Darwin Particle-in-Cell Models

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Abstract:

Electrostatic and electromagnetic PIC codes are very common. Less common is the Darwin model, which neglects the transverse displacement current in Ampere's Law. This model includes magnetic induction and Faraday's Law, but omits light waves. For many plasma problems, light waves are not important, but they impose a serious Courant condition on the time integration. If $v/c \ll 1$, the Darwin model allows one to take much bigger time steps than is possible in electromagnetic codes, and thus use more realistic values of v/c. Unfortunately, Darwin models can be numerically difficult to implement. In this tutorial, I will discuss some interesting properties of the Darwin model and how to overcome some of the numerical difficulties in building a useful code.

Darwin model: What is it?

Radiationless, or near-field electromagnetics

Neglects retardation effects

Can be derived by expansion in 1/c of Maxwell's equations:

order 1: $$\nabla \cdot E_L = 4\pi\rho$$

order $\frac{1}{c}$: $$\nabla \times B = \frac{4\pi}{c} j + \frac{1}{c}\frac{\partial E_L}{\partial t} = \frac{4\pi}{c} j_\perp$$

order $\frac{1}{c^2}$: $$\nabla \times E_\perp = -\frac{1}{c}\frac{\partial B}{\partial t} \qquad \nabla \cdot E_\perp = 0$$

Useful equation: $$\nabla^2 E_\perp = \frac{4\pi}{c^2}\frac{\partial j_\perp}{\partial t}$$

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Darwin model: Why is it useful?

Includes Ampere's and Faraday's Laws, but excludes light waves

For many plasma problems, light waves are not important, yet they impose a serious Courant condition on the time step

If $v/c \ll 1$, much larger time steps can be used in Darwin

UPIC Framework supports multiple models (Electrostatic, Darwin, Electromagnetic) to allow one to control and understand the significance of different physical processes and approximations

Darwin model: Properties

Energy Flux Equation:

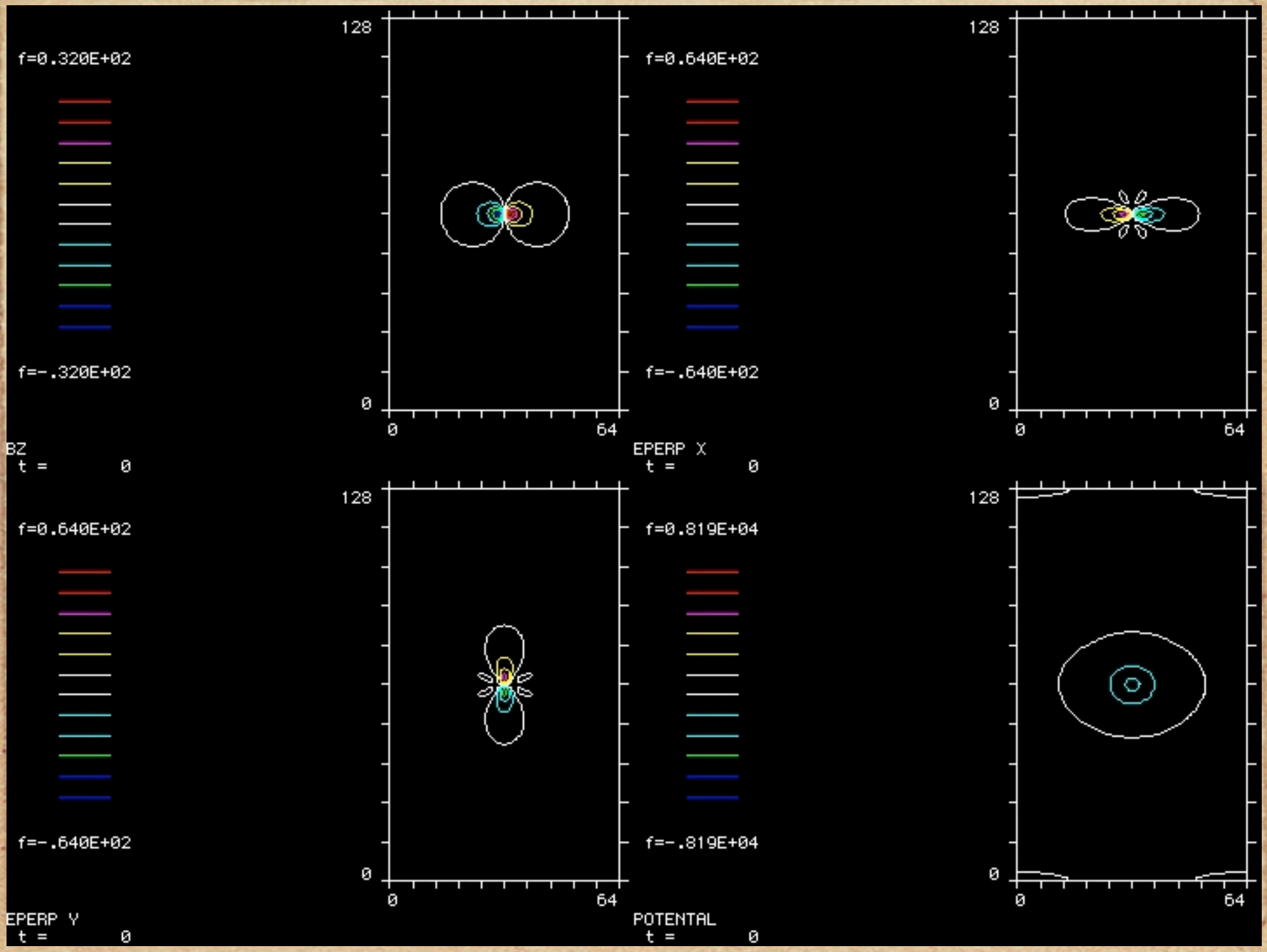
$$\frac{\partial}{\partial t}\left[\frac{E_L \cdot E_L}{8\pi} + \frac{B \cdot B}{8\pi}\right] + \nabla \cdot S = -j \bullet \left[E_L + E_\perp\right]$$

Momentum Flux Equation:

$$\frac{1}{4\pi c}\frac{\partial}{\partial t}\left[E_L \times B\right] + \rho\left(E_L + E_\perp\right) + j \times B / c = \nabla \cdot \overleftrightarrow{T}$$

Note Darwin field has momentum, and that E⊥ does not appear in the definition of energy or momentum

These flux equations are not unique, other forms are possible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BZ
t = 0
128
0
0
64
f=0.640E+02
f=-.640E+02
EPERP X
t = 0
128
0
0
64
f=0.640E+02
f=-.640E+02
EPERP Y
t = 0
128
0
0
64
f=0.819E+04
f=-.819E+04
POTENTIAL
t = 0
128
0
0
64

Darwin model: Analytic solution

For periodic systems, one can solve these equations exactly by Fourier transforming the sources

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

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

This leads to the solutions:

$$\vec{E}_L(\vec{x}_j) = 4\pi \sum_k \left[\frac{-i\vec{k}}{k^2}\right] \rho(\vec{k})\, e^{i\vec{k}\cdot\vec{x}_j} \qquad => \qquad \sum_j q_j \vec{E}_L(\vec{x}_j) = 0$$

$$\vec{B}(\vec{x}_j) = \frac{4\pi}{c}\sum_k \left[\frac{-i\vec{k}\times\vec{j}(\vec{k})}{k^2}\right] e^{i\vec{k}\cdot\vec{x}_j} \qquad => \qquad \sum_j q_j \vec{v}_j \times \vec{B}(\vec{x}_j) \neq 0$$

Darwin model: Analytic solution

To solve for E⊥ one needs the sources:

$$\frac{\partial \vec{j}(\vec{k})}{\partial t} = \frac{1}{V}\sum_i q_i\left[\frac{d\vec{v}_i}{dt} - i(\vec{k}\cdot\vec{v}_i)\vec{v}_i\right]S(k)e^{-i\vec{k}\cdot\vec{x}_i}$$

$$\vec{j}_\perp = \vec{j} + \frac{1}{4\pi}\frac{\partial \vec{E}_L}{\partial t} = \vec{j} - \left(\frac{i\vec{k}}{k^2}\right)\frac{\partial \rho}{\partial t} = \vec{j} - \frac{\vec{k}(\vec{k}\cdot\vec{j})}{k^2}$$

$$\frac{\partial \vec{j}_\perp}{\partial t} = \frac{\partial \vec{j}}{\partial t} - \frac{\vec{k}}{k^2}(\vec{k}\cdot\frac{\partial \vec{j}}{\partial t})$$

which leads to the solution:

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

Darwin model: Properties

One can show that self-forces for E_L and $v \times B$ are zero, but not for $E_\perp$. Consider an isolated particle. One can show that:

$$E_{\perp y}(\vec{x}_j) = -\frac{q_j}{c^2}\frac{dv_{jy}}{dt}k_{y0} \qquad \text{where} \qquad k_{y0} \equiv \frac{4\pi}{V}\sum_k \frac{1}{k^2}\left[1-\frac{k_y{}^2}{k^2}\right]S(k)$$

Consider gravity in the y direction. The equation of motion is:

$$\frac{dv_{jy}}{dt} = q_j E_{\perp y}(\vec{x}_j) + m_j g \qquad \text{whose solution is:} \qquad \frac{dv_{jy}}{dt} = \frac{g}{1+\frac{q_j{}^2}{m_j c^2}k_{y0}}$$

Charged particles accelerate with less than g!

Darwin model: Properties

To understand this, first we write the solution for the vector potential:

$$\nabla^2 \vec{A} = -\frac{4\pi}{c}\vec{j}_\perp \quad => \quad \vec{A}(\vec{x}_j) = \frac{4\pi}{c}\sum_k \left[\frac{\vec{j}_\perp(\vec{k})}{k^2}\right] e^{i\vec{k}\cdot\vec{x}j}$$

For an isolated particle, this becomes:

$$A_y(\vec{x}_j) = \frac{q_j v_{jy}}{c} k_{y0} \quad => \quad \frac{q_j}{c}\frac{dA_y(\vec{x}_j)}{dt} = \frac{q_j^2}{c^2}\frac{dv_{jy}}{dt} k_{y0} = -q_j E_{\perp y}(\vec{x}_j)$$

The equation of motion can then be written:

$$\frac{d}{dt}\left[m_j v_{jy} + \frac{q_j}{c} A_y(\vec{x}_j)\right] = m_j g$$

The term on the left is the canonical momentum. Thus a charged particle accelerates at less than g, because it is the total momentum that accelerates at g.

Darwin model: Properties

What is the physical meaning of $\frac{q_j}{c}\vec{A}(\vec{x}_j)$?

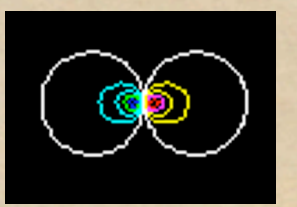
Recall that the Darwin field has momentum given by:

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

After a bit of algebra, one can prove the following identity:

$$\int \vec{S} dV = \frac{V}{4\pi c}\sum_k \vec{E}_L \times \vec{B}^* = \sum_j \frac{q_j}{c}\vec{A}(\vec{x}_j)$$

Thus one can associate $\frac{q_j}{c}\vec{A}(\vec{x}_j)$ with the Darwin field momentum



Alternative Momentum Flux Equation:

$$\frac{\partial}{\partial t}\left[\frac{\rho\vec{A}}{c}\right] + \rho\left(E_L + E_\perp\right) + j \times B / c = \nabla \cdot \overleftrightarrow{T}'$$

Darwin model: Numerical solution

Lagrangian formulation

Since $E_\perp$ depends on dv_i/dt of all the particles, and dv_i/dt depends on $E_\perp$ through the particle equation of motion

$$m_j \frac{d\vec{v}_j}{dt} = q_j\left[\vec{E}_\perp(\vec{x}_j) + \vec{E}_L(\vec{x}_j) + \vec{v}_j \times \vec{B}(\vec{x}_j)/c\right]$$

we have a coupled system of equations involving the accelerations of all the particles.

A simple iterative scheme for solving $E_\perp$

$$\nabla^2 \vec{E}_\perp = \frac{4\pi}{c^2}\frac{\partial \vec{j}_\perp}{\partial t} \qquad => \qquad \vec{E}_\perp(\vec{x}_j) = -\sum_k \left[\frac{4\pi}{k^2c^2}\right]\frac{\partial j_\perp}{\partial t} e^{i\vec{k}\cdot\vec{x}_j}$$

using old values of dv_i/dt on the right hand side is unstable when $kc < \omega_{pe}$.

Darwin model: Numerical solution

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

$$\nabla^2 \vec{E}_\perp - \frac{\omega_{p0}^2}{c^2}\vec{E}_\perp = \frac{4\pi}{c^2}\frac{\partial \vec{j}_\perp}{\partial t} - \frac{\omega_{p0}^2}{c^2}\vec{E}_\perp \qquad \text{where} \qquad \omega_{p0}^2 \equiv \frac{4\pi}{V}\sum_i \frac{q_i^2}{m_i}$$

This leads to the following solution:

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

The original scheme was unstable if the denominator $kc < \omega_{pe}$. With the new denominator, this will not generally occur.

Why does subtracting the same term from both sides make a scheme stable? Because old values are used on the right hand side and new values on the left hand side. When converged, the original equation should give the same result.

Darwin model: Numerical solution

Another problem: most PIC codes know x(t), v(t-Δt/2), but the equation for E⊥ requires v(t), and dv(t)/dt. We combine iteration for E⊥ and B with iteration for time-centering:

To initialize iteration, approximate j(t) using x(t), v(t-Δt/2). Approximate dj(t)/dt, using convective derivative only. This is a force-free approximation. Solve for initial E⊥ and B

Advance particles, but do not update. Instead calculate

$$v(t) = \frac{v(t+\Delta t/2)+v(t-\Delta t/2)}{2} \qquad \text{and} \qquad \frac{dv(t)}{dt} = \frac{v(t+\Delta t/2)-v(t-\Delta t/2)}{\Delta t}$$

Deposit j and dj/dt. Solve for improved E⊥ and B, and repeat

When converged, use normal push to update particles

Darwin model: Numerical solution

Hamiltonian formulation

Another formulation can be derived from the vector identity:

$$\frac{d\vec{A}}{dt} = \frac{\partial \vec{A}}{\partial t} + \nabla(\vec{v} \cdot \vec{A}) - \vec{v} \times (\nabla \times \vec{A})$$

which leads to the Hamiltonian equation of motion:

$$\frac{d}{dt}[m_j \vec{v}_j + \frac{q_j \vec{A}}{c}] = q_j \left[\vec{E}_L + \nabla(\frac{\vec{v}_j \cdot \vec{A}}{c}) \right]$$

The solution for A is given by:

$$\vec{A}(\vec{x}_j) = \frac{4\pi}{c} \sum_k \left[\frac{\vec{j}_\perp(\vec{k})}{k^2} \right] e^{i\vec{k} \cdot \vec{x}j} \qquad => \qquad \sum_j q_j \nabla \left[\frac{\vec{v}_j \cdot \vec{A}(\vec{x}_j)}{c} \right] = 0$$

Note that E⊥ does not appear in the equation of motion. Its role, apparently, is to partition the acceleration between the particle momentum and the field momentum.

Darwin model: Numerical solution

This equation is unstable to iteration just like the equation for E⊥, and but can be stabilized exactly the same way:

$$\nabla^2 \vec{A} - \frac{\omega_{p0}^2}{c^2}\vec{A} = -\frac{4\pi}{c}\vec{j}_\perp - \frac{\omega_{p0}^2}{c^2}\vec{A}$$

It is convenient to define an un-canonical momentum:

$$\vec{p}_j \equiv \vec{v}_j + \frac{q_j \vec{A}(\vec{x}_j)}{m_j c}$$

The discrete equation of motion:

$$\frac{1}{\Delta t}\left[\vec{p}(\mathrm{t} + \frac{\Delta t}{2}) - \vec{p}(t - \frac{\Delta t}{2})\right] = \frac{q}{m}\vec{E}_L + \frac{q}{mc}\nabla\left[\frac{1}{2}\left(\left[\vec{p}(t + \frac{\Delta t}{2}) + \vec{p}(t - \frac{\Delta t}{2})\right] - \frac{q\vec{A}}{mc}\right)\cdot\vec{A}\right]$$

Can be solved in a manner very similar to the Boris Mover:

$$\vec{p}(t + \frac{\Delta t}{2}) = \overleftrightarrow{R}\cdot\left[\vec{p}(t - \frac{\Delta t}{2}) + \frac{\vec{F}}{2}\right] + \frac{\vec{F}}{2} \quad \text{where} \quad \vec{F} = \frac{q}{m}\vec{E}_L\Delta t - \frac{\Delta t}{2}\left(\frac{q}{mc}\right)^2\nabla\left(\vec{A}\cdot\vec{A}\right)$$

Darwin model: Numerical solution

One iterates to update the canonical momentum. Initially, approximate j(t) using x(t), v(t-Δt/2). Solve for initial A and ∇A

Advance particles, but do not update. Instead calculate

$$v(t) = \frac{p(t+\Delta t/2) + p(t-\Delta t/2)}{2} - \frac{qA}{mc}$$

Deposit j. Solve for improved A and ∇A, and repeat

When converged, update the momentum. However, we cannot update position because we do not know v(t+Δt/2)!

To find v(t+Δt/2) we need to know A(t+Δt/2) and for this we need to know x(t+Δt/2). Finding x(t+Δt/2) requires another iteration! Fortunately, the second iteration is simpler.

Darwin model: Numerical solution

Initially, estimate $x(t+\Delta t/2) = x(t) + v(t)\Delta t/2$. Solve for initial $A(t+\Delta t/2)$

Calculate:

$$v(t+\Delta t/2) = p(t+\Delta t/2) - \frac{qA(t+\Delta t/2)}{mc}$$

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

Deposit j. Solve for improved A, and repeat

When converged, update the position $x(t+\Delta t)=x(t)+v(t+\Delta t/2)\Delta t$

Darwin model: Comparisons for 2-1/2D

The two methods give nearly identical results

For uniform plasma, both schemes converge in 2 iterations

For 1000 time steps, 36 particles/cell, linear interpolation

Energy Conservation: $\Delta W/W = 3.0\text{x}10\text{-}5$

Momentum Conservation: $\Delta v/|v| = 4\text{x}10\text{-}7$

Performance on 2.5 GHz Macintosh G5, NDC = 2

Lagrangian: 414 nsec/particle/step

Hamiltonian: 477 nsec/particle/step

Electromagnetic Code: 104 nsec/particle/step

Darwin model: Comparisons for 2-1/2D

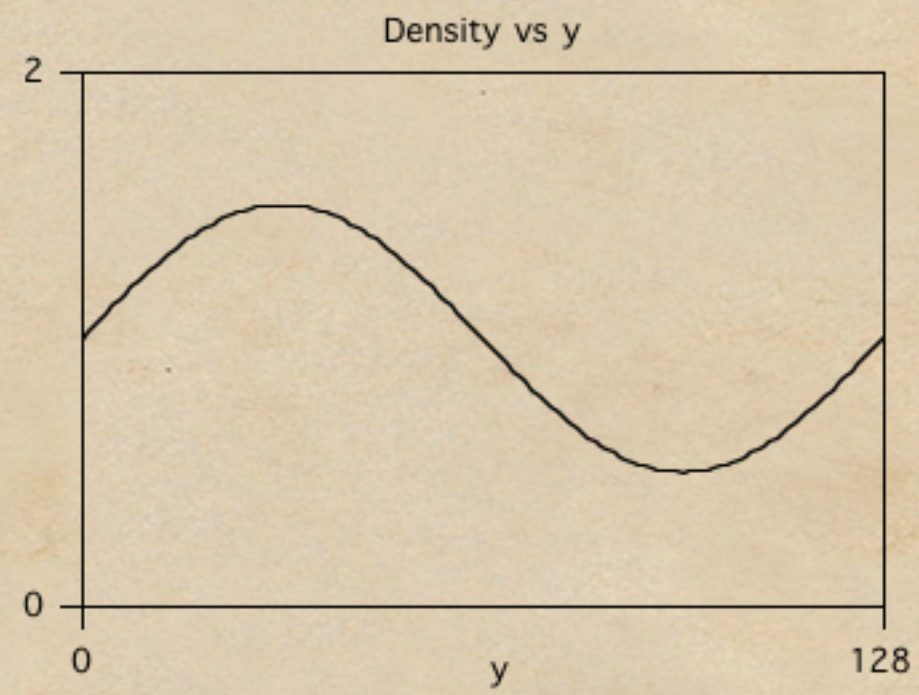
This good convergence continues so long as

$$\max(\omega_p^2(x)) < 1.5\omega_{p0}^2 \qquad \text{where} \qquad \omega_p^2(x) \equiv 4\pi \sum_{i, i\in x} \frac{q_i^{\,2}}{m_i}$$

Beyond this, more iterations are required. If

$$\max(\omega_p^2(x)) > 2\omega_{p0}^2$$

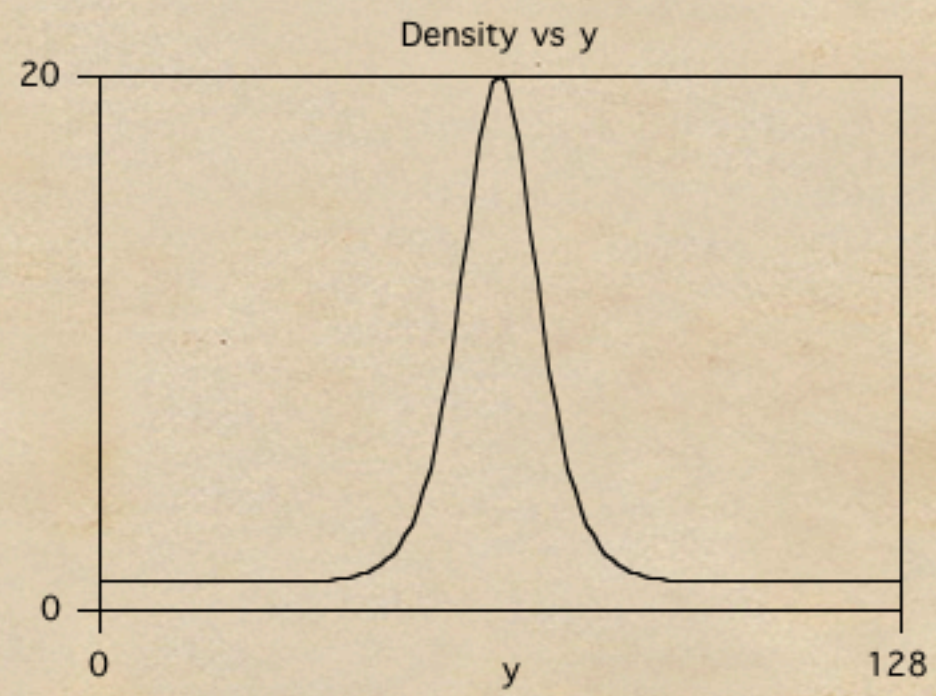
The iteration becomes unstable



Darwin model: Comparisons for 2-1/2D

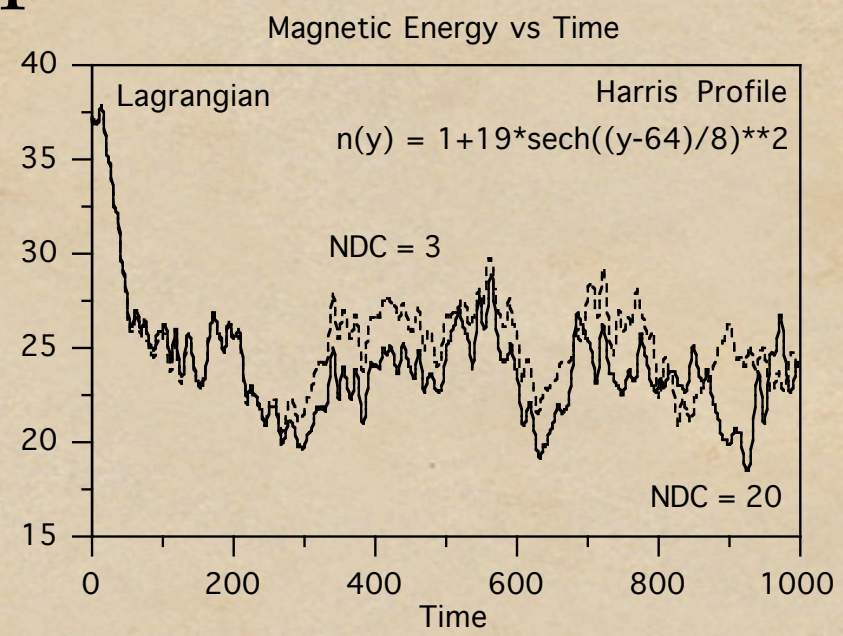
Fortunately, the iteration can easily be stabilized again if we use the constant

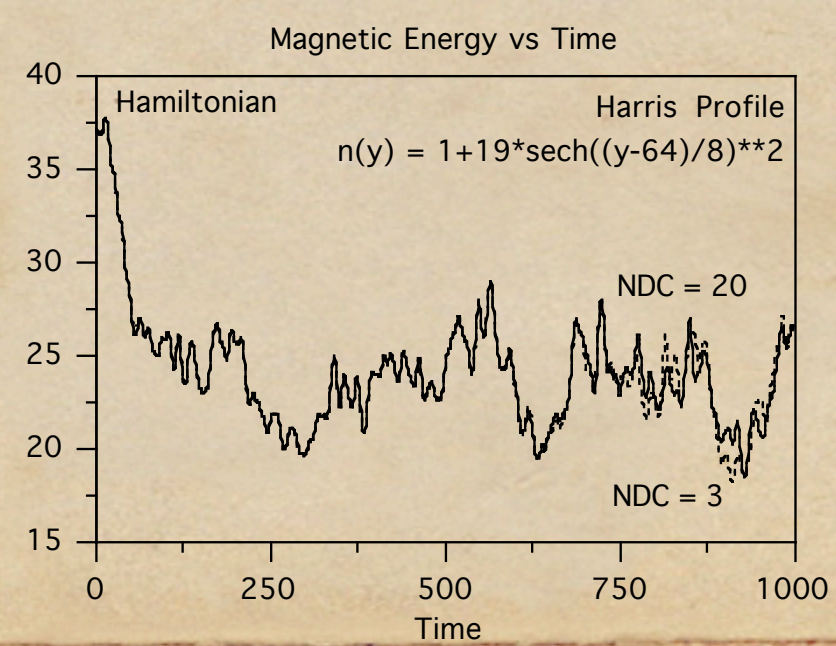
$$\omega_{pm}^2 \equiv \frac{1}{2}\left[\max(\omega_p^2(x)) + \min(\omega_p^2(x))\right] \quad \text{instead of} \quad \omega_{p0}^2$$



Darwin model: Comparisons for 2-1/2D

As the density profile becomes extreme, the Lagrangian formulation requires more and more iterations to converge



the Hamiltonian will converge in 3 iterations

For extreme density variation, the Hamiltonian is better.
For moderate variation, the Langrangian is faster