Description of Darwin Spectral Particle-in-Cell Code

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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.

Possible forces:

- Electrostatic (Coulomb)
- Electromagnetic (most complete)
- Darwin (radiationless or near field electromagnetics)
- Collisions (various kinds)

Darwin model neglects retardation effects

- Contains electric and magnetic fields induced by plasma currents
- Neglects electric and magnetic fields induced by displacement current
- We once popular in the 1970's, but were largely abandoned

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

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:

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

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:

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

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

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

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

And solve them separately:

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

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

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:

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

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

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

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

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

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

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.

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:

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

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

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:

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

Energy and Momentum Flux

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

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

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:

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

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

EM Plasma Waves in Magnetized Plasma

- S. Ichimaru gives a theory for waves propagating perpendicularly to the B field

- **In this theory the electrostatic and the electromagnetic components are coupled**

$$\beta = \frac{k^2 v_{th}^2}{\Omega_c^2} \qquad \Lambda_n(\beta) = I_n(\beta) e^{-\beta}$$

$$\epsilon_1(k,\omega) = 1 - \frac{k_D^2}{k^2} \sum_n \frac{(n\Omega_c)^2}{\omega\,(\omega - n\Omega_c)} \Lambda_n(\beta)$$

$$\epsilon_2(k,\omega) = 1 - \frac{k_D^2}{k^2} \sum_n \frac{(n\Omega_c)^2}{\omega(\omega - n\Omega_c)} \left[\Lambda_n(\beta) - \frac{2\beta^2}{n^2}\Lambda_n'(\beta)\right]$$

$$\epsilon_3(k,\omega) = 1 - \frac{\omega_p^2}{\omega^2} \sum_n \frac{\omega}{\omega - n\Omega_c} \Lambda_n(\beta)$$

$$\epsilon_x(k,\omega) = \frac{\omega_p^2}{\omega^2} \sum_n \frac{\omega}{\omega - n\Omega_c} n\Lambda'(\beta)$$

Extraordinary:

$$\left(\frac{kc}{\omega}\right)^2 = \frac{\epsilon_1\epsilon_2 - \epsilon_x^2}{\epsilon_1}$$

Ordinary:

$$\left(\frac{kc}{\omega}\right)^2 = \epsilon_3$$

Darwin Version of Theory

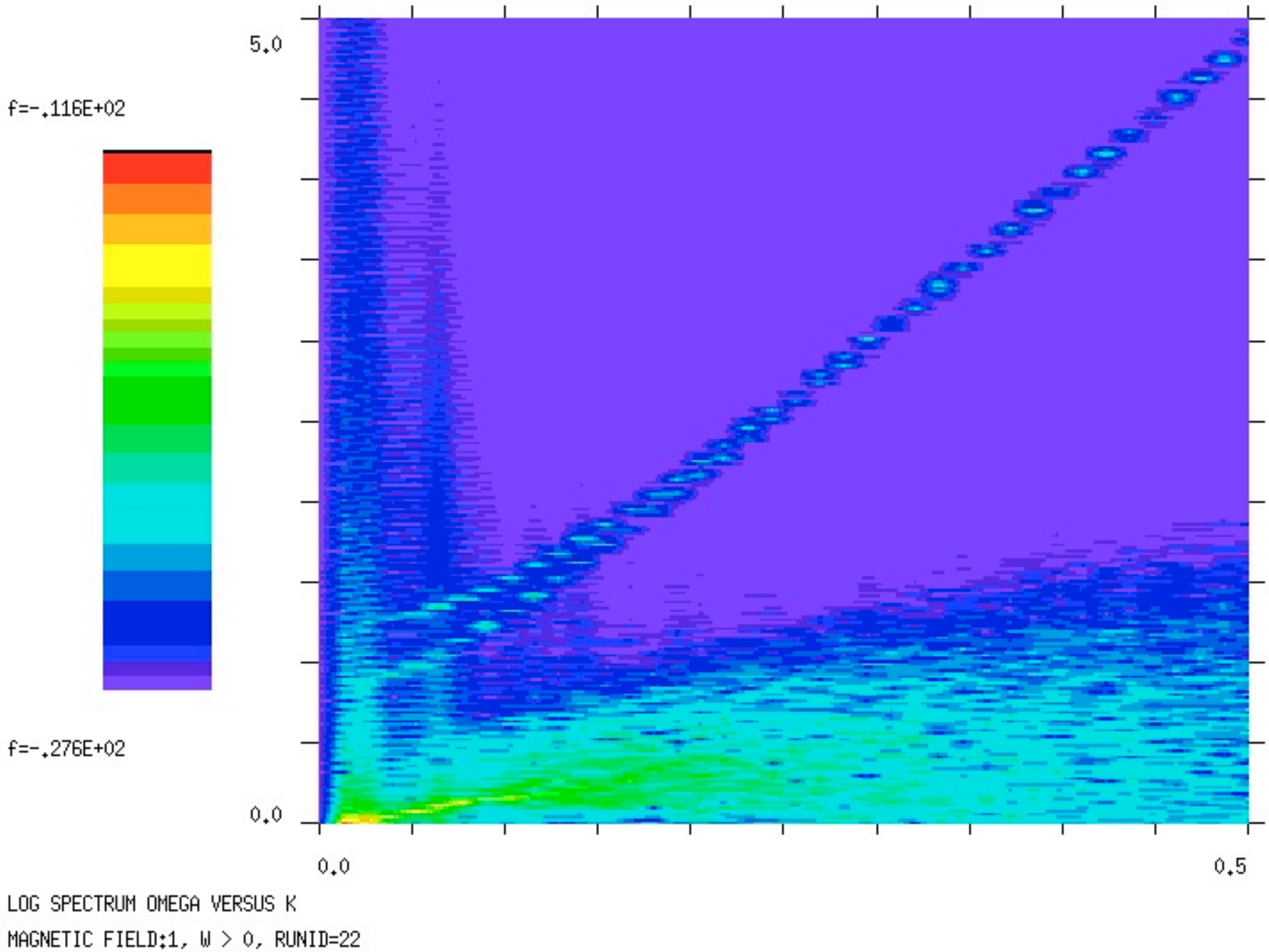
- The dispersion relation derived from the Darwin equations is similar
- The difference is that in Darwin the 1 is removed from ϵ_2 and ϵ_3

$$\epsilon_2(k,\omega) = -\frac{k_D^2}{k^2}\sum_n \frac{(n\Omega_c)^2}{\omega(\omega - n\Omega_c)}\left[\Lambda_n(\beta) - \frac{2\beta^2}{n^2}\Lambda_n'(\beta)\right]$$

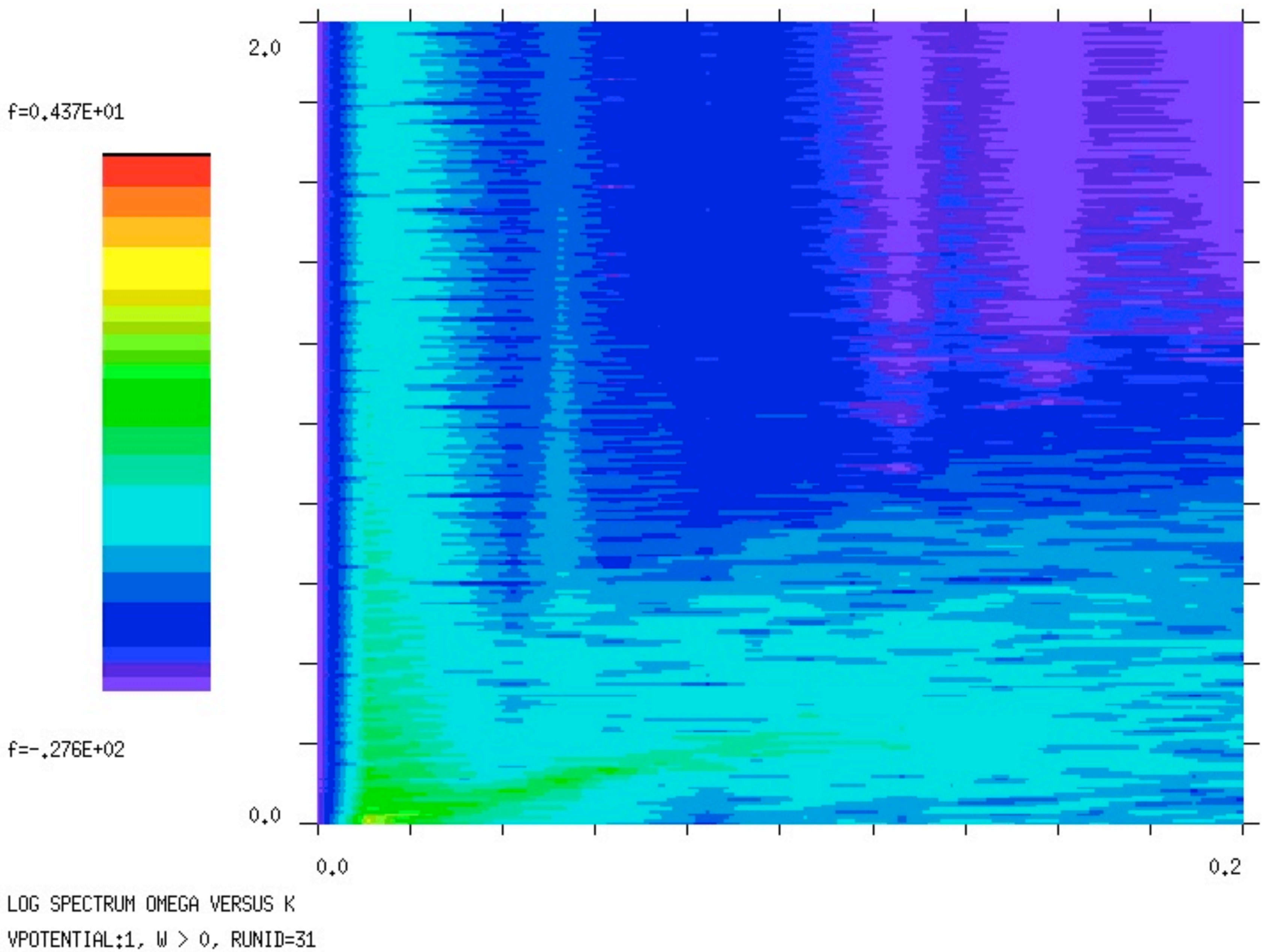
$$\epsilon_3(k,\omega) = -\frac{\omega_p^2}{\omega^2}\sum_n \frac{\omega}{\omega - n\Omega_c}\Lambda_n(\beta)$$

This modifies the extraordinary wave solutions, and removes the ordinary wave solutions

Let's look at waves in magnetized plasma, set OMX = 0.4 by copying input1.LR to input1, and executing ./new_bbeps1. To see LR waves and whistler waves, execute: ./vspectrum1



To see Whistler Waves Parallel to $\mathbf{B}_0$, $\Omega_{ce}/\omega_{pe} = 0.4$, c = 10:
copy input1.whistler, and execute: ./new_dbeps1
then ./vspectrum1



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