Multigrid Particle-in-cell Simulations of Plasma Microturbulence

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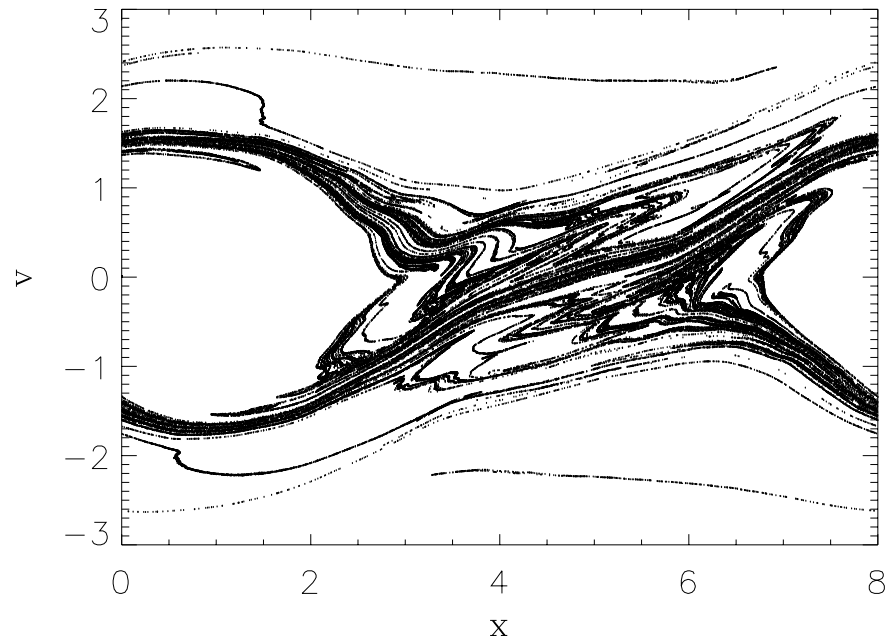


Outline

- Motivation: optimal particle-in-cell (PIC) simulations with electron dynamics
- Electron Dynamics in PIC Simulations...or how to split correctly... [1D case: this talk; progress on 3D, toroidal case using Algebraic Multigrid (EU-US TTF, September 2002)]
- Splitting Scheme and δf Scheme
- Multigrid Solver for Nonlinear Elliptic Equations
- Numerical Results; Linear Benchmarks; Nonlinear Saturation; Energy Conservation,...
- Conclusions

Motivation

- Full Kinetic Electron Response requires Global Solve for Scalar Fields at *each time step*
- Accurate treatment of electron dynamics requires efficient global solver for elliptic-type problems on toroidal grids
- Efficiency is crucial: global solution required at each time step on a grid with $N = N_\phi \times N_\theta \times N_r \sim 10^2 \times 10^3 \times 10^3 = 10^8$ points
- Geometry is important: no geometrical approximation of computational domain
- Advantages of MUGPIC: modular structure (easy to maintain); easy to parallelize (MPI + OpenMP); near-optimal efficiency;

Motivation (Remarks on δf Scheme)

Taken from Parker & Lee's paper [Phys. Fluids B5(1), 77 (1993)]

Remark 0: "In order to further minimize the noise, we have used a cut-off scheme of $w_i = \phi(x_i)$ for the fast particles with $v_{||i} \gg \omega/k_{||}$(...)

Remark 1: "It is found that the conservation of number density, momentum, and energy in the nonlinear stages of the simulations can be achieved only if we use a sufficiently large of particles (...)"

Remark 2: "In the linear stage of that simulation, the particle conservation is near perfect and the inaccuracy occurs only in the nonlinear stage due to numerical noise (...)"

Remark 3: "The implication here seems to be that one still has to use a very large number of particles with enough spatial and time resolution to obtain reasonable conservation properties (...)"

Remark 4: "Nevertheless, the errors for the conservation properties after nonlinear saturation is somewhat troublesome, since our ultimate goal is to use the scheme to study long-time steady-state phenomena (...)"

Remark 5: "We were able to obtain energy conservation. However, compared to the number needed to capture the relevant physics of the drift wave model, a very large number of particles was required(...)"

Splitting scheme removes *all* the limitations above

1D Electrostatic Drift Waves

Start from

$$\frac{dF_j}{dt} \equiv \frac{\partial F_j}{\partial t} + \left(v_{||}\widehat{\mathbf{b}}_0 + \mathbf{V}_E\right)\cdot\boldsymbol{\nabla} F_j - \frac{q_j}{m_j}\,\widehat{\mathbf{b}}_0\cdot\boldsymbol{\nabla}\Phi\frac{\partial F_j}{\partial v_{||}} = 0\ ,$$

where $\widehat{\mathbf{b}}_0 = \mathbf{B}_0/B_0$ a unit vector and $\mathbf{V}_E = c\widehat{\mathbf{b}}_0\times\boldsymbol{\nabla}\Phi/B_0$ is the $\mathbf{E}\times\mathbf{B}$ drift velocity; $\mathbf{B}_0 = B_0\left(\widehat{\mathbf{z}} + \theta\widehat{\mathbf{y}}\right)$ where $\theta \ll 1$.

Standard δf Scheme

$$F_j = F_{Mj} + \delta f_j$$

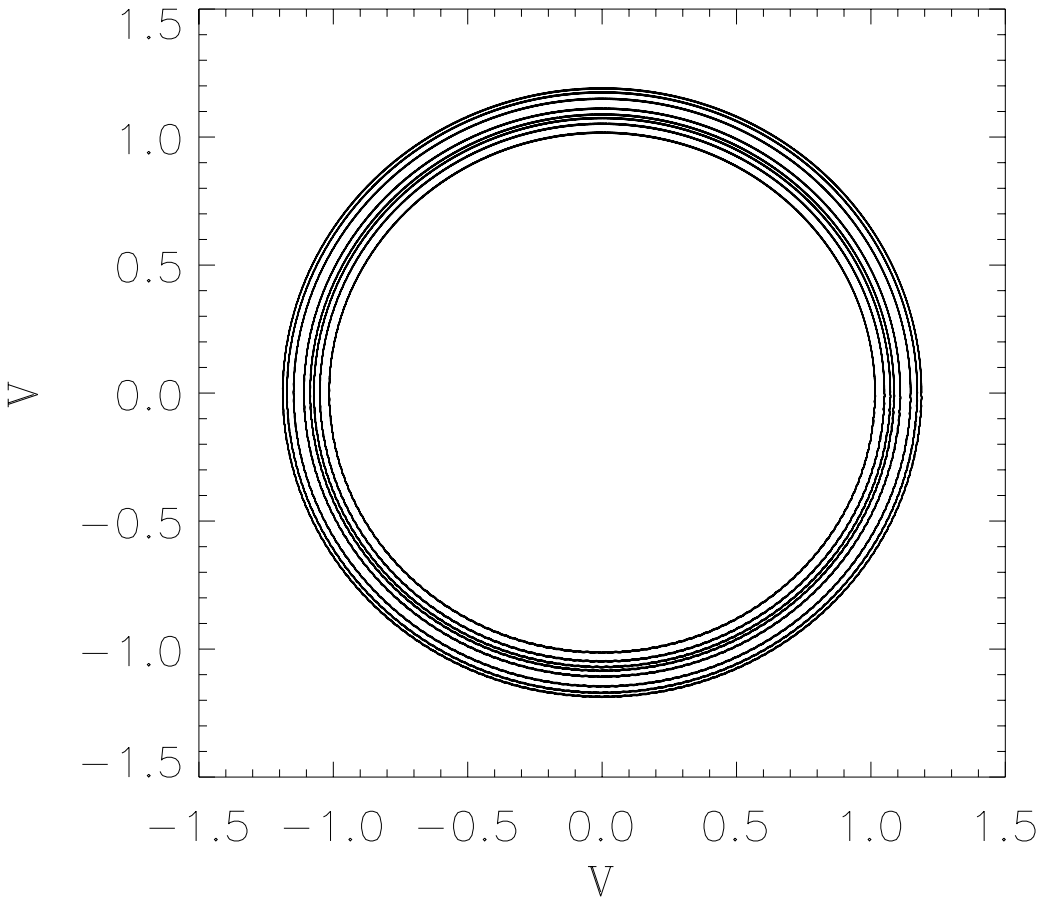
Equation for the weight $W_j \equiv \delta f_j/F_j$ (GK units)

$$\frac{dW_j}{dt} = (1 - W_j)\left[\left(\widehat{\mathbf{b}}_0\times\boldsymbol{\nabla}\Phi\right)\cdot\boldsymbol{\kappa}_j - \sigma_j v_{||}\nabla_{||}\Phi\right]\ .$$

where $\sigma_j = Z_j T_e/T_j$. The system of equations is closed with the gyrokinetic Poisson equation (in the long wavelength limit)

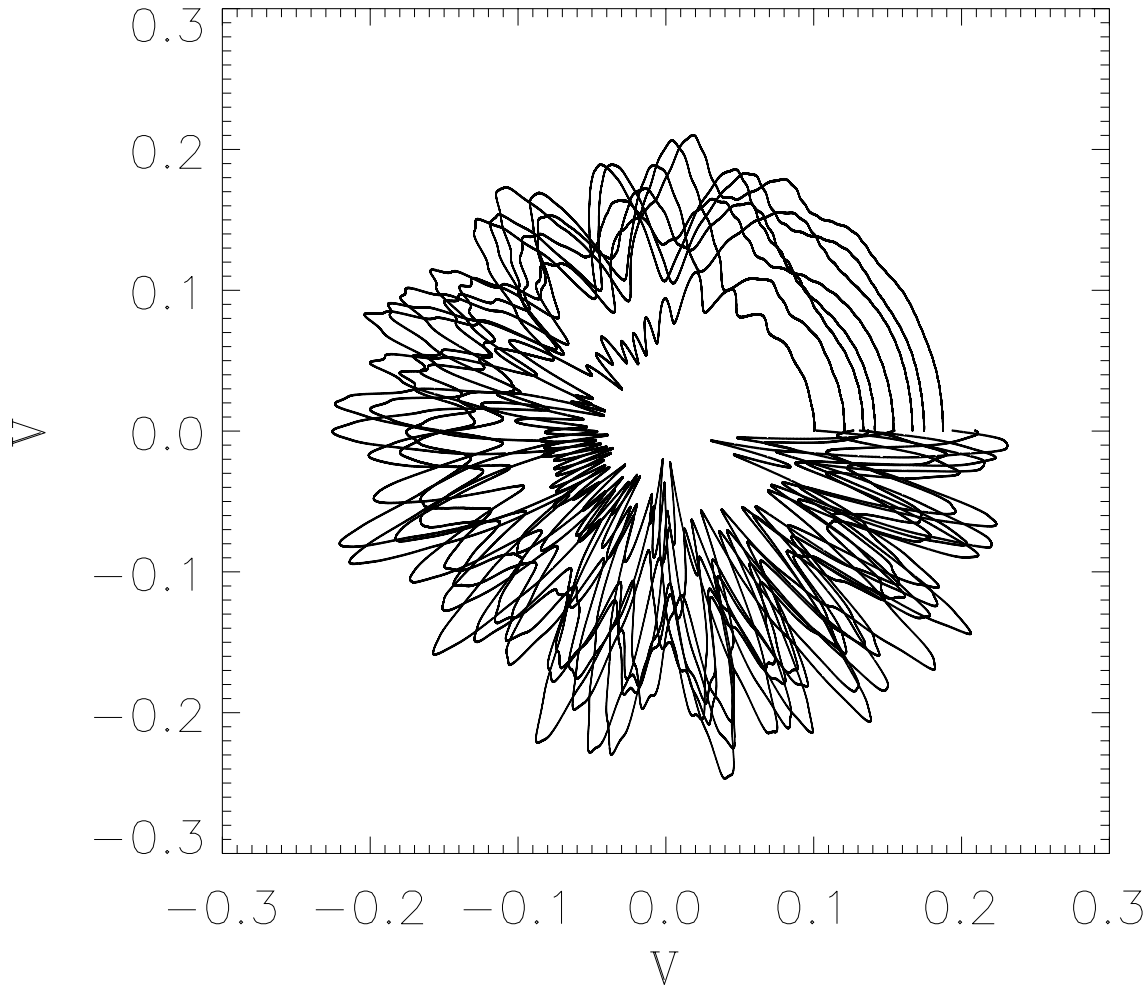
$$\nabla_\perp^2\Phi = \int_{-\infty}^{+\infty}\left(\delta f_e - \delta f_i\right)dv_{||}\ .$$

Adiabatic Electrons vs ...



Fully nonlinear simulations (no smoothing...) $(T \sim 10\tau_\ell = 10/\gamma_\ell)$

... Nonadiabatic Electrons



Fully nonlinear simulations (no smoothing...) $(T \sim 10\tau_\ell = 10/\gamma_\ell)$

How to Split Correctly?

$$F_j = H\left(\Phi\right) F_{Mj} + h_j \ ,$$

where, as before, F_{Mj} is the Maxwellian distribution for particle species j and $H\left(\Phi\right)$ is a yet undetermined function of the electrostatic potential. The so-called nonadiabatic part of the distribution function, h_j, is governed by

$$\frac{dh_j}{dt} = -H \underbrace{\mathbf{V}_E \cdot \boldsymbol{\nabla} F_{Mj}}_{\mathbf{1}} - v_{||} \nabla_{||} \Phi \underbrace{\left(H' + \frac{q_j}{T_j} H \right)}_{\mathbf{2}} F_{Mj} - \underbrace{H' F_{Mj} \frac{\partial \Phi}{\partial t}}_{\mathbf{3}} \ ,$$

Demand that term (**2**) vanishes...

$$\frac{dH}{d\Phi} = -\frac{q_j}{T_j} H$$

with solution

$$H = \exp\left(-\frac{q_j}{T_j} \Phi \right) \ .$$

Splitting Scheme

$$F_j = \exp\left(-\frac{q_j}{T_j} \Phi \right) F_{Mj} + h_j \ .$$

The equation governing the weight associated with the nonadiabatic part of the distribution function, $\overline{W}_j \equiv h_j/F_j$, is

$$\frac{d\overline{W}_j}{dt} = (1-\overline{W}_j)\left(\mathbf{V}_E\cdot\boldsymbol{\kappa}_j + \frac{q_j}{T_j}\,\varphi\right)$$

where

$$\varphi \equiv \frac{\partial\Phi}{\partial t} \quad \text{(polarization field)}$$

Note Above Equation for $\overline{W}_j$ is exact (no truncation in mode amplitude, etc..)

Nonlinear Gyrokinetic Poisson Equation

$$\nabla_\perp^2\Phi - \left(1+\frac{1}{\tau}\right)\Phi = \int_{-\infty}^{+\infty}(h_e - h_i)\,dv_{||} + Q(\Phi) \ ,$$

where

$$Q(\Phi) \equiv \exp(\Phi) - \exp(-\Phi/\tau) - (1+1/\tau)\,\Phi \ ,$$

and $\tau = T_i/T_e$.

Summary

δf Scheme

- Weight Equation with Free Streaming Term
- Linear Elliptic Problem

Splitting Scheme

- Weight Equation with **No** Free Streaming Term
- Linear Elliptic Problem
- Nonlinear Elliptic Problem

Is there is any physical justification for the additional computational work?
yes...

Multigrid Solver for Nonlinear Elliptic Problems

For a configuration with period ℓ, Nonlinear Poisson's equation is of the form

$$LF \equiv \frac{d^2F}{d\theta^2} = S\left(F, F^2, \cdots; \theta\right) \tag{1}$$

where $\theta \equiv 2\pi x/\ell$ is an angle-like coordinate with period 2π
S : is a known source term; Uniform computational grid has N_θ nodes. Problem (1) can be defined on a set of overlapping grids (or levels) as

$$L^{(p)}F^{(p)} = S^{(p)} \ ,$$

where $p = 0, 1, \cdots, Q$, and Q is the total number of levels compatible with the original number of grid points N_θ
grid spacing $(p = 0)$ is $\Delta\theta = 2\pi/N_\theta$ (finest grid)
grid spacing on coarser grids :$\delta\theta = 2^p\Delta\theta$ (for $p > 0$).

f: exact solution of Eq.(1).....$f = L^{-1}S$
F denotes an approximate solution, then the algebraic error,

$$e \equiv f - F$$

and the residual

$$r \equiv S - LF$$

and related through the $\boxed{\text{Residual Equation}}$

$$Le = r \qquad \left(\text{or } L^{(p)} e^{(p)} = r^{(p)} \ .\right) \tag{2}$$

If $A^{(p)}$ denotes an approximation to ${L^{(p)}}^{-1}$ then $F^{(p)} = A^{(p)} S^{(p)}$; in general, the approximate solution $F^{(p)}$ will depend on the initial guess $F_0^{(p)}$. Thus

$$F^{(p)} = A^{(p)} \left(S^{(p)}; F_0^{(p)}; \nu_p \right) \ , \tag{3}$$

where ν_p is the number of relaxation sweeps on level p and $F_0^{(p)}$ is the initial guess.

Intergrid Transfer Operators

$\boxed{\text{Prolongation Operator}}$ From coarse grid to fine grid

$$F^{(p)} = I\left(p+1 \mapsto p\right) F^{(p+1)}$$

$\boxed{\text{Restriction Operator}}$ From fine grid to coarse grid

$$F^{(p+1)} = I\left(p \mapsto p+1\right) F^{(p)}$$

Multigrid V Cycle

V cycle can be cast in the following algorithmic form of

MultiGrid V cycle

$$
\begin{aligned}
F^{(p)} &= A^{(p)}\left(S^{(p)}; F_0^{(p)}; \nu_p\right) \\
r^{(p)} &= S^{(p)} - L^{(p)} F^{(p)} \quad ; \quad p = 0, 1, \cdots, Q-1 \\
S^{(p+1)} &= I\left(p \mapsto p+1\right) r^{(p)} \\
\ldots\ldots &. \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
F_0^{(p)} &\Longleftarrow F^{(p)} + I\left(p+1 \mapsto p\right) F^{(p+1)} \\
F^{(p)} &= A^{(p)}\left(S^{(p)}; F_0^{(p)}; \nu_p\right)
\end{aligned}
\tag{4}
$$

Multigrid Solver: Example

Source term

$$S(\theta) = -\sum_{q=1}^{M} q^2 \left[\widehat{\alpha}_q \cos(q\theta) + \widehat{\beta}_q \sin(q\theta)\right] \ ,$$

which corresponds to the exact solution

$$f(\theta) = \sum_{q=1}^{M} \widehat{\alpha}_q \cos(q\theta) + \sum_{q=1}^{M} \widehat{\beta}_q \sin(q\theta) \ ,$$

and $M = 12$ is the total number of modes with amplitudes $\widehat{\alpha}_q = \widehat{\beta}_q = 1, \forall q$.
Initial Profile (finest grid)

$$F_0(\theta) = \pi^2 \sin(\theta/2)$$

Multigrid Solver for Nonlinear Elliptic Problems

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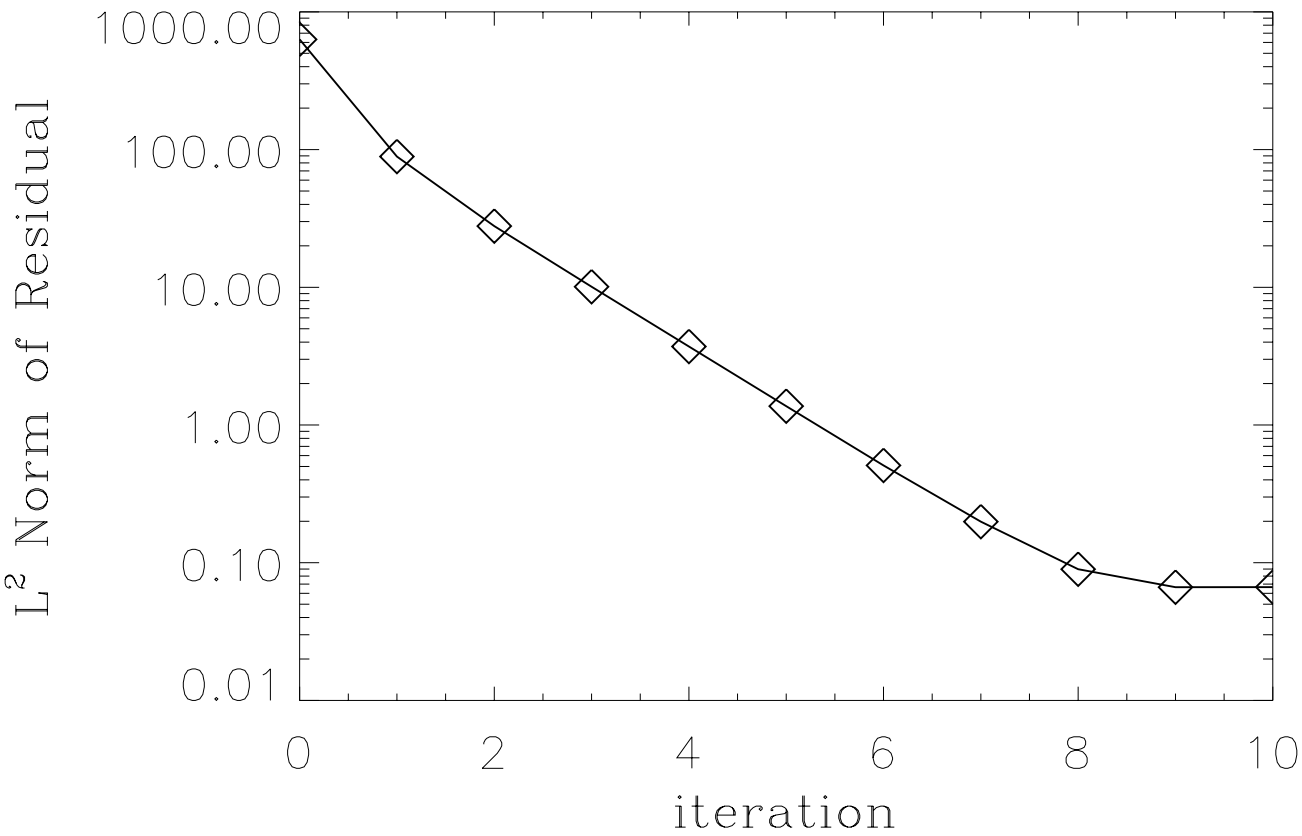

10 Multigrid V Cycles

Multigrid Solver for Nonlinear Elliptic Problems

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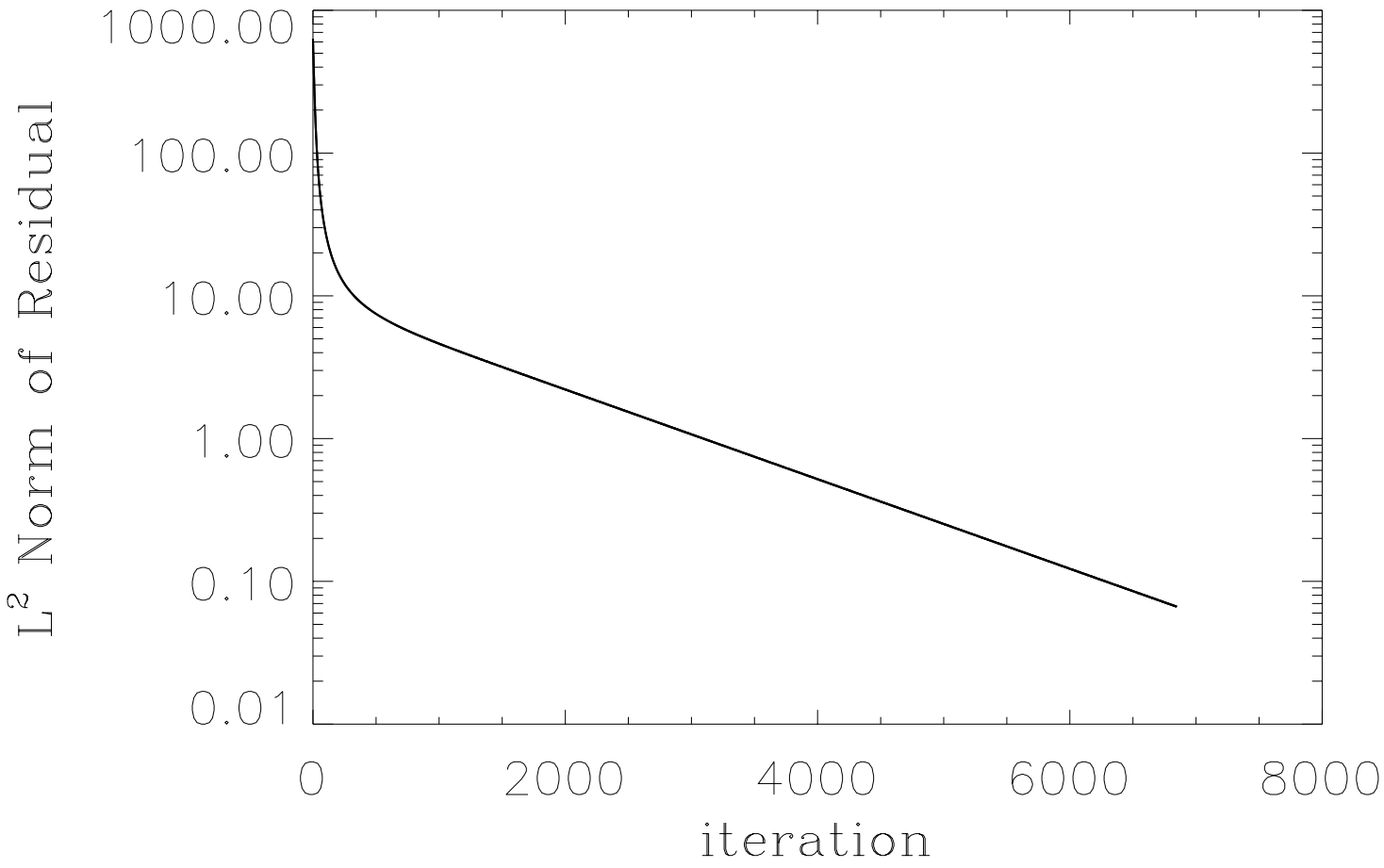

Single-grid (Jacobi) Solver

Multigrid Solver for Nonlinear Elliptic Problems

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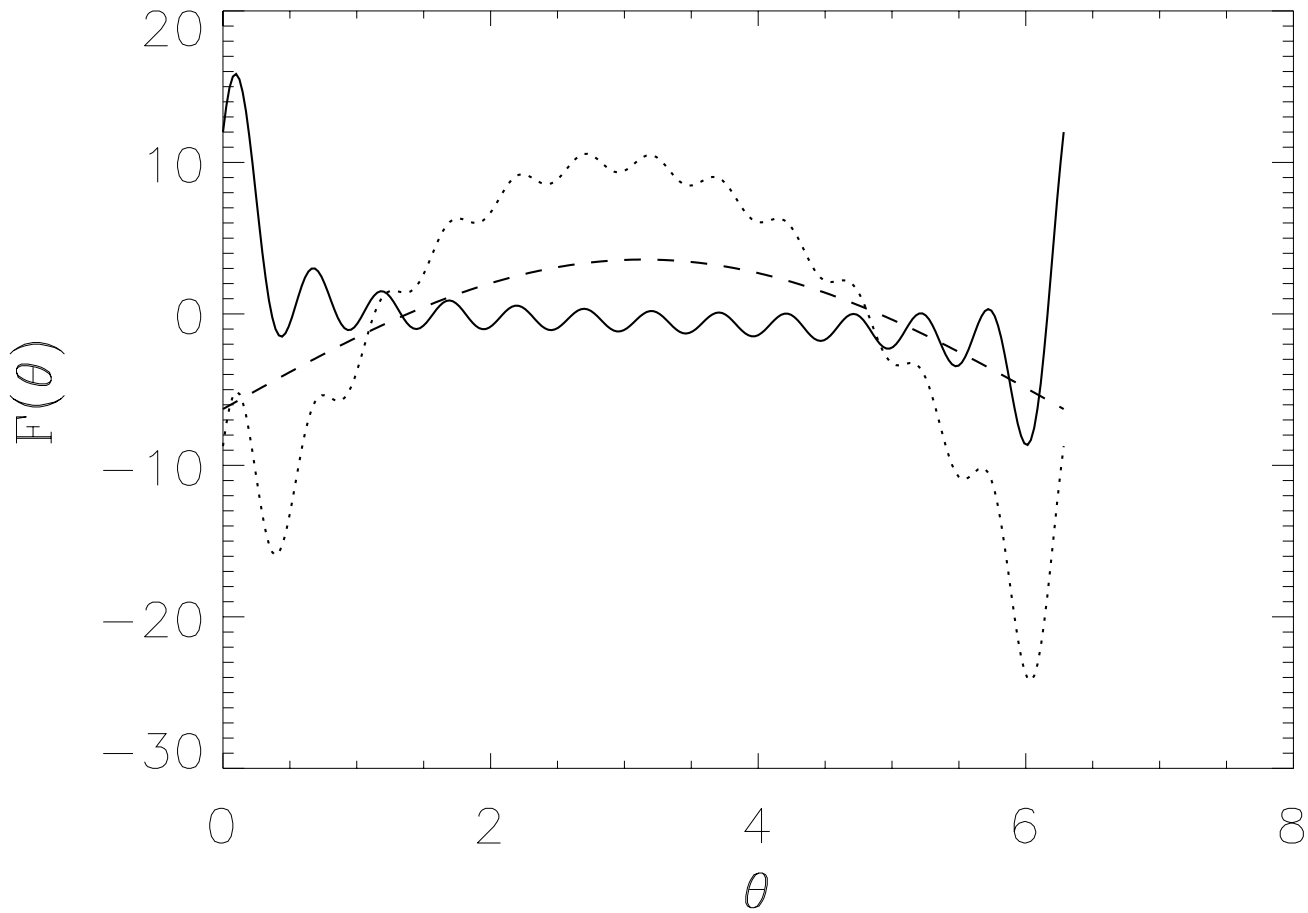

After 1 V cycle...

Multigrid Solver for Nonlinear Elliptic Problems

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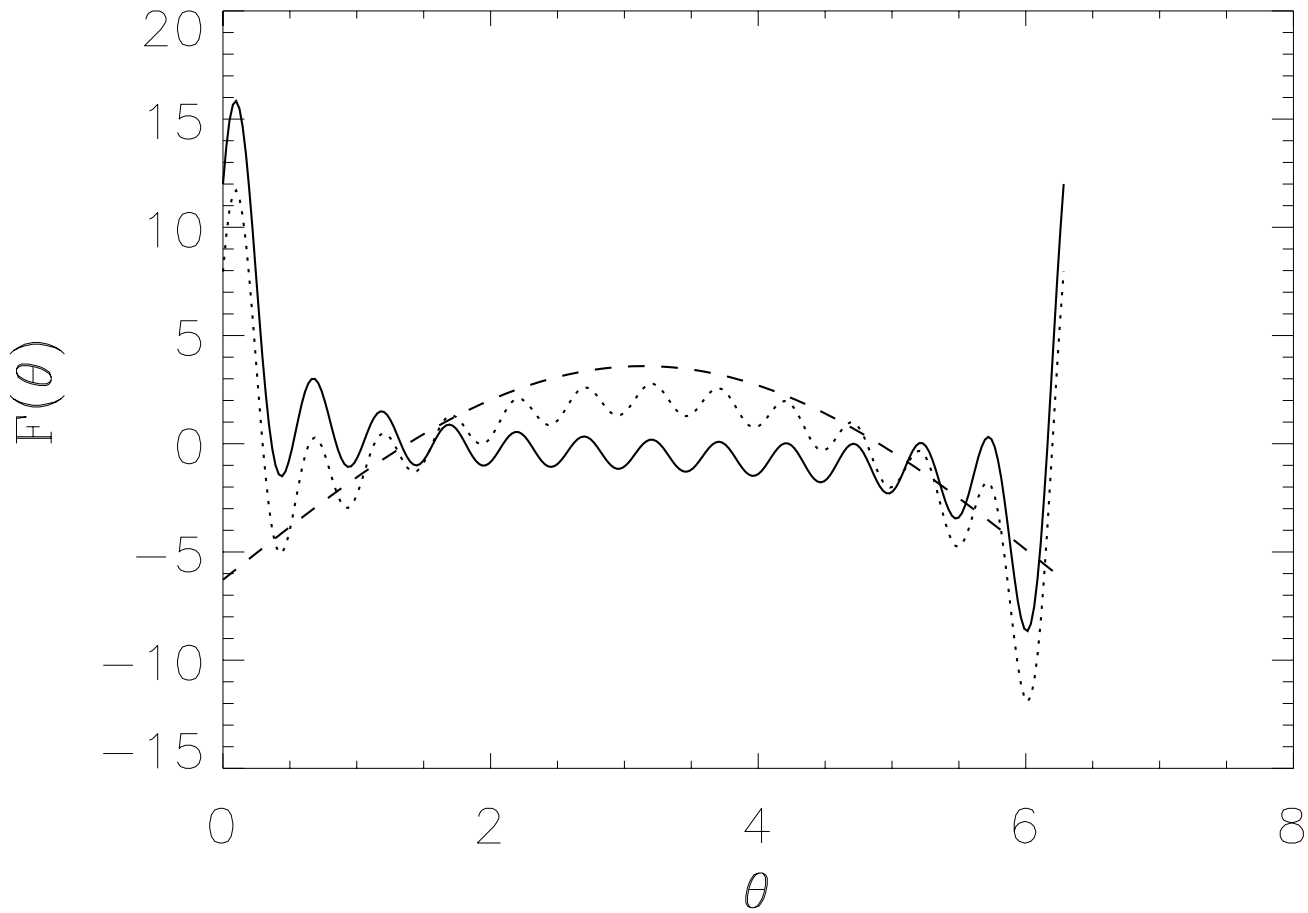

After 3 V cycles...

Multigrid Solver for Nonlinear Elliptic Problems

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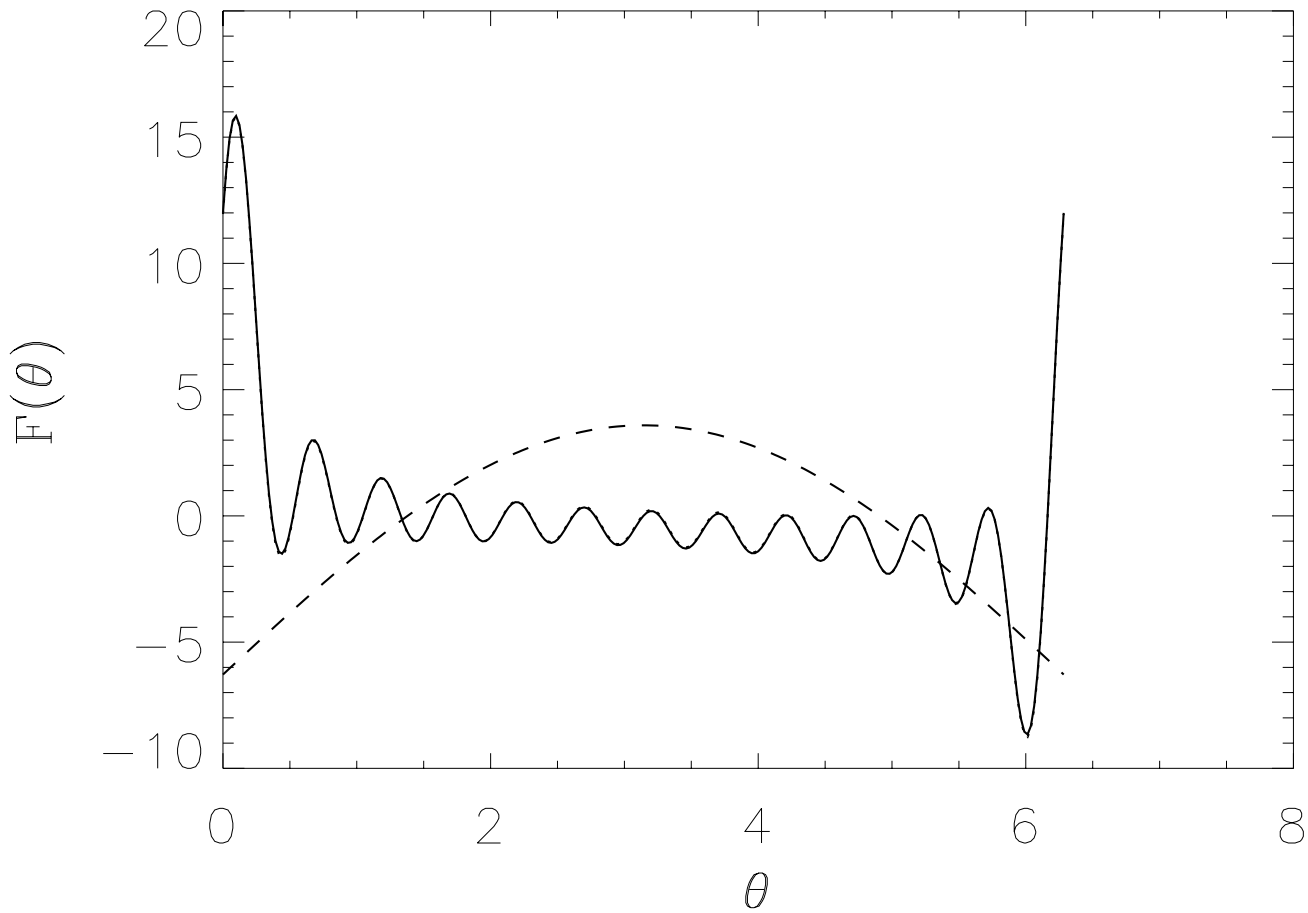


After 7 V cycles...

Linear Benchmarks (Linear Dispersion)

The distribution for species j is written as $F_j = \exp\left(-q_j\Phi/T_j\right) F_{Mj} + h_j$ where the nonadiabatic part, h_j, is governed by

$$\frac{dh_j}{dt} = \exp\left(-\frac{q_j\Phi}{T_j}\right)\left[\mathbf{V}_E\cdot\boldsymbol{\kappa}_j + \frac{q_j}{T_j}\frac{\partial\Phi}{\partial t}\right] F_{Mj} \ ,$$

where $\boldsymbol{\kappa}_j = \boldsymbol{\kappa} g_j(\overline{v}_{||})$; $g_j(\overline{v}_{||}) = 1 - \eta_j\left(1 - \overline{v}_{||}{}^2\right)/2$; and $\overline{v}_{||} = v_{||}/V_{thj}$. Assuming perturbations of the form $\exp\left(i\mathbf{k}\cdot\mathbf{r} - i\omega t\right)$ and linearizing, we get

$$h_j = \left[\omega_\star g_j(\overline{v}_{||}) + \sigma_j\omega\right]\frac{F_{Mj}}{\omega - k_{||}v_{||}}\,\widetilde{\Phi} \ , \tag{5}$$

where $\omega_\star = \left(k_y\rho_s\right)c_s/L_n$ is the drift frequency, $\sigma_j = Z_jT_e/T_j$ and $\widetilde{\Phi} = e\Phi/T_e$. Multiplying Eq.(5) by $v_{||}{}^k$ and integrating over velocity space

$$\int_{-\infty}^{+\infty} h_j v_{||}^k dv_{||} = -n_0\frac{\left(\sqrt{2}V_{thj}\right)^k}{\omega_{||j}}\left\{\left[\sigma_j\omega + \omega_\star\left(1 - \eta_j/2\right)\right]Z^{(k)}\left(\zeta_j\right) + \omega_\star\eta_j Z^{(k+2)}\left(\zeta_j\right)\right\}\widetilde{\Phi} \ ,$$

where $\omega_{||j} \equiv \sqrt{2}k_{||}V_{thj}$, $\zeta_j \equiv \omega/\omega_{||j}$; we have defined

$$Z^{(k)}\left(\zeta\right) \equiv \frac{1}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{x^k}{x-\zeta}\exp\left(-x^2\right)dx \ ,$$

for nonnegative integer k; $Z^{(0)}\left(\zeta\right) \equiv Z\left(\zeta\right)$ is the usual plasma dispersion function.

Linear Benchmarks (Dispersion Relation)

The particle density for species j is

$$\begin{aligned} n_j &= n_0 \exp\left(-\frac{q_j}{T_j}\,\Phi\right) + \int_{-\infty}^{+\infty} h_j dv_{||}\ , \\ &= n_0\left(1-\sigma_j\widetilde{\Phi}\right) + \int_{-\infty}^{+\infty} h_j dv_{||}\ . \end{aligned} \tag{6}$$

Substituting Eq.(6) in the gyrokinetic Poisson equation, ${k_y}^2{\rho_\mathrm{s}}^2\widetilde{\Phi} = \left(n_i - n_e\right)/n_0$, and using Eq.(6), we obtain the dispersion relation for electrostatic drift waves

$$\left(1+\frac{1}{\tau}\ +b\right)\omega = -\omega\left[\zeta_e Z\left(\zeta_e\right) + \frac{1}{\tau}\,\zeta_i Z\left(\zeta_i\right)\right] + \omega_\star\left[\zeta_e R\left(\zeta_e\right) - \zeta_i R\left(\zeta_i\right)\right]\ , \tag{7}$$

where $R\left(\zeta_j\right) \equiv \left(1-\eta_j/2\right) Z\left(\zeta_j\right) + \eta_j\zeta_j\left[1+\zeta_j Z\left(\zeta_j\right)\right]$, $\tau = T_i/T_e$ and $b = {k_y}^2{\rho_\mathrm{s}}^2$. In the cold ions, warm electrons limit

$$\frac{\omega}{k_{||}V_{thi}} \gg 1 \gg \frac{\omega}{k_{||}V_{the}}\ ,$$

Eq.(7) assumes the simplified form of

$$\left(1+b\right)\omega = \omega_\star + i\sqrt{\pi}\zeta_e\left[\omega_\star\left(1-\eta_e/2\right) - \omega\right]\ ,$$

which can be solved for the mode frequency

$$\omega_\mathrm{r} = \frac{\omega_\star}{1+b} \tag{8}$$

and the linear growth rate

$$\begin{aligned}\gamma &= \sqrt{\frac{\pi}{2}}\,\frac{\omega_{\mathrm{r}}}{k_{||}V_{the}}\,\frac{\omega_\star\left(1-\eta_e/2\right)-\omega_{\mathrm{r}}}{1+b} \\ &= \sqrt{\frac{\pi}{2}\,\frac{m_e}{m_i}}\,\frac{{\omega_\star}^2}{k_{||}c_s}\,\frac{\left(1+b\right)\left(1-\eta_e/2\right)-1}{\left(1+b\right)^3}\quad .\end{aligned}$$

Linear Benchmarks (Linear Dispersion)

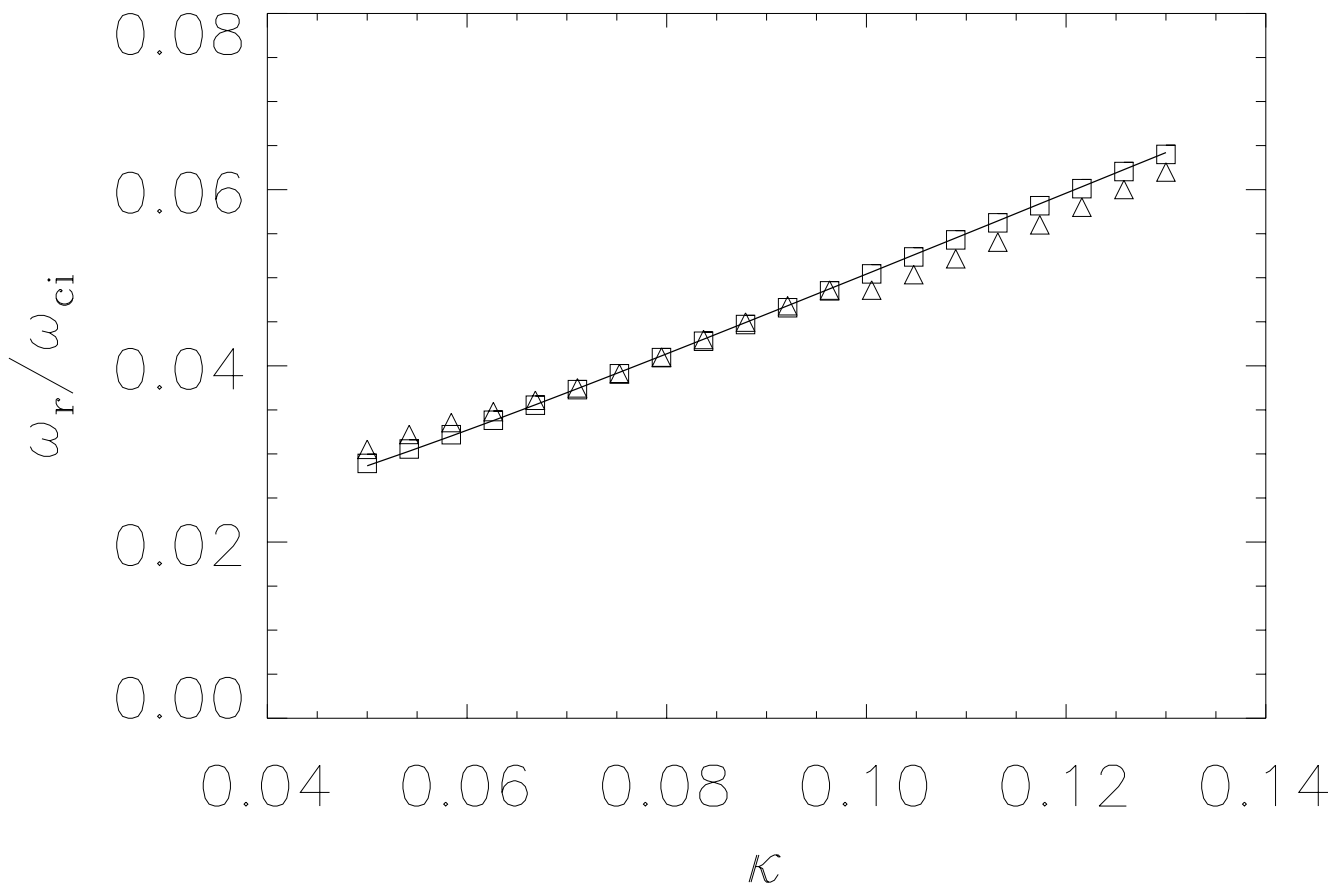
Velocity moment of linearized splitting scheme response + gyrokinetic Poisson Equation

$$\left(1+\frac{1}{\tau}+b\right)\omega=-\omega\left[\zeta_e Z\left(\zeta_e\right)+\frac{1}{\tau}\zeta_i Z\left(\zeta_i\right)\right]+\omega_\star\left[\zeta_e R\left(\zeta_e\right)-\zeta_i R\left(\zeta_i\right)\right] \ ,$$

where $R\left(\zeta_j\right)\equiv\left(1-\eta_j/2\right)Z\left(\zeta_j\right)+\eta_j\zeta_j\left[1+\zeta_j Z\left(\zeta_j\right)\right]/2$, $\zeta_j\equiv\omega/\left(\sqrt{2}k_{||}V_{thj}\right)$, $b={k_y}^2{\rho_\mathrm{s}}^2$ and $Z(\zeta)$ is the plasma dispersion function.

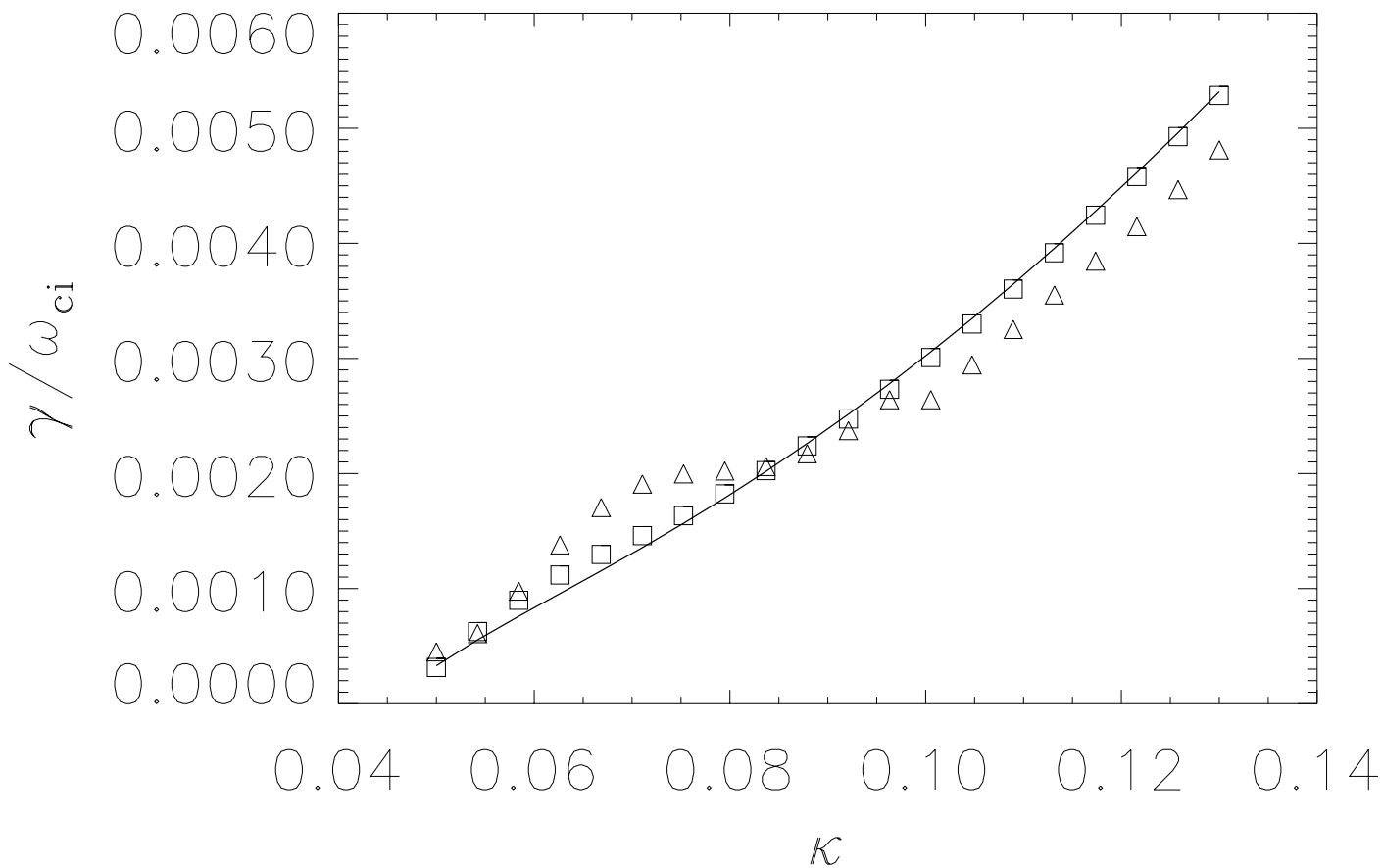
Numerical Solution: Muller's Algorithm in the complex $\omega_r-\gamma$ plane

Linear Benchmarks (Mode Frequency)



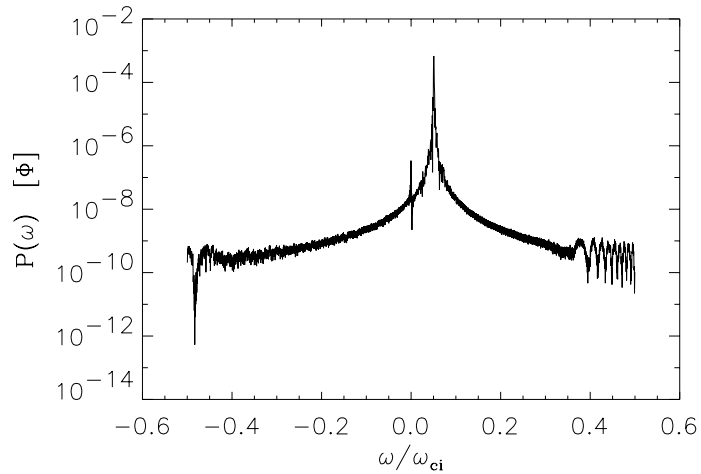
Parameters: $\theta = 0.01$, $\Delta t = 1.0$, $N_i = N_e = 6765$, $L = 8$ on a 64-grid; $\eta_e = \eta_i = 0.0$. Only $n = 1$ mode $(k_\perp \rho_s \simeq 0.78)$

Linear Benchmarks (Growth Rate)

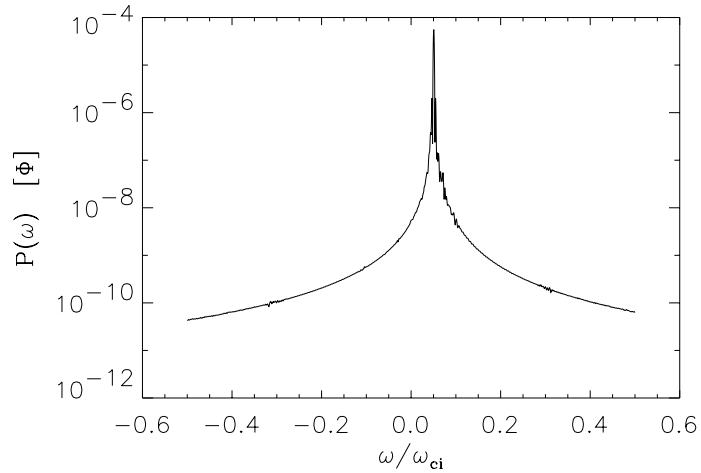


Parameters: $\theta = 0.01$, $\Delta t = 1.0$, $N_i = N_e = 6765$, $L = 8$ on a 64-grid; $\eta_e = \eta_i = 0.0$. Only $n = 1$ mode $(k_\perp \rho_s \simeq 0.78)$

Power Spectrum

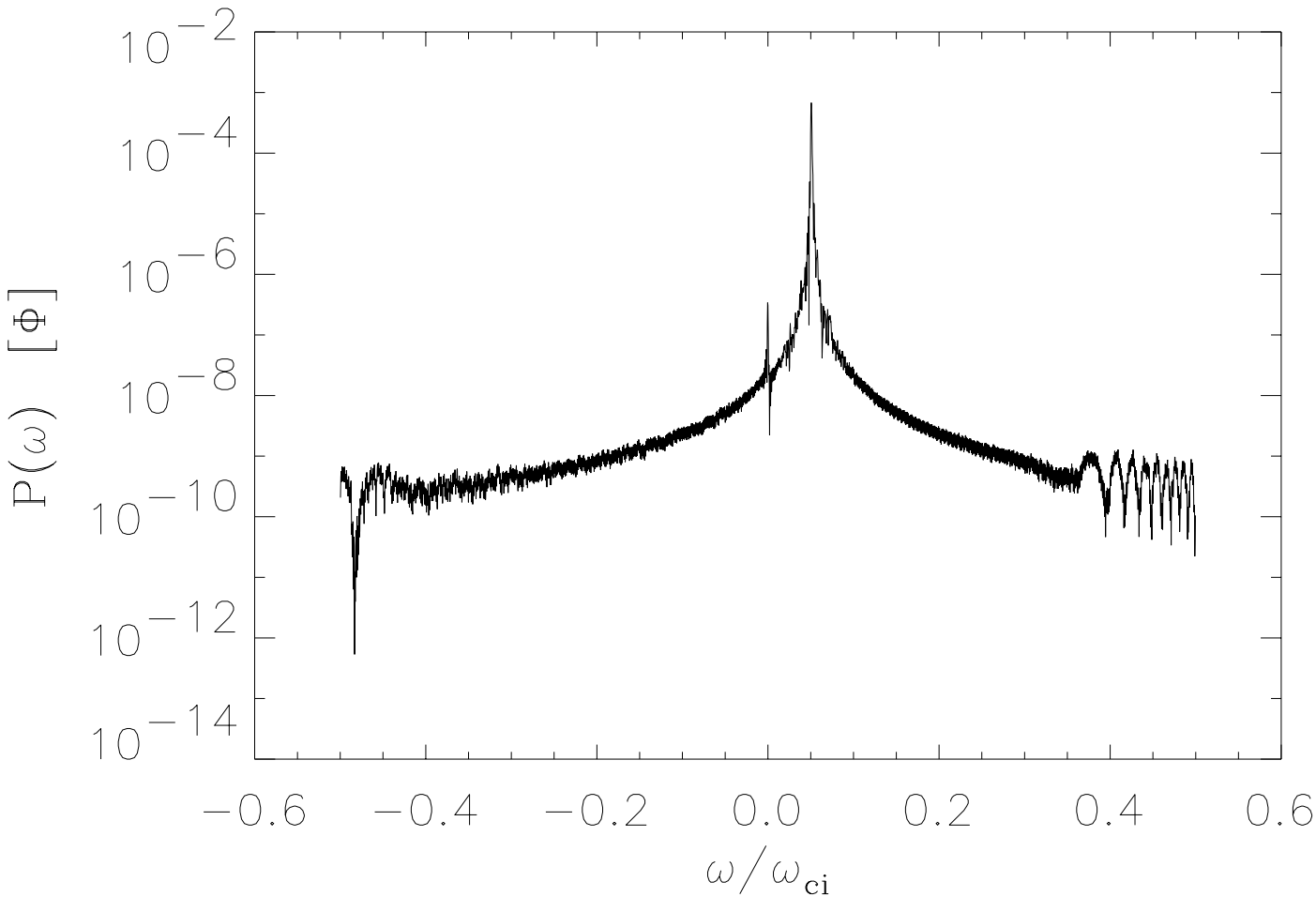


δf scheme (top), splitting scheme (bottom)



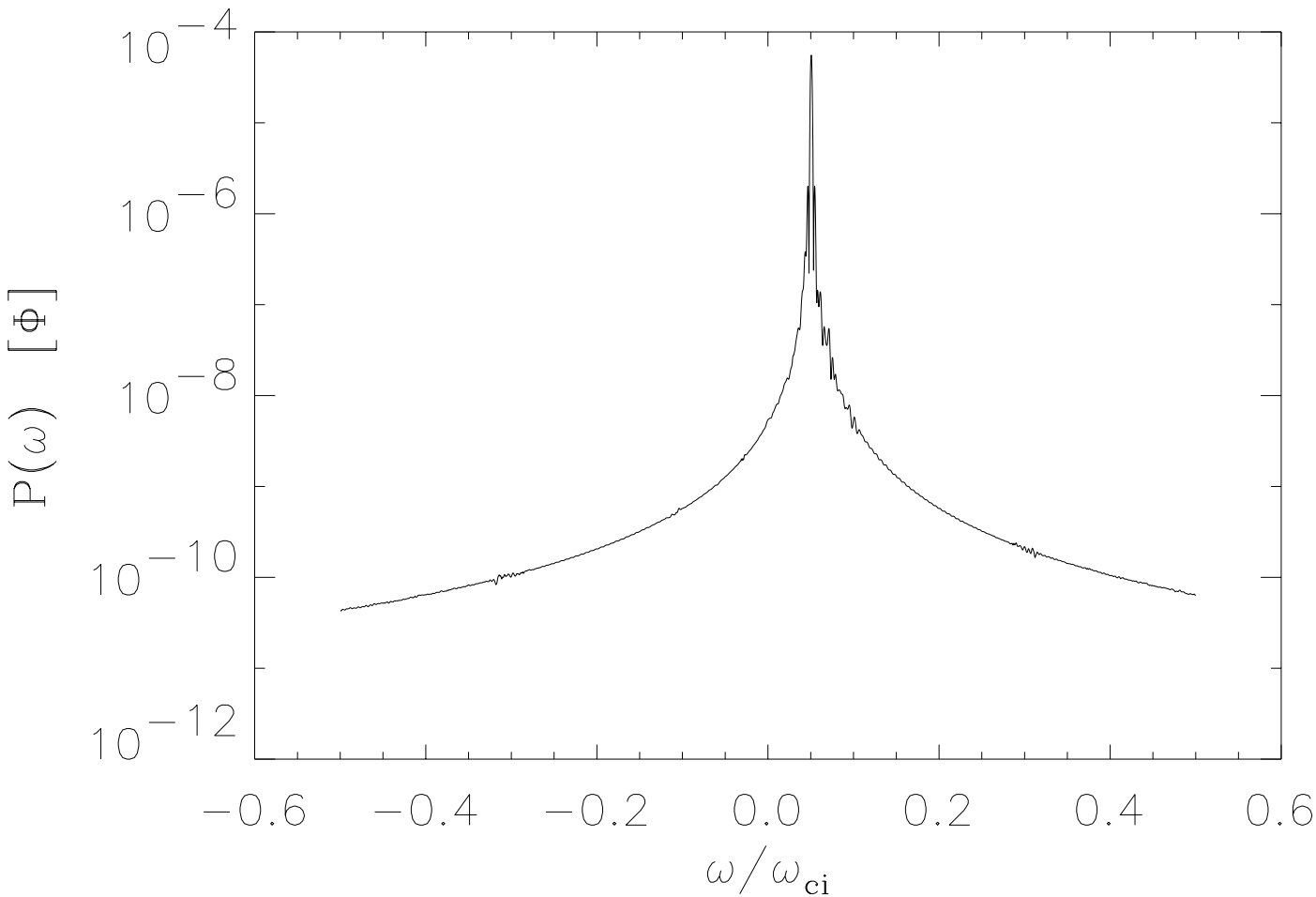
Parameters: 5000 time steps (nonlinear run); $L = 8$ on a 64-grid; $N_i = N_e = 10946$, $\kappa = 0.05$; $\eta_e = \eta_i = 0.0$; $\theta = 0.01$.

Power Spectrum (δf scheme)



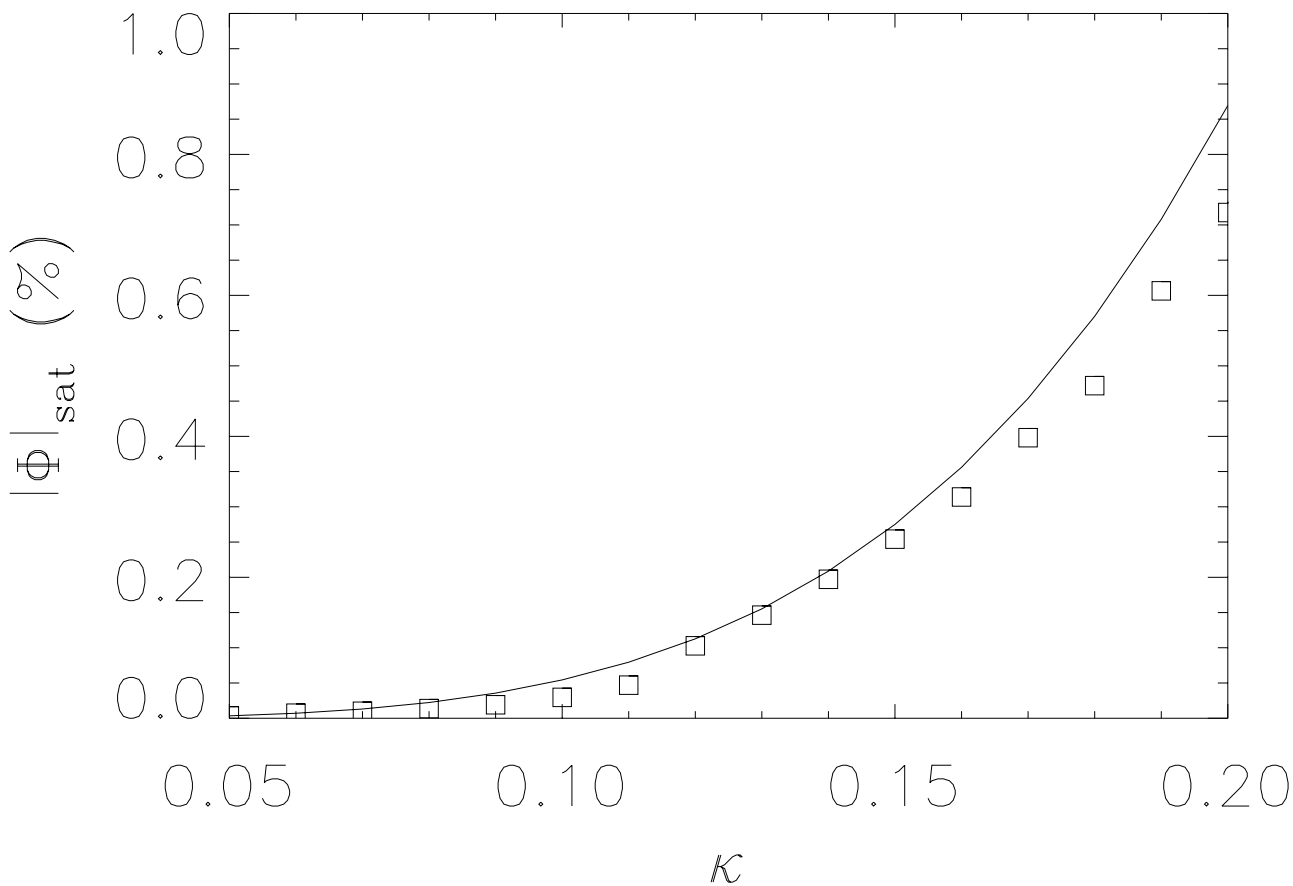
Parameters: 5000 time steps (nonlinear run); $L = 8$ on a 64-grid; $N_i = N_e = 10946$, $\kappa = 0.05$; $\eta_e = \eta_i = 0.0$; $\theta = 0.01$.

Power Spectrum (splitting scheme)



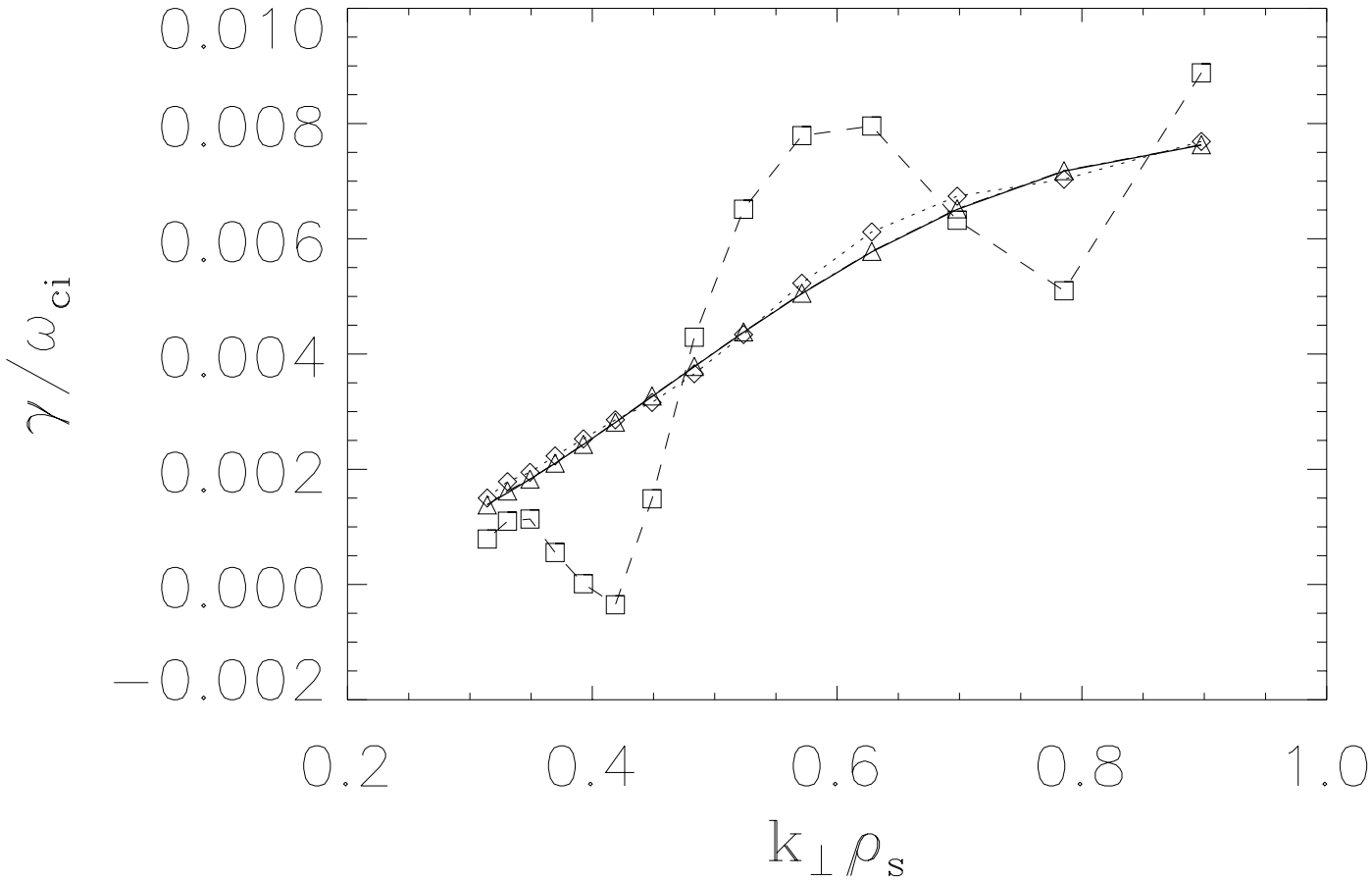
Parameters: 5000 time steps (nonlinear run); $L = 8$ on a 64-grid; $N_i = N_e = 10946$, $\kappa = 0.05$; $\eta_e = \eta_i = 0.0$; $\theta = 0.01$.

Nonlinear Saturation



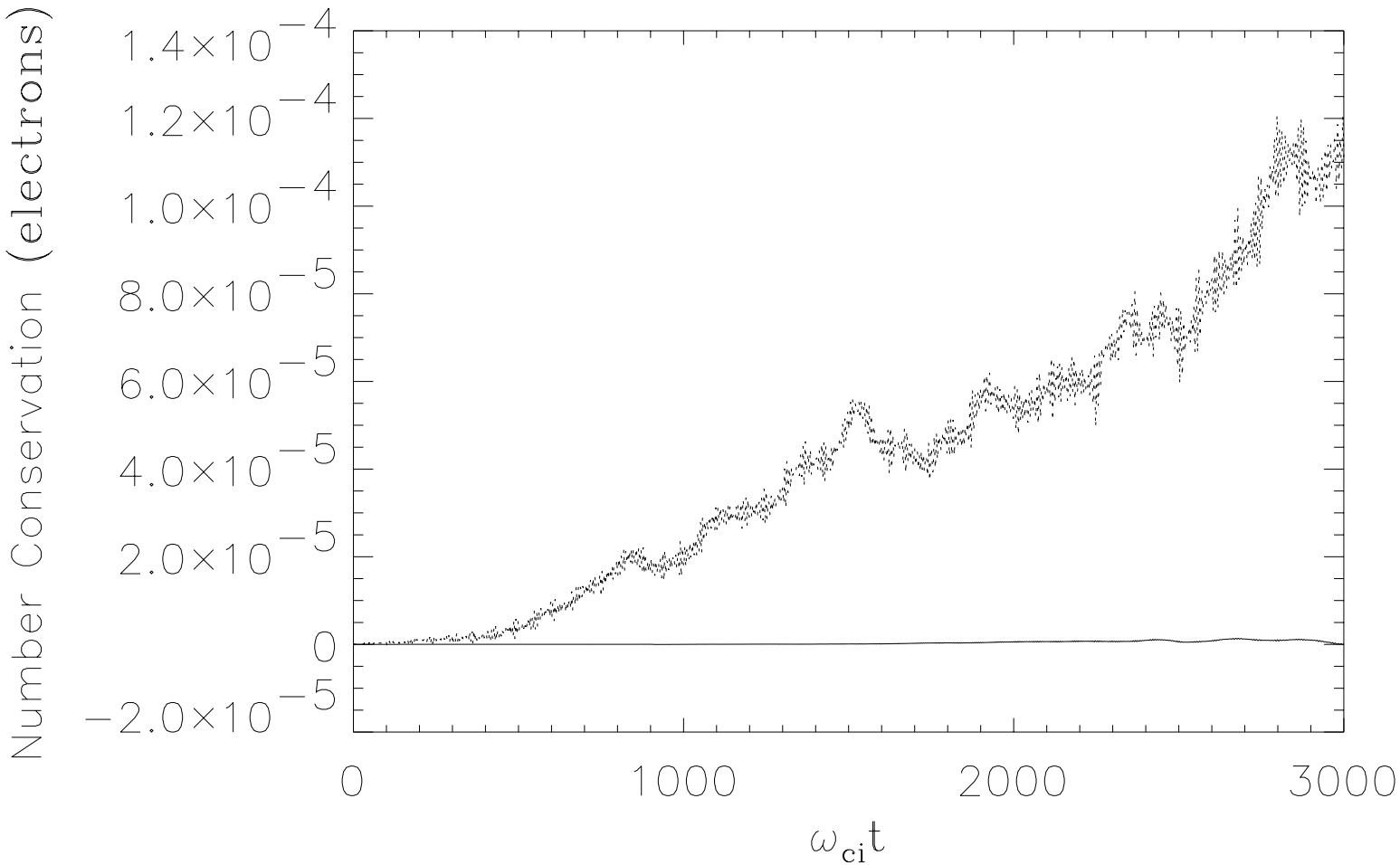
Parameters: nonlinear run with $\Delta t = 1.0$; $N_i = N_i = 6765$; $\theta = 0.01$; $L = 8$ on 64-grid. Plain line: three-wave mode coupling theory of Parker and Lee (Phys. Fuids, 1993)

Simulations with Few Electrons



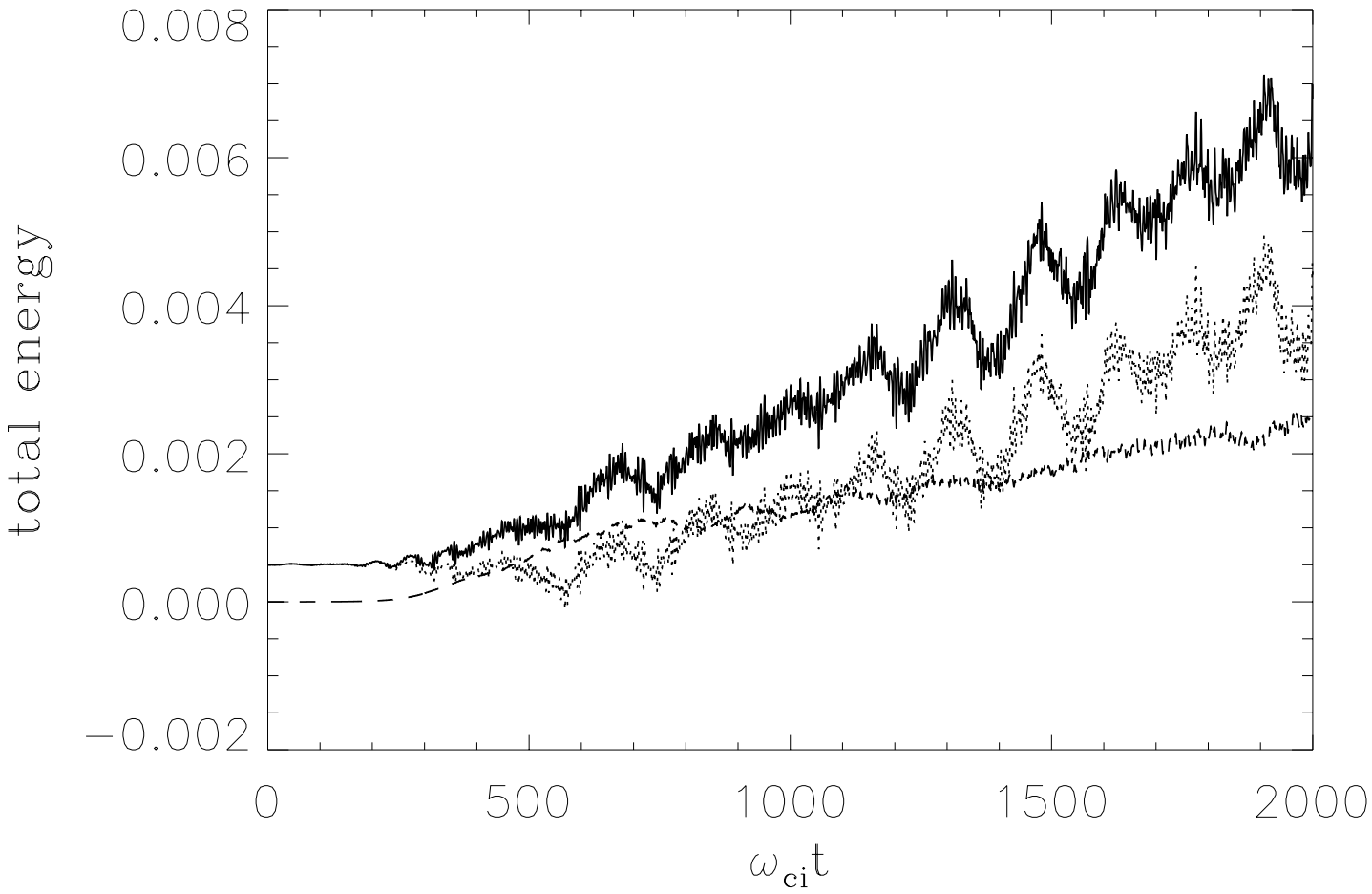
Parameters: $N_i = 10946$, $N_e = 144$ (squares), $N_e = 233$ (diamonds), $N_e = 4181$ (triangles); on a 512-grid with $\kappa = 0.15$

Number Conservation



Nonlinear Run with $N_e = N_i = 6765$...$\langle\langle W_e \rangle\rangle = 4.3\times10^{-5}$ (δf scheme)...$\langle\langle W_e \rangle\rangle = 3.2\times10^{-7}$ (splitting scheme)

Energy Conservation...δf Scheme



Nonlinear Run with $N_e = N_i = 6765$

Energy Conservation...Splitting Scheme

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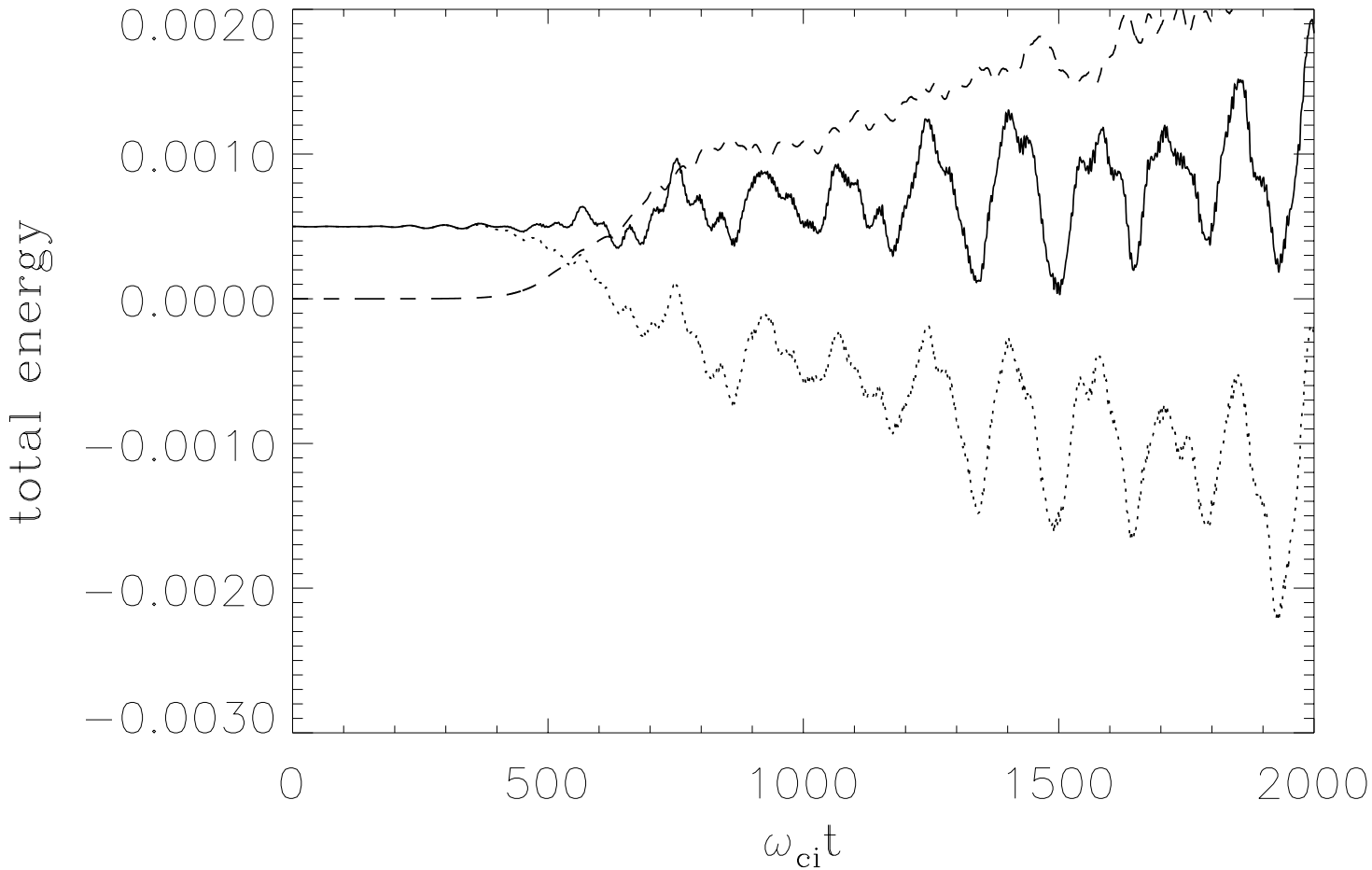

Nonlinear Run with $N_e = N_i = 6765$...no secular increase as in the δf scheme

Conclusions

- It pays off (both linear and nonlinearly) to split correctly... (splitting with Φ in the electromagnetic case is not optimal (Y. Chen's talk) , on physical and numerical grounds... (see papers by Krommes (1993) and Lee, Lewandowski *et al* (2001) re discussion on thermodynamics properties)
- Splitting scheme has favorable *linear* and *nonlinear* properties
- Simulations wih few electrons are accurate (2 electrons/cell yields good results): impact on large-scale PIC codes which routinely run at 10 markers/cell (adiabatic regime)
- Good Energy Conservation (no secular increase as in δf)
- Toroidal (axisymmetric) Case shows converged χ_i
- Electromagnetic Case is promising...(separate talk)
- Multigrid Particle-in-cell (MUGPIC) Concept: computational work scales linearly with number of markers and number of grid points in configuration space, with no sacrifice on geometry or dubious assumptions...