

How to Reduce Noise in Particle Simulation

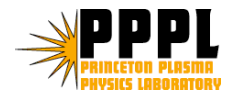
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(August 2005)

- Introduction
 - Efficiency and Scalability of Particle Codes on Parallel Computers
- Thermodynamic Properties of a Simulation Plasma
 - Fluctuation Dissipation Theorem for an Equilibrium Plasma
 - Noise Properties in an Unstable Plasma
- Why do we want to get rid of the Noise?
 - Linear Simulation: Resonant Broadening Effects
 - Nonlinear long time simulation
- Methods to Reduce Particle Noise
 - Quasineutral Simulation
 - Perturbative Particle Simulation
- Particle Simulation vs. Vlasov Simulation
- Entropy Balance, Collisionless Dissipation and Collisional Dissipation
- Conclusions



**Testimony of Dr. Raymond L. Orbach, Director, Office of Science, U.S.
Department of Energy before the U.S. House of Representatives
Committee on Science
July 16, 2003**

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Looking to the future, we are beginning a **Fusion Simulation Project** to build a computer model that will fully simulate a burning plasma to both predict and interpret ITER performance and, eventually, assist in the design of a commercially feasible fusion power reactor. Our best estimate, however is that success in this effort will require at least **50 teraFLOPS** of sustained computing power.

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Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas

SciDAC - Advanced Simulation of Fusion Plasmas

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AMR Project for
Multiscale Gyrokinetic Particle Simulation
of Magnetized Plasmas

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and

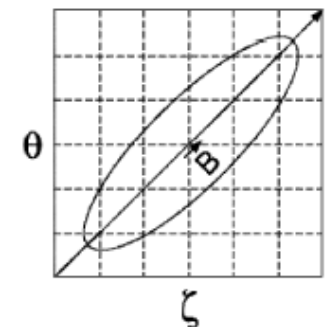
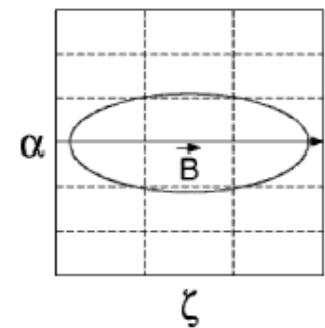
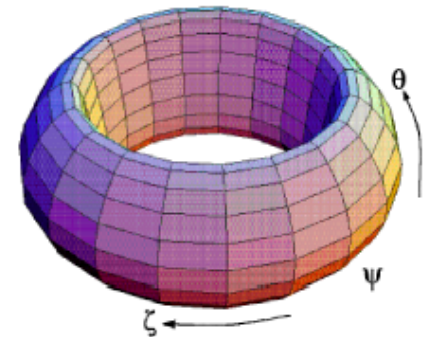
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Global Gyrokinetic Toroidal Particle Simulation Code: GTC

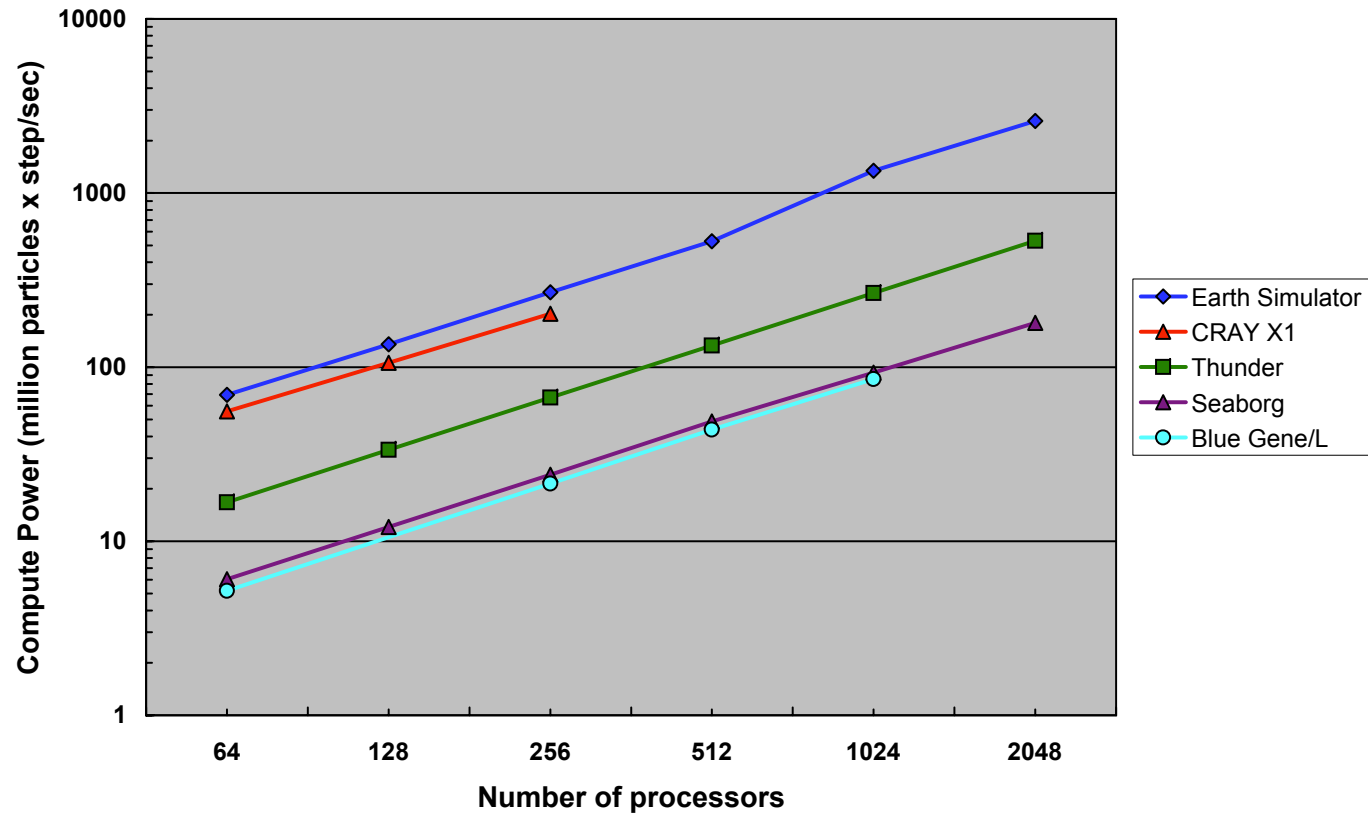
[Z. Lin, T. S. Hahm, W. W. Lee, W. M. Tang and R. B. White, *Science* (1998)]

- Magnetic coordinates (ψ, θ, ζ) [Boozer, 1981]
- Guiding center Hamiltonian [Boozer, 1982; White and Chance, 1984]
- Non-spectral Poisson solver [Lin and Lee, 1995]
- Global field-line coordinates: $(\psi, \alpha, \zeta), \alpha = \theta - \zeta/q$
 - Microinstability wavelength: $\lambda_{\perp} \propto \rho_i, \lambda_{\parallel} \propto qR$
 - With field-line coordinates: Grid # $N \propto a^2$, a : minor radius, $\Delta\zeta \propto R$
 - Without field-line coordinates: grid # $N \propto a^3$, $\Delta\zeta \propto \rho$
 - Larger time step: no high k_{\parallel} modes
- Collisions: e-i, i-i and e-e
- Neoclassical Transport Code: GTC-neo [W. X. Wang, 2004]



GTC performance on MPP platforms - S. Ethier

Number of particles (in million) that move 1 step in 1 second



- Gyrokinetic particle codes are portable, scalable and efficient on both cache-based and vector-parallel MPP platforms

GTC performance

# of proc.	#part (Billion)	IBM SP 3 (Seaborg)		Itanium 2 + Quadrics		Opteron + Infiniband		CRAY X1		ES	
		Gflop	%Pk	Gflop	%Pk	Gflop	%Pk	Gflop	%Pk	Gflop	%Pk
64	0.207	9.0	9.3	25.0	6.9	37.8	13.3	82.6	10.1	102.4	20.0
128	0.414	17.9	9.3	49.9	6.9	75.5	13.3	156.2	9.6	199.7	19.5
256	0.828	35.8	9.3	97.3	6.9	145.9	13.1	299.5	9.1	396.8	19.4
512	1.657	71.7	9.4	194.6	6.8	261.1	11.6			783.4	19.1
1024	3.314	143.4	8.7	378.9	6.7					1,925	23.5
2048	6.627	266.2	8.4	757.8	6.7					3,727	22.7

3.7 Teraflops achieved on the Earth Simulator with 2,048 processors using 6.6 billion particles!!

Numerical Schemes

- Vlasov - Poisson System

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

$$\nabla^2 \phi = -4\pi \sum_{\alpha} q_{\alpha} \int F_{\alpha} d\mathbf{v}$$

- Particle Codes: need only spatial grid

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v}_j$$

$$\frac{d\mathbf{v}_j}{dt} = \frac{q}{m} \mathbf{E}(\mathbf{x}_j)$$

$$F(\mathbf{x}, \mathbf{v}, t) = \sum_{j=1}^N \delta[\mathbf{x} - \mathbf{x}_j(t)] \delta[\mathbf{v} - \mathbf{v}_j(t)]$$

- Vlasov Codes: need spatial grid and velocity grid

$$\frac{d\mathbf{x}_g}{dt} = \mathbf{v}_g$$

$$\frac{d\mathbf{v}_g}{dt} = \frac{q}{m} \mathbf{E}(\mathbf{x}_g)$$

$$F(\mathbf{x}_g + d\mathbf{x}_g, \mathbf{v}_g + d\mathbf{v}_g, t + dt) = F(\mathbf{x}_g, \mathbf{v}_g, t)$$

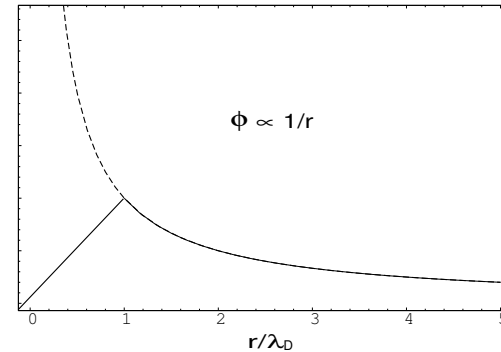
NOISE R US

- *One man's noise is another man's signal [Birdsall & Langdon].*
- *Without noise, there would be no particle simulation.*
- *Without proper treatment of noise, there would still be no particle simulation.*

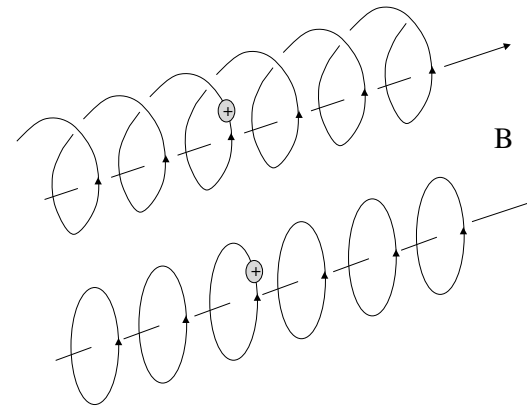


Modified Dynamics for Particle Pushing

- Finite-size particles
[Dawson et al. '68; Birdsall et al. '68]
 - Coulomb interactions are collisionless
 - Collisional effects are subgrid phenomena



- Gyrokinetic particles
[Lee PF '83]
 - Gyromotion becomes motion of rotating charged rings
 - Polarization Effects in the field equation



- Efficient numerical methods to account for finite Larmor radius effects
[Lee JCP '87; Lee and Qin PP '03]

Gyrokinetic Vlasov-Maxwell Equations in Toroidal Geometry

- GK Vlasov equation - in gyrocenter coordinates

[T. S. Hahm et al. PF '88; T. S. Hahm PF '88; Brizard PF '88; Brizard J. Plas. Phys. '89]

$$\frac{\partial F_{\alpha gc}}{\partial t} + \frac{d\mathbf{R}}{dt} \cdot \frac{\partial F_{\alpha gc}}{\partial \mathbf{R}} + \frac{dv_{\parallel}}{dt} \frac{\partial F_{\alpha gc}}{\partial v_{\parallel}} = 0,$$

$$\frac{d\mathbf{R}}{dt} = v_{\parallel} \mathbf{b}^* + \frac{v_{\perp}^2}{2\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times \nabla \ln B_0 - \frac{c}{B_0} \nabla \bar{\phi} \times \hat{\mathbf{b}}_0$$

$$\frac{dv_{\parallel}}{dt} = -\frac{v_{\perp}^2}{2} \mathbf{b}^* \cdot \nabla \ln B_0 - \frac{q_{\alpha}}{m_{\alpha}} \left(\mathbf{b}^* \cdot \nabla \bar{\phi} + \frac{1}{c} \frac{\partial \bar{A}_{\parallel}}{\partial t} \right)$$

$$\mu_B \equiv v_{\perp}^2 / 2B_0 \approx \text{cons.}$$

$$\mathbf{b}^* \equiv \mathbf{b} + \frac{v_{\parallel}}{\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times (\hat{\mathbf{b}}_0 \cdot \nabla) \hat{\mathbf{b}}_0, \quad \mathbf{b} = \hat{\mathbf{b}}_0 + \frac{\nabla \times \bar{\mathbf{A}}}{B_0}$$

$$\begin{pmatrix} \bar{\phi} \\ \bar{\mathbf{A}} \end{pmatrix} (\mathbf{R}) = \langle \int \begin{pmatrix} \phi \\ \mathbf{A} \end{pmatrix} (\mathbf{x}) \delta(\mathbf{x} - \mathbf{R} - \rho) d\mathbf{x} \rangle_{\varphi},$$

$$F_{\alpha gc} = \sum_{j=1}^{N_{\alpha}} \delta(\mathbf{R} - \mathbf{R}_{\alpha j}) \delta(\mu - \mu_{\alpha j}) \delta(v_{\parallel} - v_{\parallel \alpha j})$$

GK Equations in Toroidal Geometry (cont.)

- GK Poisson's equation - in laboratory coordinates [Lee JCP '87]

$$\cancel{\nabla^2} \phi + \frac{\tau}{\lambda_D^2} [\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x})] = -4\pi \rho_{gc}(\mathbf{x}) \quad \xrightarrow{k_{\perp} \rho_s \ll 1} \quad \frac{\rho_s^2}{\lambda_D^2} \nabla_{\perp}^2 = -4\pi \rho_{gc}(\mathbf{x})$$

Quasineutral

$$\tilde{\phi}(\mathbf{x}) \equiv \langle \int \bar{\phi}(\mathbf{R}) F_i(\mathbf{R}, \mu, v_{\parallel}) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} d\mu dv_{\parallel} \rangle_{\varphi}$$

$$\rho_{gc}(\mathbf{x}) = \sum_{\alpha} q_{\alpha} \langle \int F_{\alpha gc}(\mathbf{R}) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} dv_{\parallel} d\mu \rangle_{\varphi}$$

- GK Ampere's law -- in laboratory coordinates [Qin et al. PP '99]

$$\nabla^2 \mathbf{A} - \frac{1}{v_A^2} \cancel{\frac{\partial^2 \mathbf{A}_{\perp}}{\partial t^2}} = -\frac{4\pi}{c} \mathbf{J}_{gc} \quad \omega^2 / k^2 v_A^2 \ll 1$$

$$\mathbf{J}_{gc}(\mathbf{x}) = \mathbf{J}_{\parallel gc}(\mathbf{x}) + \mathbf{J}_{\perp gc}^M(\mathbf{x}) + \mathbf{J}_{\perp gc}^d(\mathbf{x})$$

$$= \sum_{\alpha} q_{\alpha} \langle \int (\mathbf{v}_{\parallel} + \mathbf{v}_{\perp} + \mathbf{v}_d) F_{\alpha gc}(\mathbf{R}) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} dv_{\parallel} d\mu \rangle_{\varphi}$$

$$\mathbf{v}_d \equiv \frac{v_{\parallel}^2}{\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times (\hat{\mathbf{b}}_0 \cdot \nabla) \hat{\mathbf{b}}_0 + \frac{v_{\perp}^2}{2\Omega_{\alpha 0}} \hat{\mathbf{b}}_0 \times \nabla \ln B_0$$

Simple Linear Dispersion Relations

$$\epsilon \equiv 1 + [1 + \xi_e Z(\xi_e) + \tau + \tau \xi_i Z(\xi_i)] / (k \lambda_{De})^2 = 0$$

$$\xi_\alpha \equiv \omega / \sqrt{2k} v_{t\alpha} \quad , \quad v_{t\alpha} \equiv \sqrt{\frac{T_\alpha}{m_\alpha}} \quad , \quad \lambda_{De} \equiv \sqrt{T_e / 4\pi n_0 e^2}$$

Damped Normal Modes

- cold ion and cold electron limit

$$\omega = \pm \omega_{pe} \sqrt{1 + 3k^2 \lambda_{De}^2} \quad , \quad \omega_{pe} = \sqrt{4\pi n_0 e^2 / m_e}$$

- cold ion and warm electron limit

$$\omega = \pm \omega_s \quad , \quad \omega_s = \frac{kc_s}{\sqrt{1 + k^2 \lambda_{De}^2}}$$

Fluctuation-Dissipation Theorem and Particle Simulation

$$L|E(k, \omega)|^2/8\pi = -(T/\omega)Im(1/\epsilon)$$

- Fluctuations per k -mode

$$L|E(k)|^2/8\pi = \int (d\omega/2\pi)L|E(k, \omega)|^2/8\pi = (T/2)[1/\epsilon(k, \omega = \infty) - 1/\epsilon(k, \omega = 0)].$$

→

$$L|E(k)|^2/8\pi = (T/2)/(1 + k^2\lambda_D^2)$$

- Fluctuations residing in normal modes for $k^2\lambda_D^2 \ll 1$

$$L|E(k, \omega)|^2/8\pi = T\pi\delta(\omega Re \epsilon)$$

$$L|E(k)|^2/8\pi = \sum_{\Omega} L|E(k, \Omega)|^2/8\pi = (T/2) \sum_{\Omega} \frac{1}{|\partial\omega Re \epsilon/\partial\omega|_{\Omega}}.$$

→

$$L|E(k, \omega_{pe})|^2/8\pi = T/2,$$

$$L|E(k, \omega_s)|^2/8\pi = (T/2) \frac{k^2\lambda_{De}^2}{1 + k^2\lambda_{De}^2}.$$

→

$$|e\Phi(k, \omega_{pe})/T_e|_{th} = \frac{1}{\sqrt{N}k\lambda_{De}},$$

$$|e\Phi(k, \omega_s)/T_e|_{th} = \frac{1}{\sqrt{N}}$$

Fluctuation-Dissipation Theorem and Particle Simulation

- Plasma Waves and Finite-Size Particles [Langdon and Birdsall, PF **13**, 2115 (1970)]

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = \frac{T/2}{1 + k^2 \lambda_D^2 / S^2} \rightarrow T/2, \quad V \text{ -- volume, } S \text{ -- particle shape}$$

- Gyrokinetic Particle Simulation [Krommes et al., PF '86; Lee, JCP '87]

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = \frac{\lambda_D^2}{\rho_s^2} (T/2) \quad \text{for } k\rho_i \ll 1$$

- Shear-Alfven Waves in Gyrokinetic Plasmas Lee et al., PP '01]

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = \frac{\lambda_D^2}{\rho_s^2} \frac{T/2}{1 + \omega_{pe}^2 / c^2 k^2}, \quad \text{cold electrons}$$

$$V \frac{|\mathbf{E}(\mathbf{k})|^2}{8\pi} = k^2 \lambda_D^2 \frac{T/2}{1 + k^2 \rho_s^2}, \quad \text{warm electrons}$$

- Compressional-Alfven Waves in Gyrokinetic Plasmas

$$\frac{A_{\perp}}{A_{\parallel}} \sim \frac{\omega^2}{k^2 v_A^2} \ll 1$$

Why do we want to get rid of the Particle Noise?

- Suppression of linear growths due to Resonant Broadening [Lee, JCP '87]:

$$\gamma_L > \Delta\omega \approx k^2 D$$

$$D \approx (\Delta x)^2 / \Delta t \quad \text{-- random walk due to particle noise}$$

- Particle noise in the simulation of unstable modes [Kadomtsev, Plasma Turbulence, '65]
-- noise level remains the same in the nonlinear steady state

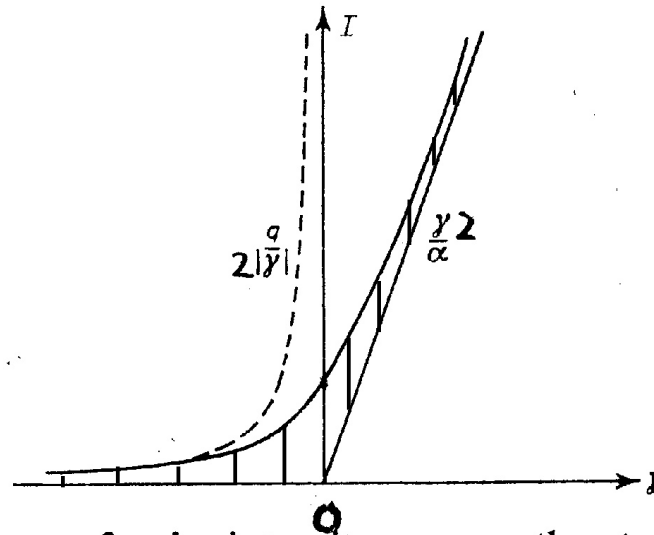


FIG. 11. Dependence of noise intensity on growth rate of small oscillations

Perturbative Particle Simulation

- δf simulation schemes:

-- [Dimits and Lee, JCP '93; Parker and Lee, PF '93; Hu and Krommes, PoP '94]

$$\text{Let } F = F_0 + \delta f \longrightarrow \frac{d\delta f}{dt} = -\frac{dF_0}{dt}$$

$$\text{Let } w \equiv \frac{\delta f}{F} \longrightarrow \delta f = \sum_{j=1}^N w_j \delta(\mathbf{R} - \mathbf{R}_j) \delta(\mu - \mu_j) \delta(v_{\parallel} - v_{\parallel j})$$

$$\text{Noise reduction: } |E|^2 \propto w^2$$

-- [Aydemir, PoP '94]

$$F = F_0 + \delta f \longrightarrow w \equiv \frac{\delta n}{n}$$

- Split-weight schemes: [Manuilskiy and Lee, PoP '00; Lee et al., PoP '01]

$$F = F_0 + \psi F_0 + \delta h \quad \psi = \phi + \frac{1}{c} \int \frac{\partial A_{\parallel}}{\partial t} dx_{\parallel 0}$$

- Time step is determined by zeroth order transit time of the electrons along the field line.

- CFL conditions can be violated with impunity.

- Perturbative Scheme: $F = F_0 + \delta f \longrightarrow w \equiv \frac{\delta f}{F}$

$$\frac{dF}{dt} \equiv \frac{\partial F}{\partial t} + x \frac{\partial F}{\partial x} + \frac{q}{m} E \frac{\partial F}{\partial v} = 0$$

$$\frac{d\delta f}{dt} = -\frac{q}{m} \frac{\partial F_0}{\partial v} \longrightarrow \frac{dw}{dt} = -\frac{q}{m} (1-w) E \frac{1}{F_0} \frac{\partial F_0}{\partial v}$$

$$\nabla^2 \phi = -4\pi \sum_{\alpha} q_{\alpha} \sum_{j=1}^N w_{\alpha j} \delta(x - x_{\alpha j})$$

- Split-Weight Scheme: $F = F_0 + \phi F_0 + \delta h \longrightarrow w^{NA} \equiv \frac{\delta h}{F}$

$$\frac{d\delta h_e}{dt} = -(1 + \phi) F_{0e} \frac{\partial \phi}{\partial t} \longrightarrow \frac{dw^{NA}}{dt} = -(1 - w^{NA}) \frac{\partial \phi}{\partial t}$$

$$\cancel{\nabla^2} \phi - \phi / \lambda_D^2 = -4\pi e \int (\delta f_i - \delta h_e) dv$$

quasineutral simulation

$$\nabla^2 \frac{\partial \phi}{\partial t} = 4\pi e \frac{\partial}{\partial x} \int v (\delta f_i - \delta h_e) dv$$

Thermal Noise in Particle Simulation of Drift Waves in ID - Parker & Lee, PFB '93

$N_{particle} = 987$
 $N_{grid} = 16$

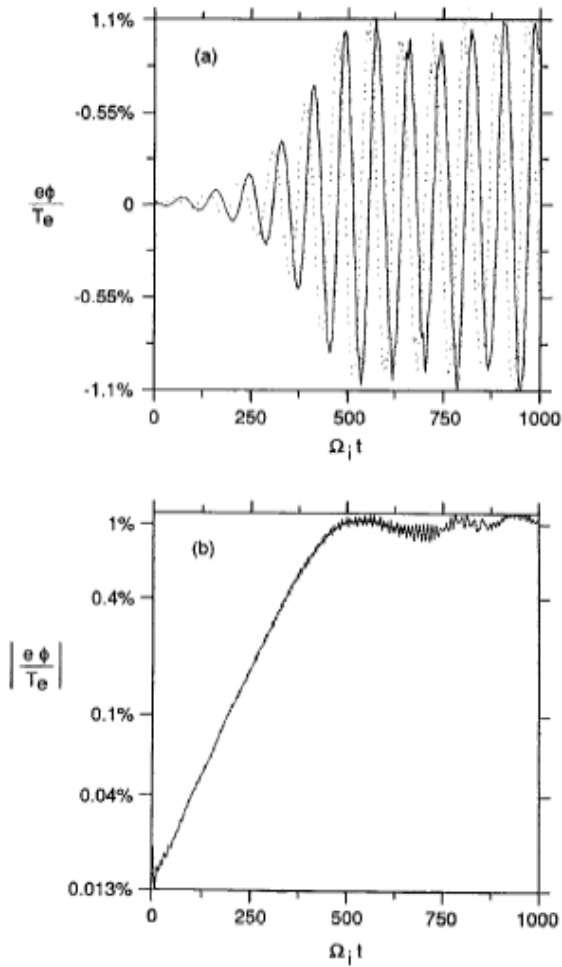


FIG. 1. The $n=1$ drift instability ($k_{\parallel} \rho_s = 0.8$) for the run with 987 particles on a 16-grid system. (a) The time history for the real (solid line) and imaginary (dashed line) parts of the electrostatic potential and (b) the corresponding amplitude evolution.

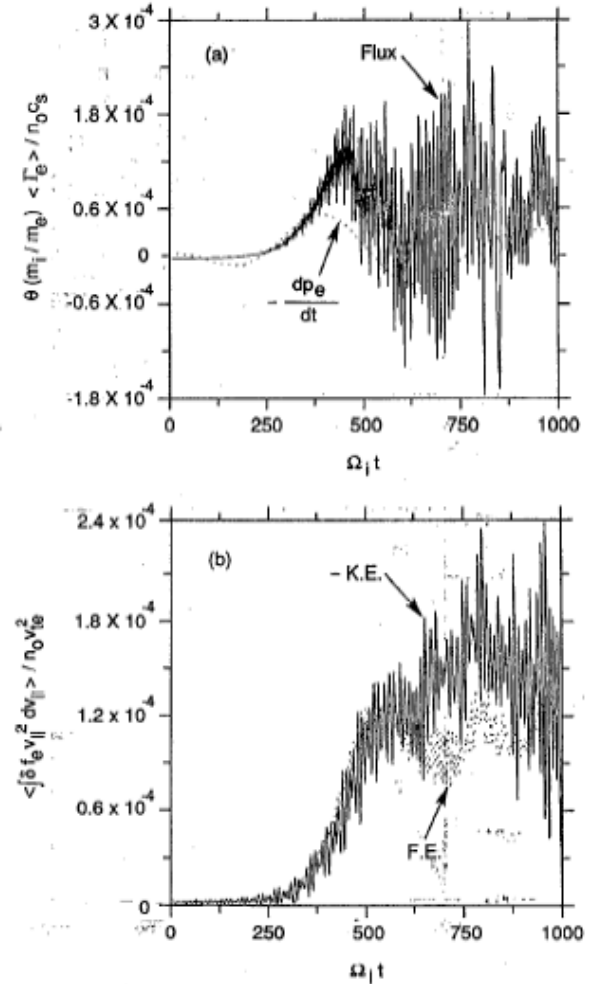


FIG. 3. The 987 particle run. (a) Time history for the electron particle flux (solid line) and the time rate of change for the electron parallel momentum (dashed line) and (b) the time evolution for the perturbed electron kinetic energy (solid line) and the field energy (dashed line).

$$e\phi/T_e)_{noise} \approx w_{rms} / (\sqrt{N_p} k_{\perp} \rho_s) \approx 0.3\%$$

$$\omega_H = \sqrt{m_i/m_e} (k_{\parallel}/k_{\perp}) \Omega_i \approx 0.43 \Omega_i$$

Thermal Noise in Particle Simulation of Drift Waves in ID (cont.) - Parker & Lee, PFB '93

$N_{particle} = 46368$
 $N_{grid} = 64$

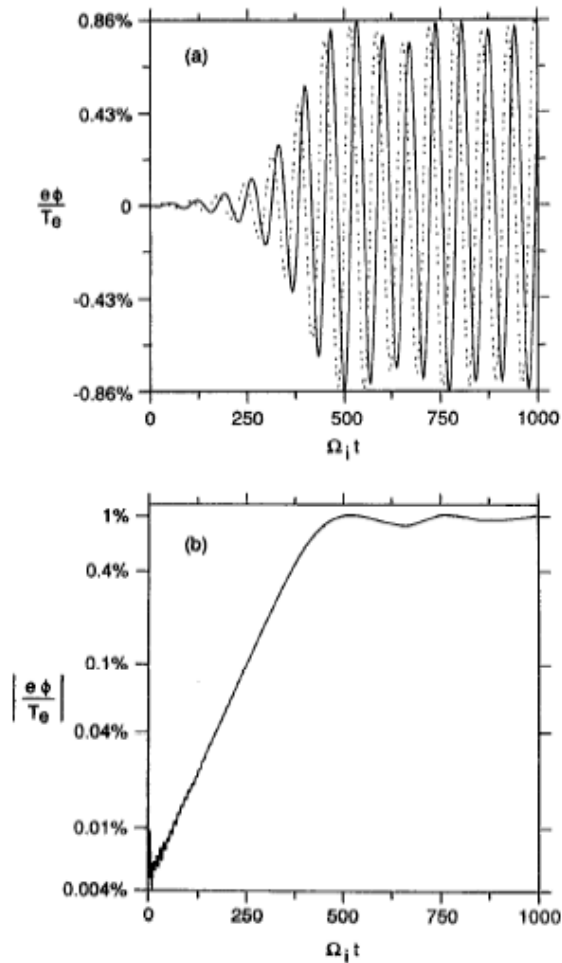


FIG. 4. The $n=1$ drift instability ($k_1 \rho_e \approx 0.8$) for the run with 46 368 particles on a 64-grid system. (a) The time history for the real (solid line) and imaginary (dashed line) parts of the electrostatic potential and (b) the corresponding amplitude evolution.

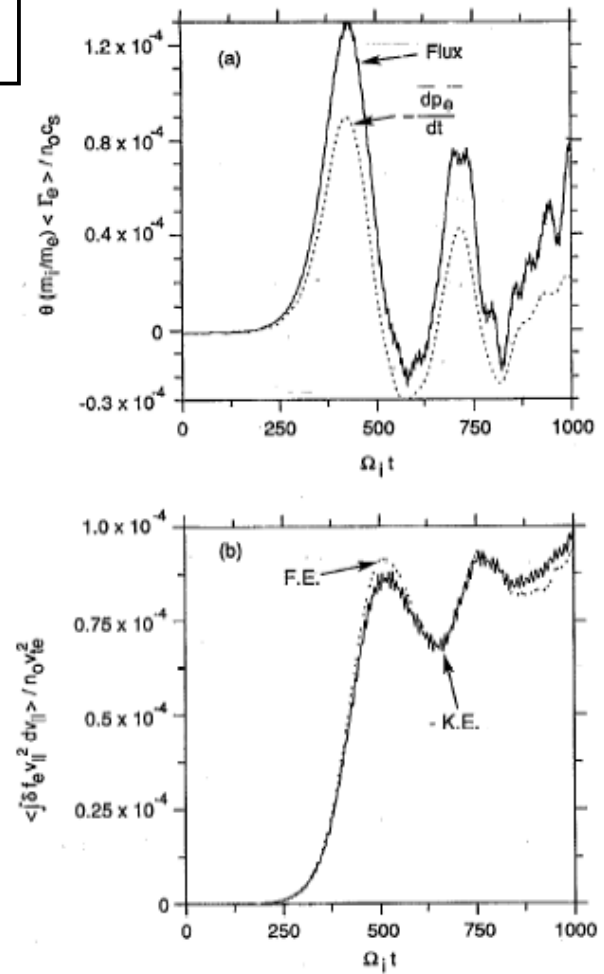
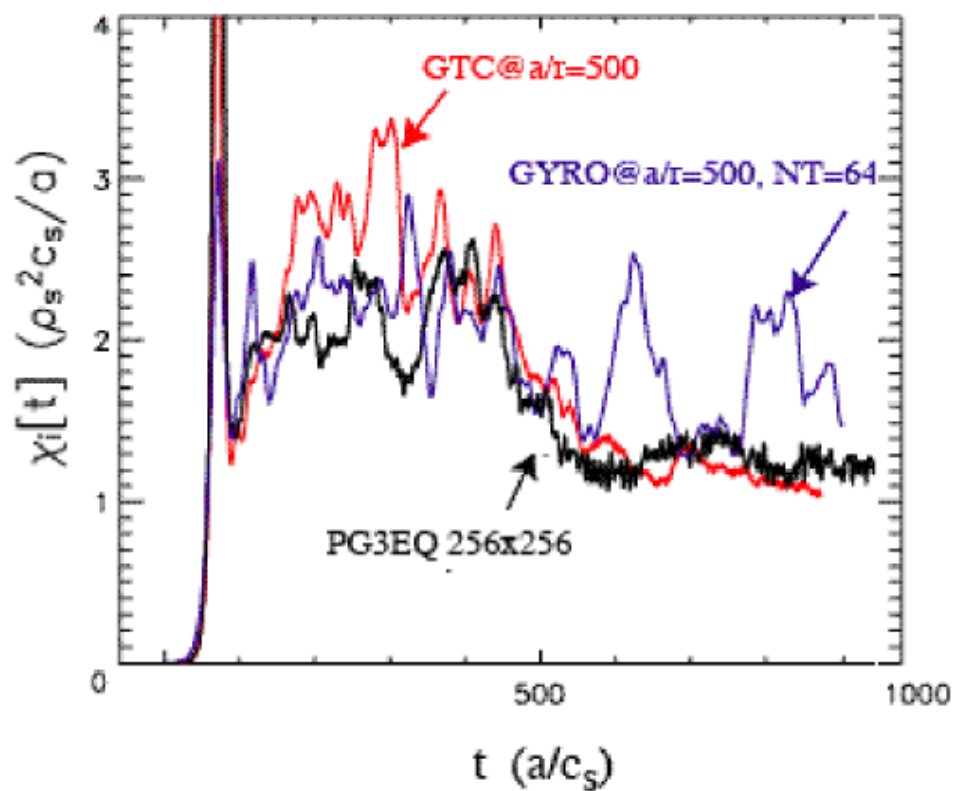


FIG. 6. The 46 368 particle run. (a) Time history for the electron particle flux (solid line) and the time rate of change for the electron parallel momentum (dashed line) and (b) the time evolution for the perturbed electron kinetic energy (solid line) and the field energy (dashed line).

Recent PMP Code Comparisons and Controversies

(W. M. Nevins, 04)



Code Comparisons:

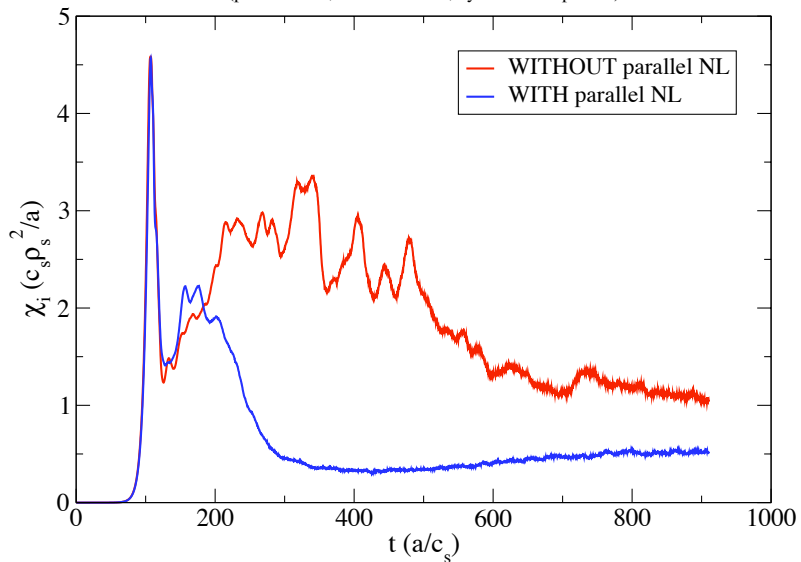
GTC - Particle Code

GYRO - Continuum Code

PG3EQ - Particle Code

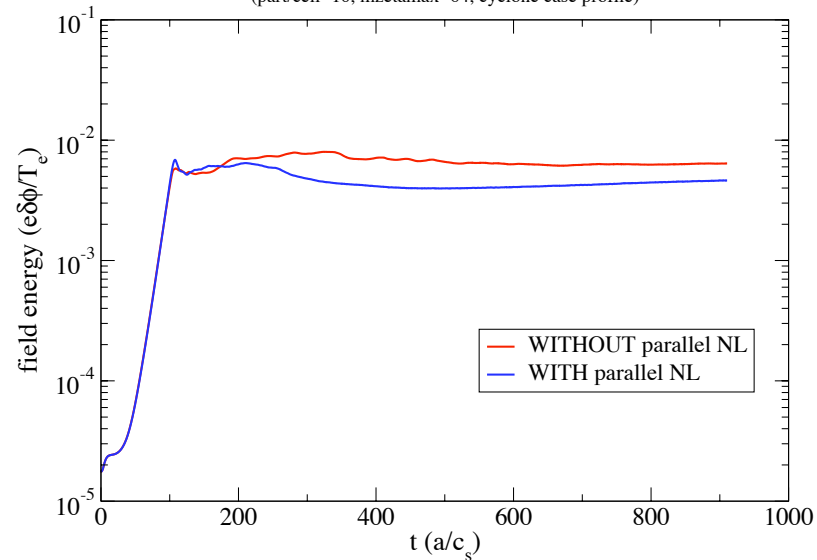
Peak χ_i (bin 3) - $a/\rho_i=500$

(part/cell=10, mzetamax=64, cyclone case profile)



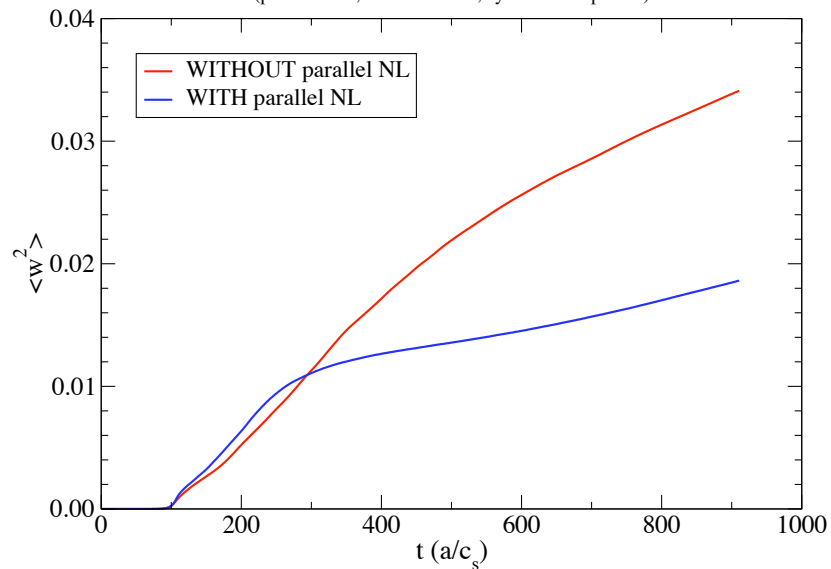
Field Energy - $a/\rho_i=500$

(part/cell=10, mzetamax=64, cyclone case profile)



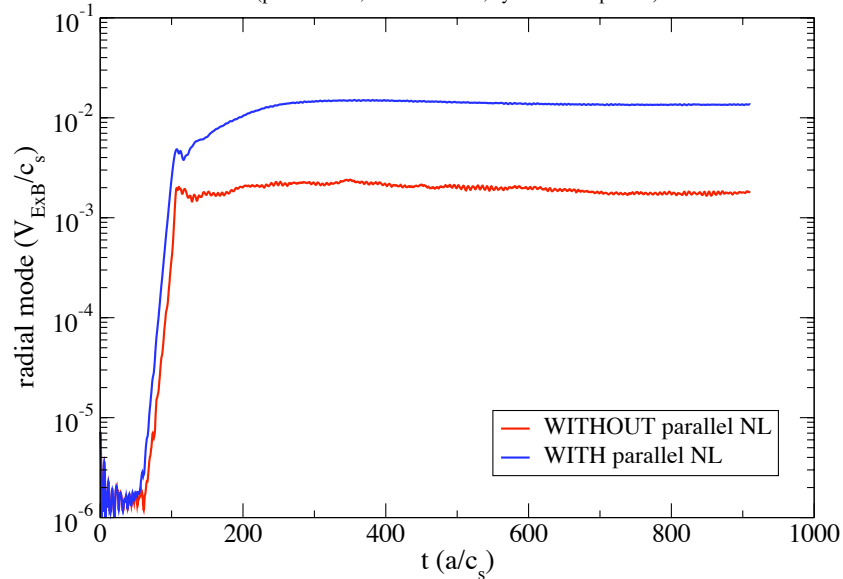
Time evolution of $\langle \text{weight}^2 \rangle$ ($a/\rho_i=500$)

(part/cell=10, mzetamax=64, cyclone case profile)



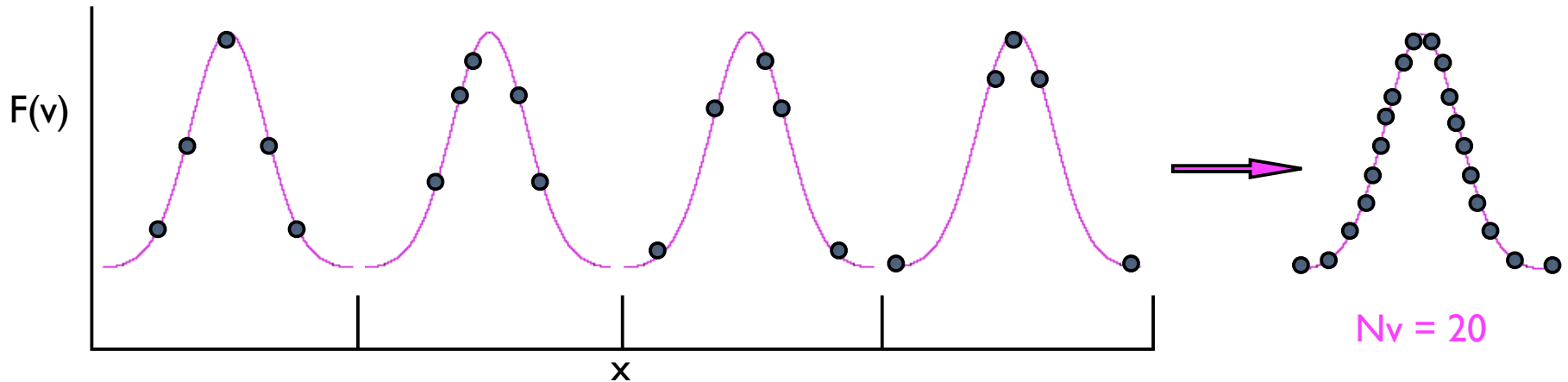
Radial Mode (Zonal Flow) - $a/\rho_i=500$

(part/cell=10, mzetamax=64, cyclone case profile)

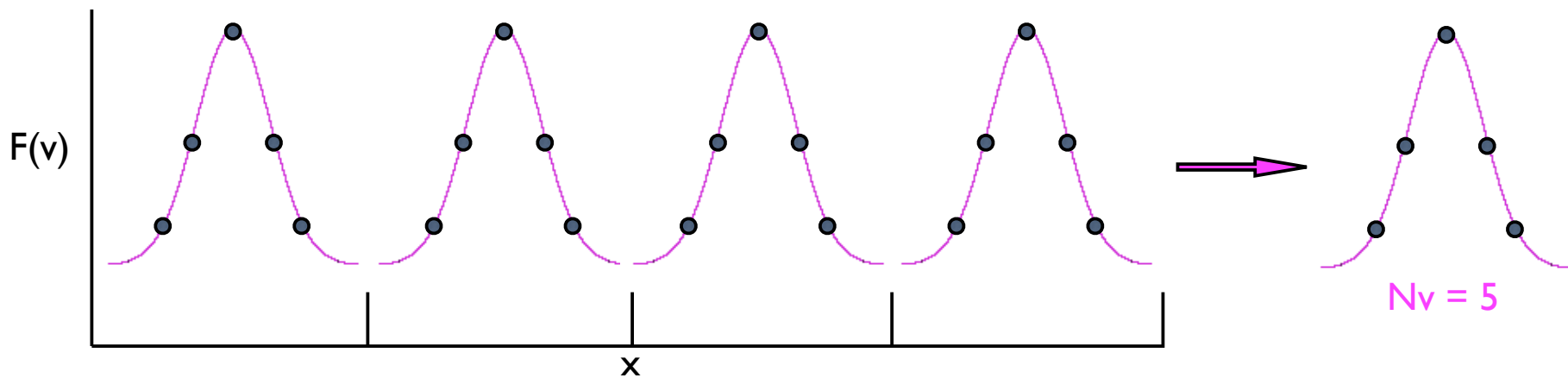


Velocity Space Resolution: Particle vs. Vlasov Codes

- More accurate for Particle Codes: $N_x N_p N_n = (4)(5)(2)$



- Less accurate for Continuum Codes: $N_x N_v = (4)(5)$



- Artificial dissipation in Vlasov Codes due to coarse grid in long time simulations

Entropy Production - ITG modes

- δf -formulation: $F_i = F_{0i} + \delta f_i$, ν is the collision frequency, and Q_{ix} is the radial ion energy flux

$$\frac{\partial}{\partial t} \left\langle \int \frac{\delta f_i^2}{F_{0i}} dv_{\parallel} + \tau \phi^2 + \tau |\nabla_{\perp} \phi|^2 \right\rangle + \left\langle \tau \frac{\partial \phi}{\partial x_{\parallel}} \int v_{\parallel} \frac{\delta f_i^2}{F_{0i}} dv_{\parallel} + 2\tau \nu \int \frac{dv_{\parallel}}{F_{0i}} \left(\frac{\partial \delta f_i}{\partial (v_{\parallel}/v_{ti})} + \frac{v_{\parallel}}{v_{ti}} \delta f_i \right)^2 \right\rangle = \kappa_{Ti} \langle Q_{ix} \rangle$$

$$\tau \equiv T_e/T_i, \quad \kappa_{Ti} \equiv -d \ln T_{0i} / dx, \quad \langle \dots \rangle \equiv \frac{1}{V} \int d\mathbf{x},$$

- Let $w \equiv \delta f_i / F_{0i}$, $E_{\parallel} \equiv -\partial \phi / \partial x_{\parallel}$, $\partial \delta f_i / \partial (v_{\parallel}/v_{ti}) \approx -\beta \delta f_i$, $\beta \ll 1$, N is the particle number,

$$\frac{\partial}{\partial t} \sum_{j=1}^N \frac{w_j^2}{1-w_j} + \tau \frac{\partial}{\partial t} \langle \phi^2 + |\nabla_{\perp} \phi|^2 \rangle + \sum_{j=1}^N \left[-\tau E_{\parallel j} v_{\parallel j} + 2\nu \tau (1-\beta)^2 \left(\frac{v_{\parallel j}}{v_{ti}} \right)^2 \right] \frac{w_j^2}{1-w_j} = \kappa_{Ti} \langle Q_{ix} \rangle$$

- Energy balance:

$$\sum_{j=1}^N E_{\parallel j} v_{\parallel j} w_j = \frac{1}{2} \frac{\partial}{\partial t} \sum_{j=1}^N v_{\parallel j}^2 w_j \approx \frac{1}{2} \frac{\partial}{\partial t} \sum_{j=1}^N \alpha v_{ti}^2 w_j, \quad \alpha \approx 1$$

- In the steady state ($\partial / \partial t \langle \phi^2 + |\nabla \phi|^2 \rangle = 0$), with $w \ll 1$:

$$\frac{\partial}{\partial t} \sum_{j=1}^N \left(1 - \frac{\alpha}{4} \right) w_j^2 + 2\nu \tau (1 - \beta^2) \alpha \sum_{j=1}^N w_j^2 = \kappa_{Ti} \langle Q_{ix} \rangle$$

Velocity-Space nonlinearity reduces ion energy flux, but collisions enhance it.

Conclusions

- Particle codes are very suitable for both cache-based and vector-parallel MPP platforms.
- Noise problems can be mitigated through quasineutral and/or perturbative schemes (or just use more particles).
- We have not yet encountered noise problem in steady state gyrokinetic particle simulations.
- If noise becomes an issue in long time simulation, we can always use a reset scheme of particle weights on a phase space grid at every m step, where $m \gg 1$. It is still more efficient than the Vlasov code simulation.
- There is no free lunch in the Vlasov-Maxwell simulation. Every technique has good and bad aspects.