E}_T$:

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

And solve them separately:

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

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

3. Advance particle's co-ordinates using Lorentz force

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

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$$

Darwin Codes

Periodic analytic solution (gridless):

1. Fourier transform charge, current and current derivative:

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

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

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

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

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

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

Darwin Codes

Periodic analytic solution (gridless):

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

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

$$\boldsymbol{B}_S(\boldsymbol{x}_j) = V \sum_{\boldsymbol{k}=-\infty}^{\infty} \boldsymbol{B}(\boldsymbol{k}) S(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{x}_j}$$

Darwin Codes

Time-Difference field equations require iteration: no leap-frog

$\mathbf{E}_\mathrm{T}$ depends on $d\mathbf{v}_j/dt$ and $d\mathbf{v}_j/dt$ depends on $\mathbf{E}_\mathrm{T}$!

Simple iteration using old values of $d\mathbf{v}_j/dt$ to update $\mathbf{E}_\mathrm{T}$:

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

is unstable when $kc < \omega_{pe}$.

To stabilize the iteration, subtract a shift constant from both sides:

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

where the shift constant is the average plasma frequency:

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

The solution is:

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

Darwin Codes

To obtain second order accuracy need to know velocities and accelerations at time t. This is obtained from leap-frog as follows:

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

Iteration starts by calculating $\mathbf{E}_L(t)$ from $\mathbf{x}(t)$
setting $\boldsymbol{v}_j(t+\Delta t/2) = \boldsymbol{v}_j(t-\Delta t/2)$
and solving for initial $\mathbf{E}_T(t)$ and $\mathbf{B}(t)$

Iteration has two parts:
Advance particles, calculate $d\mathbf{v}_j(t)/dt$ and $\mathbf{v}_j(t)$, deposit $d\mathbf{j}/dt$ and $\mathbf{j}$
Do not update particles
Solve for improved $\mathbf{E}_T(t)$ and $\mathbf{B}(t)$

When converged, use Boris Mover to update particles

Darwin Codes

Iteration converges in about 2 iterations if density does not vary too much, specifically if $\max(\omega_p^2(\boldsymbol{x})) < 1.5\omega_{p0}^2$

Beyond that, number of iterations 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 becomes more extreme, the number of iterations again increases, but appears to remain stable.

Radiative and Darwin Fields

Transverse parts of Maxwell's equation are:

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

where $\mathbf{E} = \mathbf{E}_{\mathrm{L}} + \mathbf{E}_{\mathrm{T}}$.

Transverse parts of Darwin subset are:

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

Separate transverse Maxwell fields into two parts,

$\mathbf{E}_{\mathrm{T}} = \mathbf{E}_{\mathrm{D}} + \mathbf{E}_{\mathrm{R}}$, $\mathbf{B} = \mathbf{B}_{\mathrm{D}} + \mathbf{B}_{\mathrm{R}}$.

Subtracting the Darwin equations from Maxwell's equations gives the equations for radiative parts:

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

The Darwin fields are driven by plasma current, the Radiative fields are driven by displacement current.

Radiative and Darwin Fields

Similar expressions can be derived for the vector potential in the Coulomb gauge:

$$\nabla^2 \boldsymbol{A}_D = -\frac{4\pi}{c}\boldsymbol{j}_\perp \qquad \nabla^2 \boldsymbol{A}_R = \frac{4\pi}{c}\boldsymbol{j}_\perp - \nabla \times \boldsymbol{B}$$

where $\mathbf{A} = \mathbf{A}_D + \mathbf{A}_R$. The Radiative and Darwin field then follow:

$$\boldsymbol{B}_D = \nabla \times \boldsymbol{A}_D \qquad \boldsymbol{B}_R = \nabla \times \boldsymbol{A}_R$$

$$\boldsymbol{E}_D = -\frac{1}{c}\frac{\partial \boldsymbol{A}_D}{\partial t} \qquad \boldsymbol{E}_R = -\frac{1}{c}\frac{\partial \boldsymbol{A}_R}{\partial t}$$

These decompositions are useful as filters for diagnostics, illuminating physical processes in plasmas.

Energy and Momentum Flux

For the electromagnetic model, energy flux equation is well known:

$$\nabla \cdot \boldsymbol{S} + \frac{\partial}{\partial t}\left[\frac{\boldsymbol{E} \cdot \boldsymbol{E}}{8\pi} + \frac{\boldsymbol{B} \cdot \boldsymbol{B}}{8\pi}\right] = -\boldsymbol{j} \cdot \boldsymbol{E} \qquad \boldsymbol{S} = \frac{c}{4\pi}\boldsymbol{E} \times \boldsymbol{B}$$

where **S** is the Poynting vector. This equation is not unique.

Less well known is the energy flux equation for the electrostatic model:

$$\nabla \cdot \boldsymbol{S} + \frac{\partial}{\partial t}\left[\frac{\boldsymbol{E}_L \cdot \boldsymbol{E}_L}{8\pi}\right] = -\boldsymbol{j} \cdot \boldsymbol{E}_L \qquad \boldsymbol{S} = \left[\boldsymbol{j} - \frac{1}{4\pi}\nabla\frac{\partial \phi}{\partial t}\right]\phi$$

For the Darwin model the energy flux equation is:

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

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

An important point to notice is the the transverse electric field $\mathbf{E}_T$ does not enter into the definition of the field energy.

Energy and Momentum Flux

For the electromagnetic model, the momentum flux equation is also useful:

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

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

where **T** is the Maxwell stress tensor, and $\mathbf{S}/c^2$ is the momentum of the electromagnetic field. This equation is also not unique.

In the electrostatic model there is no field momentum and the equation reduces to:

$$\nabla \cdot \overleftrightarrow{\mathrm{T}} = \rho \boldsymbol{E} \qquad \overleftrightarrow{\mathrm{T}} = \frac{1}{4\pi}\left[\boldsymbol{E}\boldsymbol{E} - \frac{1}{2}(\boldsymbol{E} \bullet \boldsymbol{E})\,\overleftrightarrow{\mathrm{I}}\right]$$

Energy and Momentum Flux

For the Darwin model, the momentum flux equation is also formerly the same as 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 different:

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

and **T** is the Maxwell stress tensor is also different:

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

Notes:

- There is momentum in Darwin field, but no radiation.
- E_T does not contribute to the field momentum.
- The Poynting vector for momentum differs from the one for energy