Verification and Convergence Properties of a Particle-In-Cell Code

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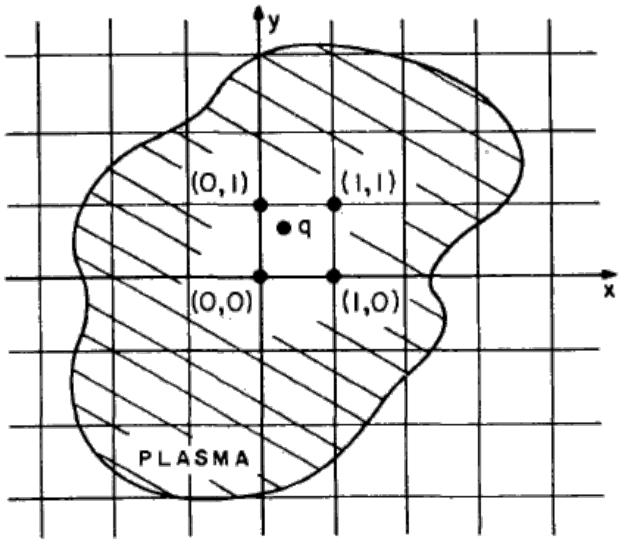
Introduction

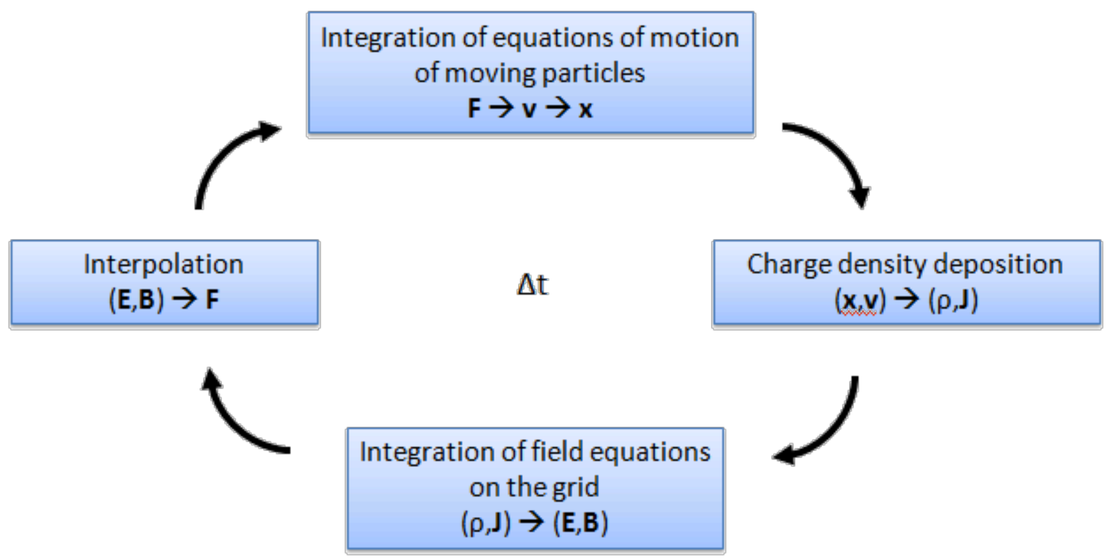


*Birdsall and Langdon [1985]

- Particle-in-cell (PIC) codes have been widely used throughout plasma physics for over 50 years

- They are used when kinetic effects are important and continuum fluid models are inadequate

- Basic PIC code loop:



But… What mathematical model do PIC codes represent?

- Statistical model such as the Vlasov equation?

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} = 0$$

  – Are particles phasespace markers, does the PIC code represent an ensemble average?

- Molecular dynamics model represented by a Klimontovich equation?

$$\frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial F}{\partial \mathbf{v}} = 0$$

$$F(\mathbf{x}, \mathbf{v}, t) = \sum_i S(\mathbf{x} - \mathbf{x}_i(t)) S(\mathbf{v} - \mathbf{v}_i(t))$$

  – Not an ensemble average but a numerical experiment of a single instance?

- We hypothesize that the mathematical model behind PIC codes is a Klimontovich equation with finite-size particles
- We verify that the PIC code converges to this model as numerical parameters are varied

Preliminaries

- Our computational model for the Klimontovich equation for finite-size particles is the "gridless PIC" code
  - We evolve a given number of particles with Maxwell's equations but without a grid
  - Spectral
    - For a periodic system, one can solve the model for a given number of particles with infinite Fourier series.
    - We truncate the infinite Fourier series at a maximum wavenumber
    - Allows comparison with a gridded PIC code
  - Gaussian particle shape function
  - Finite time step

		Gridded	Gridless
$\lvert k_{min}\rvert$	$=$	$2\pi/L$	$2\pi/L$
$\lvert k_{max}\rvert$	$=$	π/Δ	$(2\pi/L)N_{max}$

- Gridless code with finite-size particles
  - Description
  - Convergence properties
- Conventional PIC code*
  - Does it converge to the gridless code?
  - The dispersion relation of electron plasma waves

*from the UPIC Framework, Decyk, Computer Phys. Comm. (2007)

Simulation Set-up

- 1D, periodic, thermal plasma
- 18432 electrons with exactly the same initial positions and velocities
- Fixed ion background
- $L = 512\lambda_D$
- Electrostatic, $dt = 0.1\omega_p^{-1}$
- Electromagnetic, $dt \sim 0.01\omega_p^{-1}$, $v_{th}/c = 0.1$

- We further specify:
  - a = particle size
  - N_{max} = number of modes
  - λ_D = Debye length
  - Δ = grid size

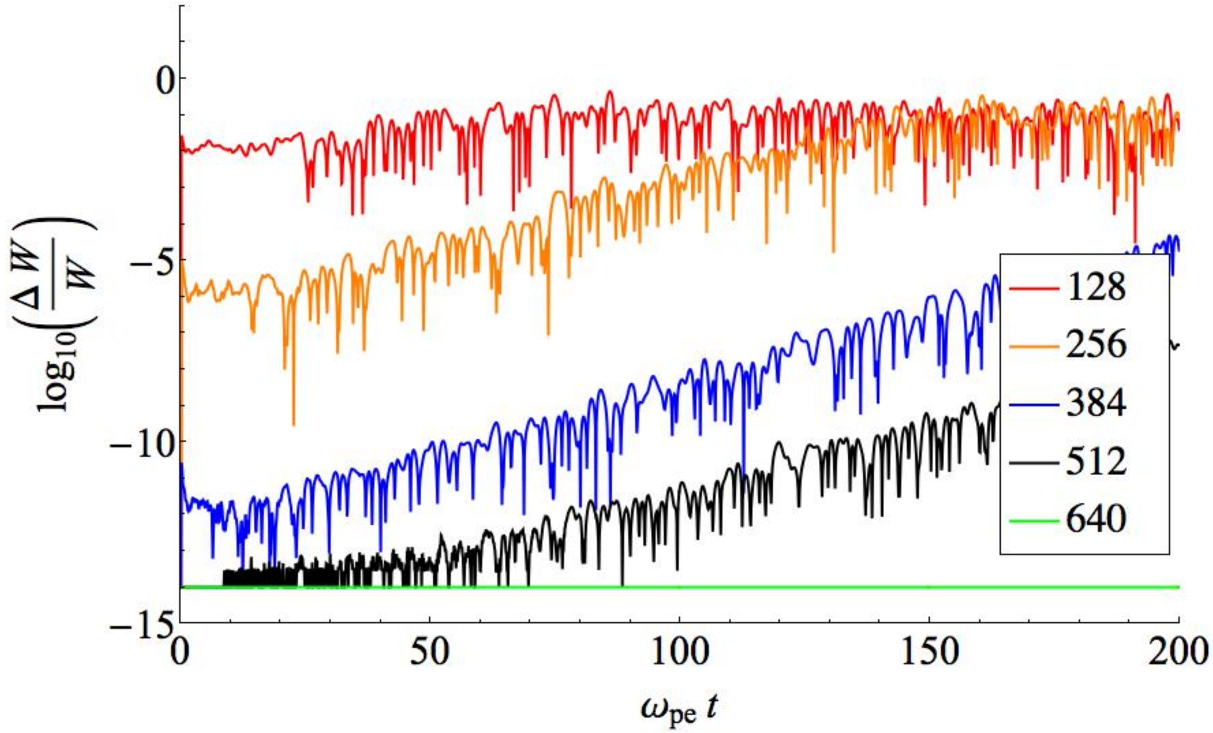
    Δ can also be used as a normalizing length to relate the gridless to gridded codes

- Our metric for comparisons: time history of the total field energy
    - Electrostatic field energy
    - Longitudinal electric, transverse electric, and magnetic field energies

Testing convergence of the electrostatic gridless code

Gridless code convergence with number of modes

Baseline case: $L = 512\lambda_D$, $a=\lambda_D$, $N_{max} = 1024$



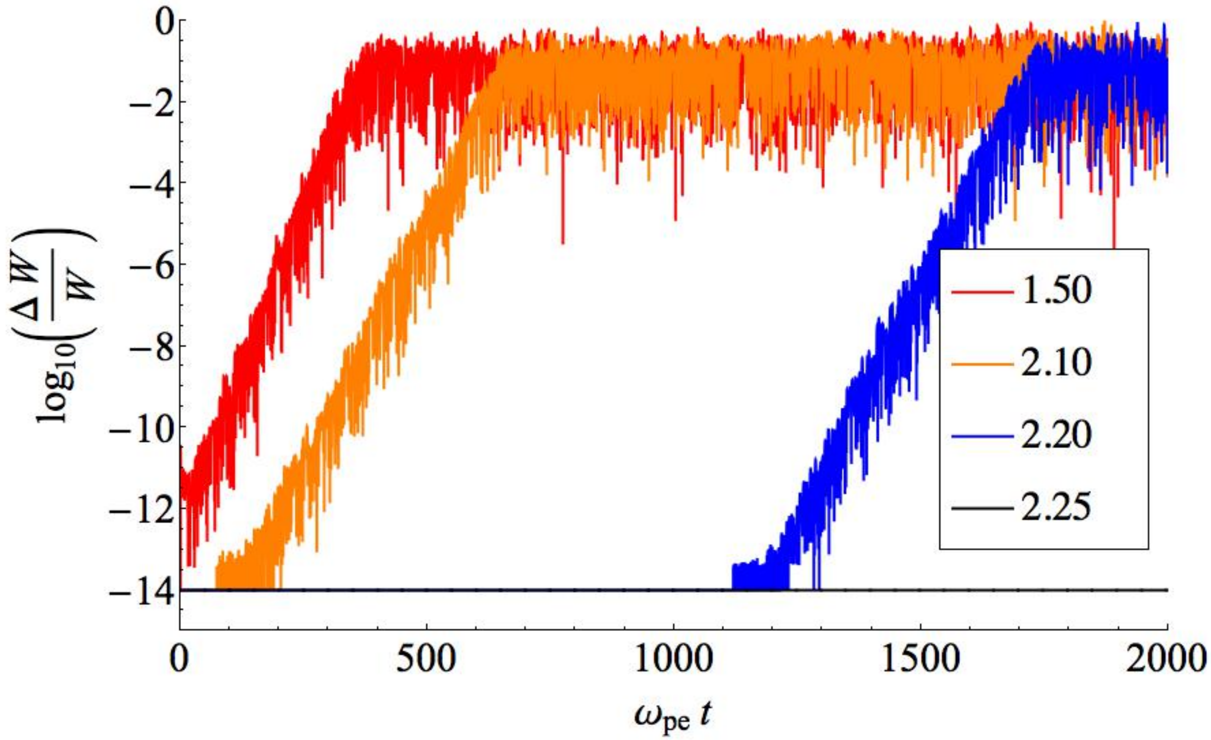
N_{max}

[We add 10^{-14} which falls at the machine precision; this follows similarly on following slides]

Gridless Code convergence with particle size

- A conventional PIC code with L = 512λ_D, a = λ_D, and Δ = λ_D would have N_{max}=256.
- Is convergence found for a fixed number of modes by varying particle size?

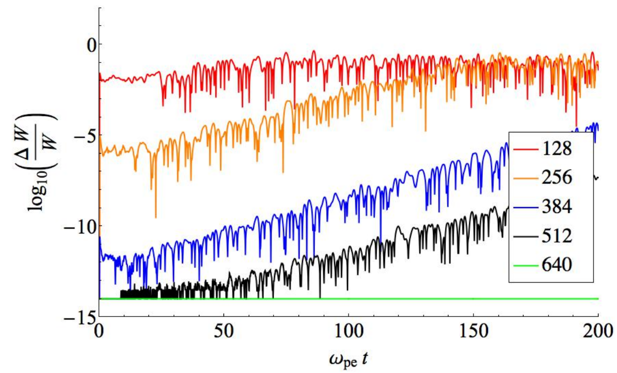
Comparison case: L = 512λ_D, N_{max} = 256, variable a
Baseline case: L = 512λ_D, N_{max} = 1024, similar a



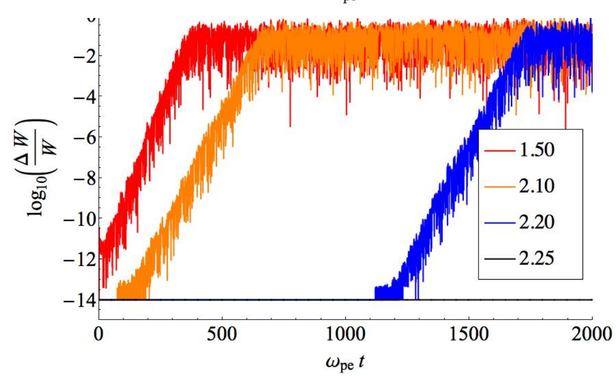
a/λ_D

Gridless Code convergence depends on $k_{max}a$

- Whether varying number of modes (k_{max}) or particle size (a):



$$\rightarrow k_{max} \geq \left(\frac{2\pi}{512\lambda_D}\right) 640$$



$$\rightarrow a \geq 2.25\lambda_D,$$
$$k_{max} = \pi/\lambda_D$$

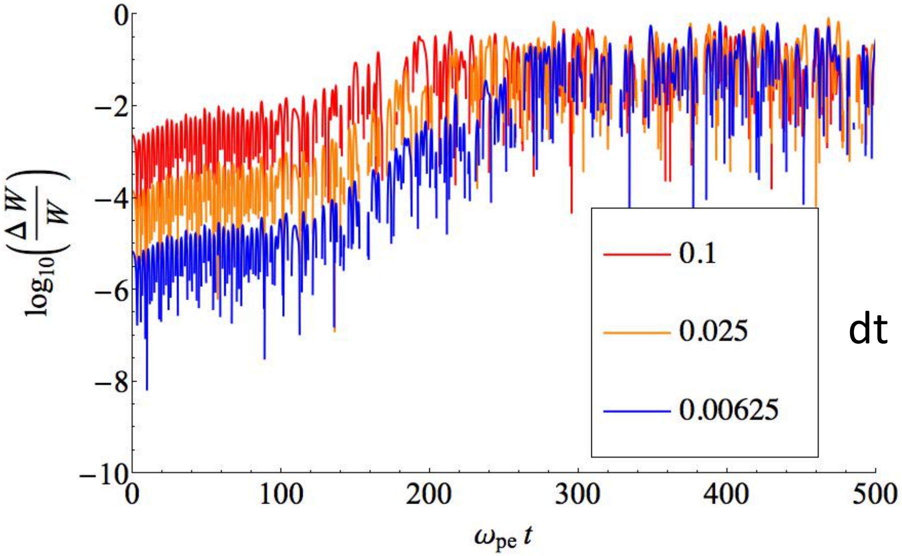
$$k_{max}a \gtrsim \frac{5}{2}\pi$$

- Key consideration: At some $k_m a$, S(k) reduces all Fourier modes with k > k_m by a ratio smaller than double precision can resolve

$$S(k) = e^{-k^2a^2/2} \lesssim 10^{-14}$$

Gridless Code convergence with time step

- The previous convergence is maintained for long times
  - Approximately 50000 time steps
  - a=2.25λ_D, N_{max}=256 vs 1024
- Energy differences with the same parameters and a very small time step (dt = 0.003125 ω_p^{-1}) also show convergence
  - Slower, quadratic vs exponential
  - Such small time steps are unnecessary, but it's reassuring to see that nothing unreasonable occurs



Testing convergence of the electrostatic gridded PIC code with the gridless code

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Convergence of the gridded code with gridless code

- **Aliasing:** particle density perturbations with $k > \pi/\Delta$ get mapped unphysically to shorter wavelengths

- **Interpolation**: we use linear, quadratic, and cubic B-spline functions
  - Particle shape is a product of the interpolation function and filter function used to suppress aliasing
  - With m the order of interpolation:

$$W_m(k) = [\sin(k\Delta/2)/(k\Delta/2)]^{m+1}$$
$$S_g(k) = e^{-(ka_g)^2/2}$$
$$S_{eff}(k) = W_m(k)S_g(k)$$

- To compare gridded with gridless code, we take $S_{eff}(k) \approx S(k)$

$$a_g = \sqrt{a^2 - \Delta^2/\alpha}$$

  - α = 6, 4, and 3 for linear, quadratic, and cubic, respectively

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Higher order interpolation gives better convergence

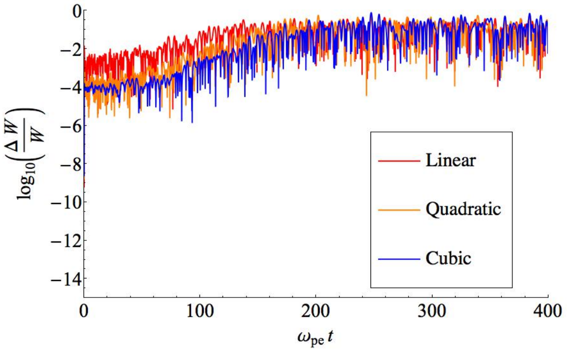
Comparison case:

Gridded PIC code, L = $512\lambda_D$, N_{max} = 256, a=2.25Δ, $\lambda_D = \Delta$

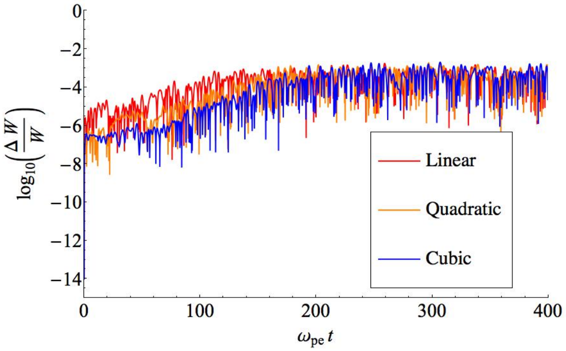
Baseline case:

Gridless code, L = $512\lambda_D$, N_{max} = 256, $\lambda_D = \Delta$

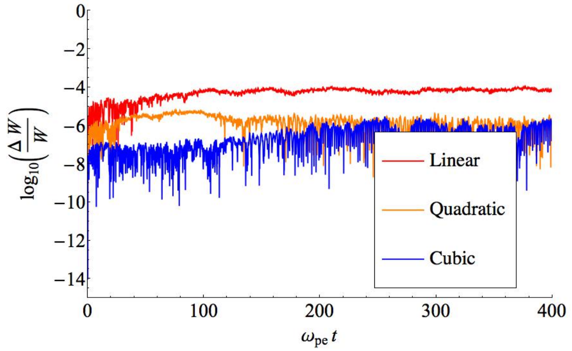
Electrostatic Field Energy



Particle Kinetic Energy



Total Energy



The higher the order of interpolation, the more the aliased modes are reduced

The gridded code converges to the gridless code as the ratio of grid size to particle size is decreased

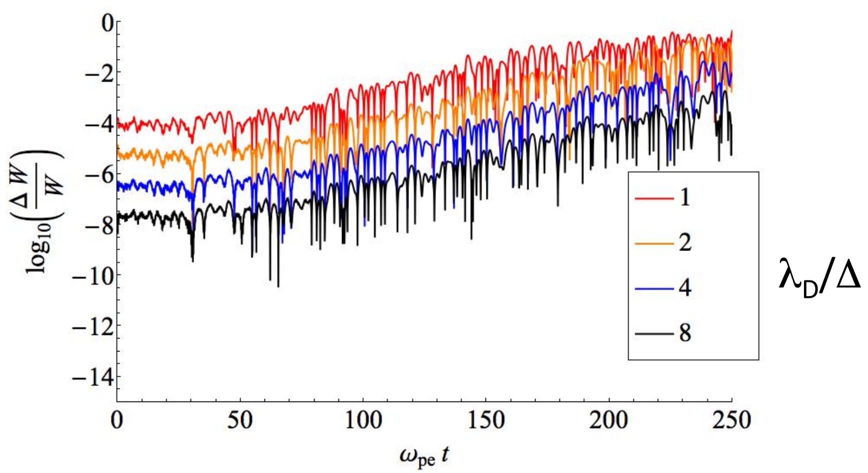
Comparison case:

Gridded PIC code, L = 512λ_D, N_{max} = 256, λ_D/Δ = variable, cubic interpolation

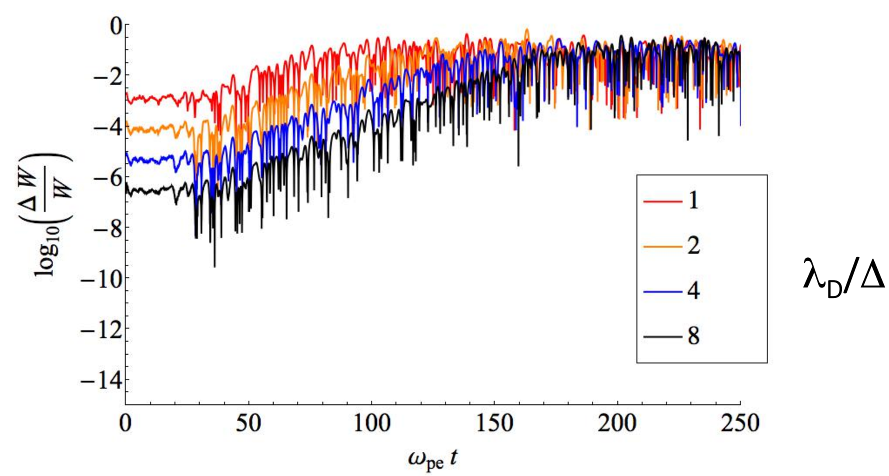
Baseline case:

Gridless code, L = 512λ_D, N_{max} = 256

a=2.25λ_D



a=λ_D



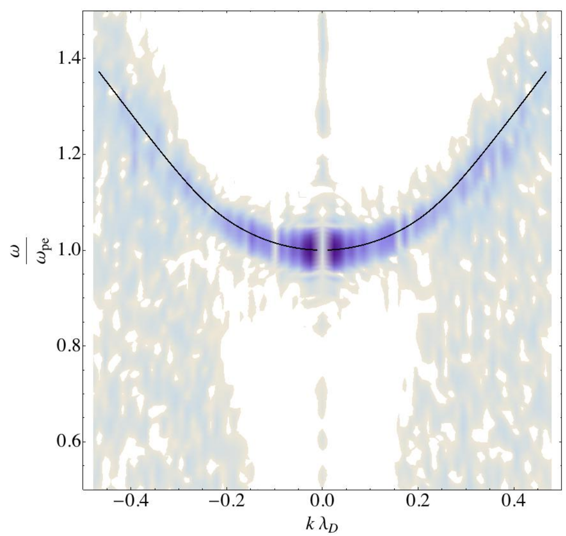
A physical question:
Do electron plasma waves have the proper dispersion relation?

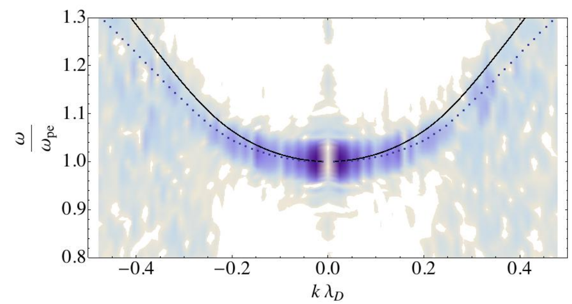
- The shape function affects the electron charge and thereby the plasma frequency
- The change in the dispersion relation can be determined simply by

$$\omega_{pe}^2 \Rightarrow \omega_{pe}^2 S(k) \text{ or } \omega_{pe}^2 \Rightarrow \omega_{pe}^2 S_{eff}(k)$$

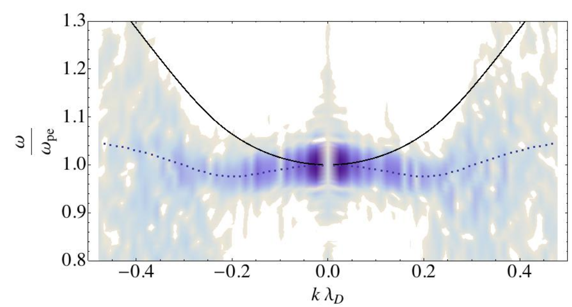
For example, $\omega^2 = \omega_{pe}^2 + 3k^2 v_{th}^2$ becomes $\omega^2 \approx \omega_{pe}^2 + \left[3 - \dfrac{a_g^2 + \Delta^2/\alpha}{\lambda_D^2}\right] k^2 v_{th}^2$

Gridless code,
L = 512λ_D,
N_{max} = 256,
a=0





Gridded code,
L = 512λ_D,
Δ = λ_D,
a = Δ



Δ = λ_D,
a = 2.25λ_D

Solid line: Kinetic dispersion relation

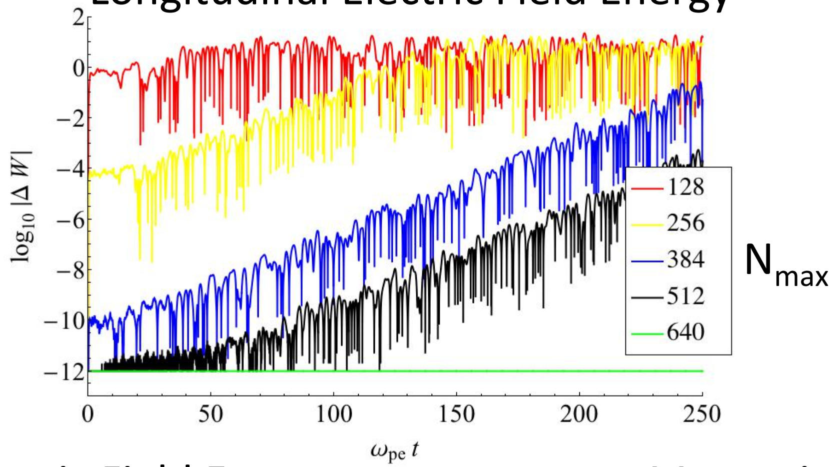
Dashed line: Kinetic dispersion relation with correction for finite-shape-particles

Testing convergence of the electromagnetic gridless code

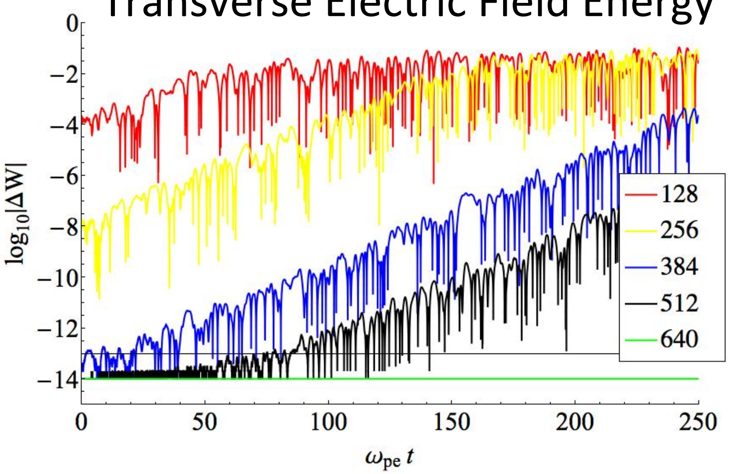
Gridless code convergence with number of modes

Baseline case: $L = 512\lambda_D$, $a=\lambda_D$, $N_{max} = 1024$

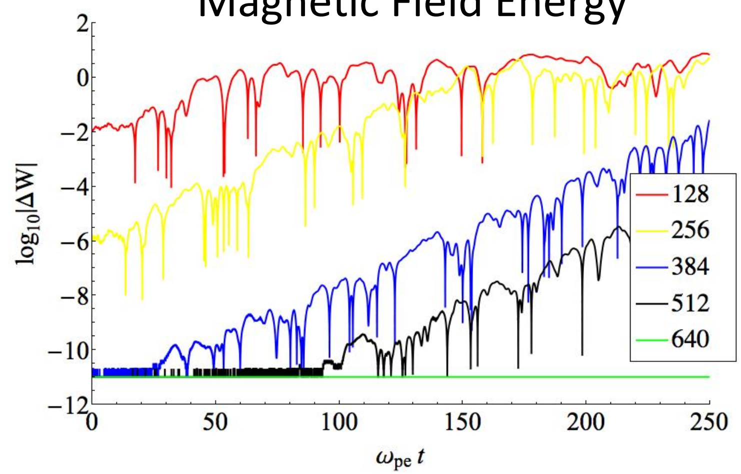
Longitudinal Electric Field Energy



Transverse Electric Field Energy



Magnetic Field Energy



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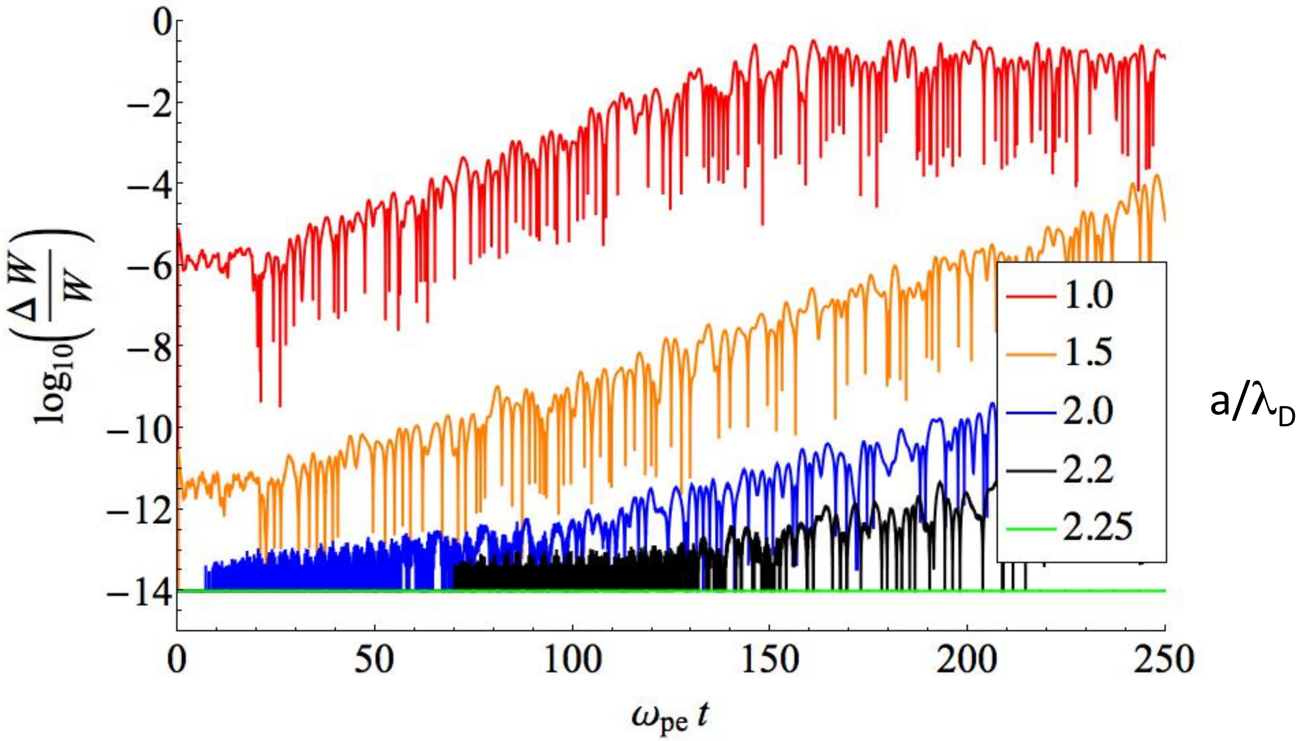
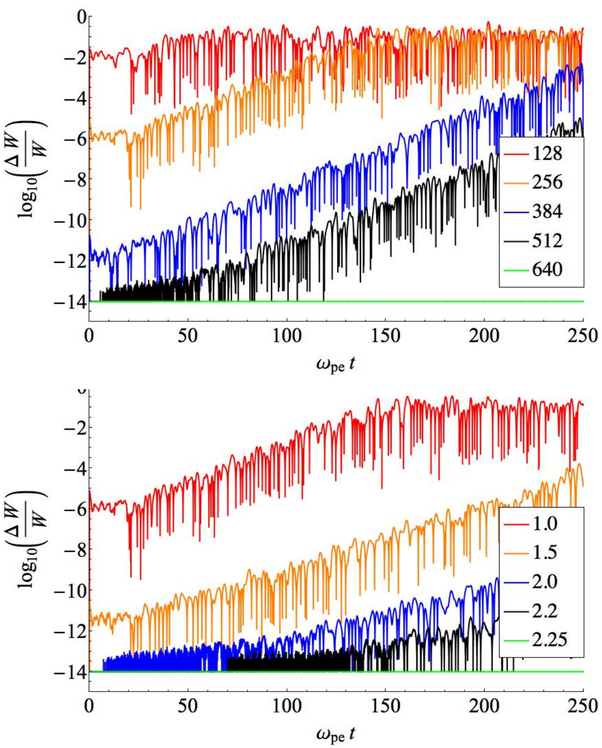


Gridless Code convergence depends on $k_{max}a$

- Whether varying number of modes (k_{max}) or particle size (a):



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$$\rightarrow a \geq 2.25\lambda_D,$$
$$k_{max} = \pi/\lambda_D$$

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- Key consideration: again, when does the shape factor fall below machine precision

$$S(k) = e^{-k^2a^2/2} \lesssim 10^{-14}$$

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with the gridless code

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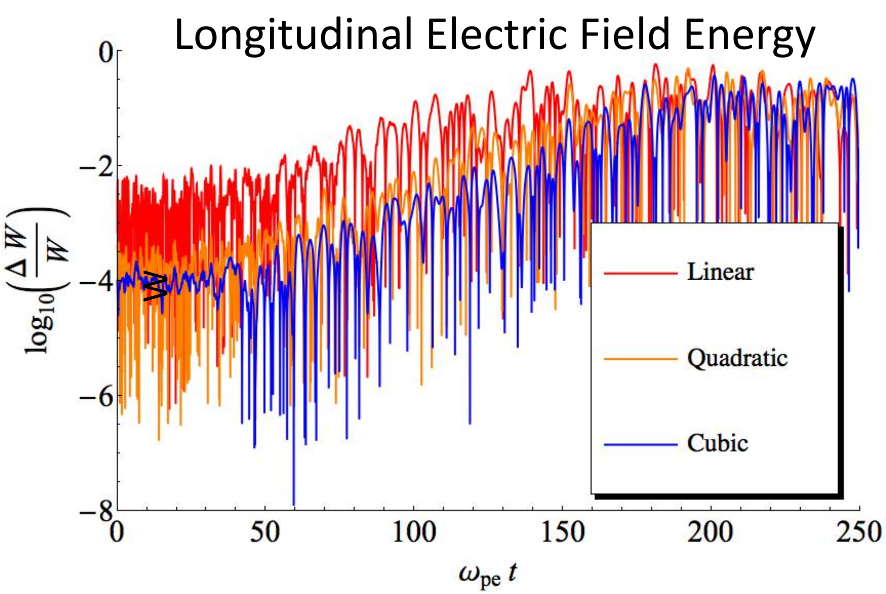
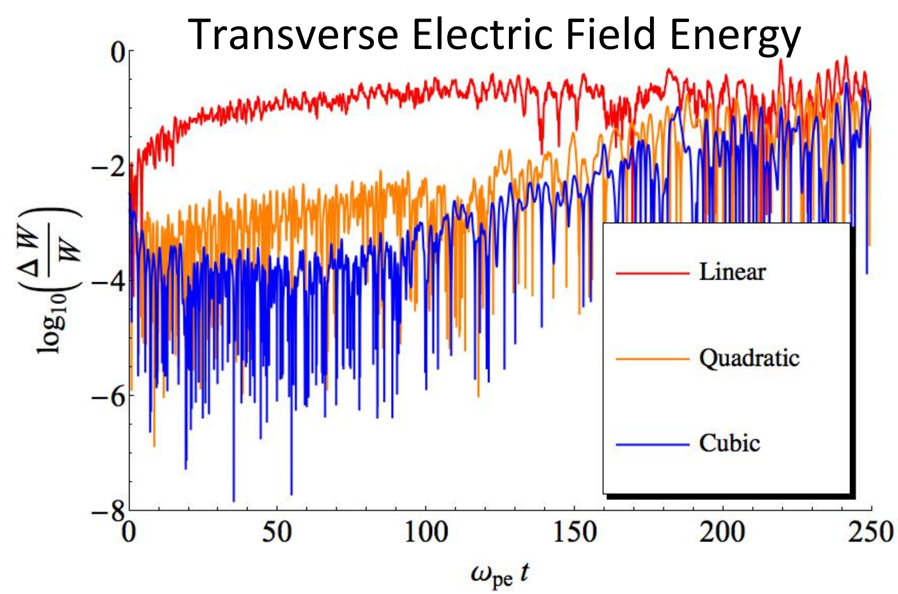
Higher order interpolation gives better convergence





- The higher the order of interpolation, the more the aliased modes are reduced
- The transverse electric field energy is not quite as convergent, but both longitudinal and transverse energies show improved convergence as the interpolation increases from linear to cubic

The gridded code converges to the gridless code as the ratio of grid size to particle size is decreased

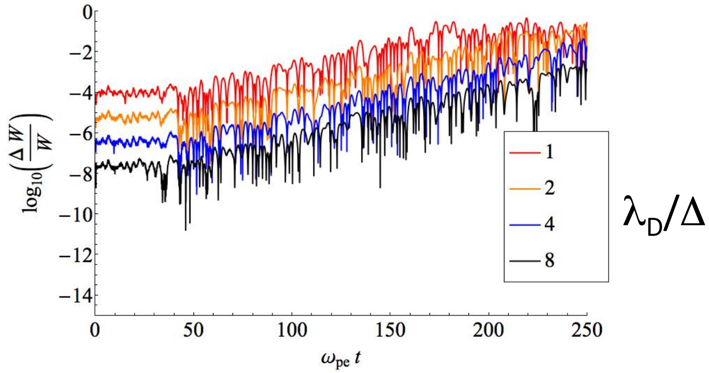
Comparison case:

Gridded PIC code, L = 512λ_D, N_{max} = 256, λ_D/Δ = variable, cubic interpolation

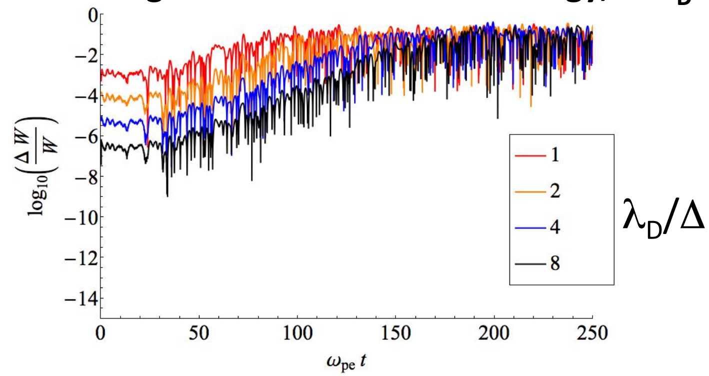
Baseline case:

Gridless code, L = 512λ_D, N_{max} = 256

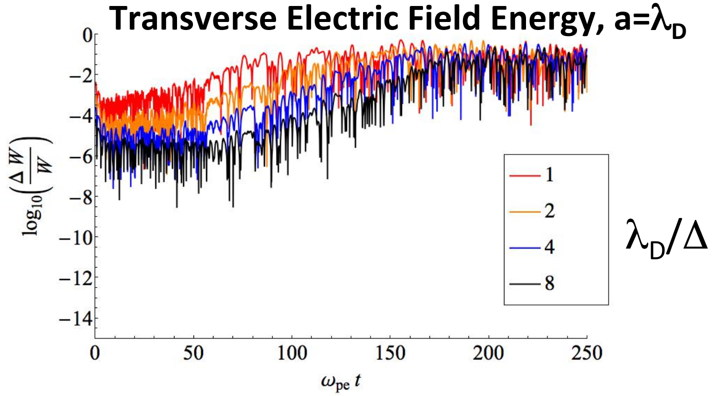
Longitudinal Electric Field Energy, a=2.25λ_D



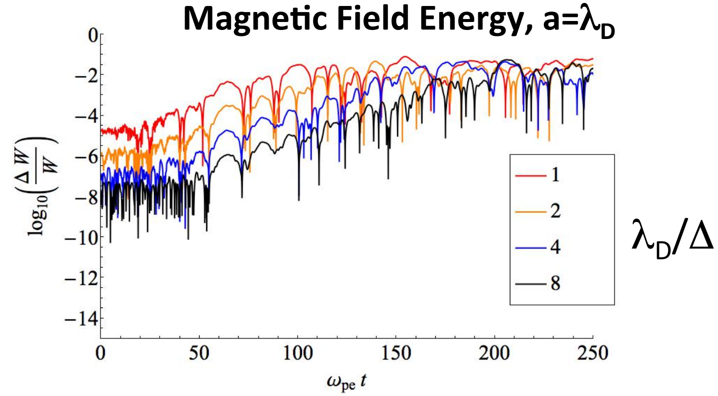
Longitudinal Electric Field Energy, a=λ_D



Transverse Electric Field Energy, a=λ_D



Magnetic Field Energy, a=λ_D



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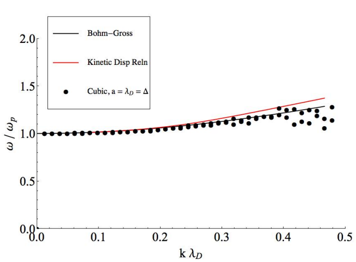

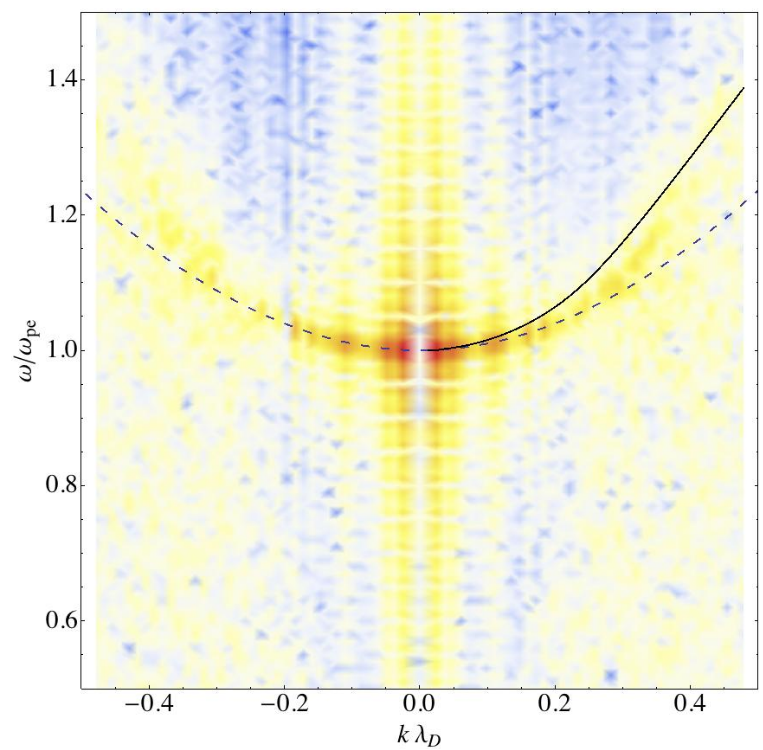

Gridded PIC code

Cubic interpolation

L = 512λ_D

a=Δ

λ_D=Δ

Conclusions

- For 1D electrostatic and electromagnetic codes, we have found convergence
  - The gridless code converged for $k_{max}a \gtrsim \frac{5}{2}\pi$
- We found that a spectral PIC code converged to the gridless code
  - Convergence occurred as “a” and λ_D increased relative to Δ.
  - These are interesting results, since we normally use PIC code with $a=\Delta= \lambda_D$.
  - With $k_{max\_PIC} = \pi/\Delta$, the gridless result implies using $a > 5/2\ \Delta$
  - For $a=\lambda_D$, this implies using a PIC code with $\Delta \sim 0.5\ \lambda_D$.
- We conclude that the mathematical model behind the PIC code is the Klimontovich model with finite-size particles