Integrated Gyrokinetic Particle Simulation*

W. W. Lee

Princeton Plasma Physics Laboratory, Princeton, NJ 08543

- Electromagnetic Gyrokinetic Vlasov-Maxwell Equations
- Shear and compressional Alfvén Waves
- Steady State Transport using GTC
- Recent Improvements in GTC
- Integrated Simulations in Time and Space

* Supported by the USDOE SciDAC Center for Gyrokinetic Particle Simulation.

Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas*

SciDAC - Advanced Simulation of Fusion Plasmas

W. W. Lee, S. Ethier, T. S. Hahm, J. L. V. Lewandowski, G. Rewoldt, W. X. Wang

Princeton Plasma Physics Laboratory, Princeton, NJ

S. E. Parker, Y. Chen, University of Colorado, Boulder, CO

Z. Lin, L. Chen, Y. Nishimura, University of California, Irvine, CA

V. K. Decyk, University of California, Los Angeles, CA

Scientific Application Partnership Program

D. E. Keyes, Columbia University, New York, NY

K.-L. Ma, University of California, Davis, CA

M. Beck, Uniersity of Tennessee, Knoxville, TN

S. Klasky, Princeton Plasma Physics Laboratory, Princeton, NJ

PPPL
PRINCETON PLASMA PHYSICS LABORATORY

Governing Equations for Microturbulence and Kinetic-MHD

- The gyrokinetic Vlasov equation in $(\mathbf{R} \equiv \mathbf{x} - \rho, v_\parallel, \mu \equiv v_\perp^2/2B, t)$ coordinates,

$$\frac{\partial F_{\alpha gc}}{\partial t} + \frac{d\mathbf{R}}{dt} \cdot \frac{\partial F_{\alpha gc}}{\partial \mathbf{R}} + \frac{dv_\parallel}{dt}\frac{\partial F_{\alpha gc}}{\partial v_\parallel} = 0. \tag{1}$$

- In general geometry including EM and toroidal effects for finite $k_\perp \rho_\alpha$ [Lee and Qin, 2003],

$$\frac{d\mathbf{R}}{dt} = v_\parallel \mathbf{b}^* + \frac{v_\perp^2}{2\Omega_{\alpha 0}}\hat{\mathbf{b}}_0 \times \nabla lnB_0 - \frac{c}{B_0}\nabla\bar{\phi} \times \hat{\mathbf{b}}_0,$$

$$\frac{dv_\parallel}{dt} = -\frac{v_\perp^2}{2}\mathbf{b}^* \cdot \nabla lnB_0 - \frac{q_\alpha}{m_\alpha}\left(\mathbf{b}^* \cdot \nabla\bar{\phi} + \frac{1}{c}\frac{\partial \bar{A}_\parallel}{\partial t}\right),$$

$$\mu \equiv \frac{v_\perp^2}{2B_0}\left(1 - \frac{mc}{e}\frac{v_\parallel}{B_0}\hat{\mathbf{b}}_0 \cdot \nabla \times \hat{\mathbf{b}}_0\right) \approx cons.,$$

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

$$\mathbf{b} = \hat{\mathbf{b}}_0 + \frac{\nabla \times \bar{\mathbf{A}}}{B_0},$$

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

N_α is the total number of particles, ρ_α is the gyroradius of the species α, $\Omega_{\alpha 0} \equiv q_\alpha B_0/m_\alpha c$.

Governing Equations (cont.)

- The gyrophase averaged potentials are

$$\begin{pmatrix} \bar{\phi} \\ \bar{\mathbf{A}} \end{pmatrix}(\mathbf{R}) = \langle \int \begin{pmatrix} \phi \\ \mathbf{A} \end{pmatrix}(\mathbf{x})\delta(\mathbf{x}-\mathbf{R}-\rho)d\mathbf{x}\rangle_\varphi, \quad \langle\cdots\rangle_\varphi \equiv \oint d\varphi/2\pi.$$

- Gyrokinetic Poisson's equation can be written as

$$(\tau/\lambda_D^2)[\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x})] = -4\pi\rho_{gc}, \tag{2}$$

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

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

- Gyrokinetic Ampere's law becomes

$$\nabla^2\mathbf{A} - \frac{1}{v_A^2}\frac{\partial^2\mathbf{A}_\perp}{\partial t^2} = -\frac{4\pi}{c}\mathbf{J}_{gc}, \tag{3}$$

$$\mathbf{J}_{gc}(\mathbf{x}) = \mathbf{J}_{\parallel gc}(\mathbf{x}) + \mathbf{J}^M_{\perp gc}(\mathbf{x}) + \mathbf{J}^d_{\perp gc}(\mathbf{x}), \tag{4}$$

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

$$\mathbf{v}_d \equiv \frac{v_\parallel^2}{\Omega_{\alpha 0}}\hat{\mathbf{b}}_0 \times (\hat{\mathbf{b}}_0\cdot\nabla)\hat{\mathbf{b}}_0 + \frac{v_\perp^2}{2\Omega_{\alpha 0}}\hat{\mathbf{b}}_0 \times \nabla lnB_0.$$

Governing Equations (cont.)

- For $\omega^2 \ll k^2 v_A^2$, we can simply ignore the time derivative term in gyrokinetic Ampere's law without having to invoke any further geometric simplifications.

- The gyrophase averages in Eqs. (1) - (4) can be calculated by using the 4-point scheme for a rotating charged ring, namely,

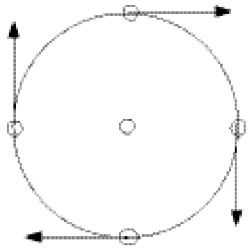
$$\begin{pmatrix} \bar{\phi} \\ \bar{\mathbf{A}} \end{pmatrix} (\mathbf{R}_{\alpha j}) = \langle \begin{pmatrix} \phi \\ \mathbf{A} \end{pmatrix} (\mathbf{x}_{\alpha j}) \rangle_\varphi,$$

$$\rho_{gc}(\mathbf{x}) = \sum_\alpha q_\alpha \sum_{j=1}^{N} \langle \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_\varphi,$$

$$\mathbf{J}_{\parallel gc}(\mathbf{x}) = \sum_\alpha q_\alpha \sum_{j=1}^{N} v_{\parallel \alpha j} \langle \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_\varphi,$$

$$\mathbf{J}^d_{\perp gc}(\mathbf{x}) = \sum_\alpha q_\alpha \sum_{j=1}^{N} \mathbf{v}_{d\alpha j} \langle \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_\varphi,$$

$$\mathbf{J}^M_{\perp gc}(\mathbf{x}) = \sum_\alpha q_\alpha \sum_{j=1}^{N} \langle \mathbf{v}_{\perp \alpha j} \delta(\mathbf{x} - \mathbf{x}_{\alpha j}) \rangle_\varphi.$$



Governing Equations (cont.)

- The significance here is that the FLR effects can now be accounted for by using the scheme for all the field quantities including the perpendicular current.

- Since we assume that $\rho/L_{eq} \sim o(\epsilon)$, the magnetic drift and diamagnetic currents, in the limit of small $k_\perp \rho_i$, can be calculated explicitly as

$$\mathbf{J}^d_{\perp gc} = \frac{c}{B_0} \sum_\alpha \left[p_{\alpha\parallel} (\nabla \times \hat{\mathbf{b}}_0)_\perp + p_{\alpha\perp} \hat{\mathbf{b}}_0 \times (\nabla lnB_0) \right],$$

$$\mathbf{J}^M_{\perp gc} = -\sum_\alpha \nabla \times \frac{c\hat{\mathbf{b}}_0}{B_0} p_{\alpha\perp},$$

$$\begin{pmatrix} p_{\alpha\parallel} \\ p_{\alpha\perp} \end{pmatrix} = m_\alpha \int \begin{pmatrix} v_\parallel^2 \\ v_\perp^2/2 \end{pmatrix} F_{\alpha gc}(\mathbf{x}) dv_\parallel d\mu.$$

- For $p = p_{\alpha\parallel} = p_{\alpha\perp}$, we recover the usual pressure balance equation as

$$\mathbf{J}_{\perp gc} = \frac{c}{B_0} \sum_\alpha \hat{\mathbf{b}}_0 \times \nabla p_\alpha.$$

- These equations can be solved via existing particle simulation techniques on massively parallel computers.

Kinetic-MHD Equations

[Lee and Qin, 2003]

- General Geometry

$$\frac{d}{dt}\nabla_\perp^2\phi + \frac{v_A^2}{c}(\hat{\mathbf{b}}\cdot\nabla)\nabla^2 A_\parallel - 4\pi\frac{v_A^2}{c^2}\nabla_\perp\cdot\mathbf{J}^d_{\perp gc} = 0 \tag{5}$$

$$\frac{1}{c}\frac{\partial A_\parallel}{\partial t} + \mathbf{b}\cdot\nabla\phi = 0. \tag{6}$$

$$\frac{dp_\alpha}{dt} = 0$$

$$\mathbf{J}^d_{\perp gc} = \frac{c}{B_0}\sum_\alpha\left[p_\alpha(\nabla\times\hat{\mathbf{b}}_0)_\perp + p_\alpha\hat{\mathbf{b}}_0\times(\nabla lnB_0)\right], \tag{7}$$

- Slab Geometry: more general than Strauss' equations [1976]

$$\frac{d\nabla_\perp^2\phi}{dt} + \frac{v_A^2}{c}(\mathbf{b}\cdot\nabla)\nabla^2 A_\parallel = 0. \tag{8}$$

$$\frac{1}{c}\frac{\partial A_\parallel}{\partial t} + \mathbf{b}\cdot\nabla\phi = 0. \tag{9}$$

Thermodynamic/Numerical properties of Alfvén Waves

[Lee et al., 2002]

- Fluctuation-Dissipation Theorem for $A_\parallel$: $\psi = \phi + (1/c)\int \partial A_\parallel/\partial t dx_\parallel$ N – no. of particles
  - Total Noise

$$\left|\int \frac{e\psi}{T} d\omega\right| = \frac{1}{\sqrt{N} k\rho_s}$$

  - Noise from Alfvén Waves with cold electrons

$$\left|\frac{e\psi}{T}\right| = \frac{1}{\sqrt{N} k\rho_s} \frac{1}{\sqrt{1+\omega_{pe}^2/c^2k^2}}$$

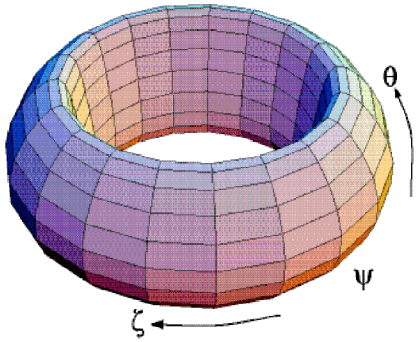
  - Noise from Alfvén Waves with warm electrons

$$\left|\frac{e\psi}{T}\right| = \frac{1}{\sqrt{N} k\rho_s} \frac{1}{\sqrt{1+k^2\rho_s^2}}$$

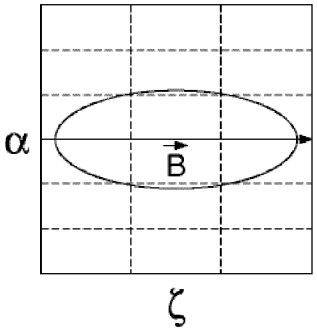
- Compressional Alfvén Waves: $|A_\perp/A_\parallel| \sim (\omega/kv_A)^2$

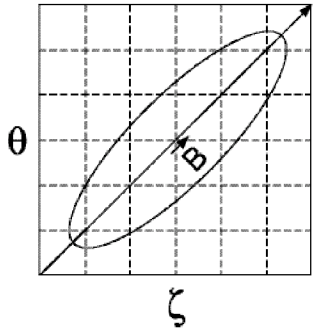
Global Gyrokinetic Toroidal Particle Simulation Code: GTC

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



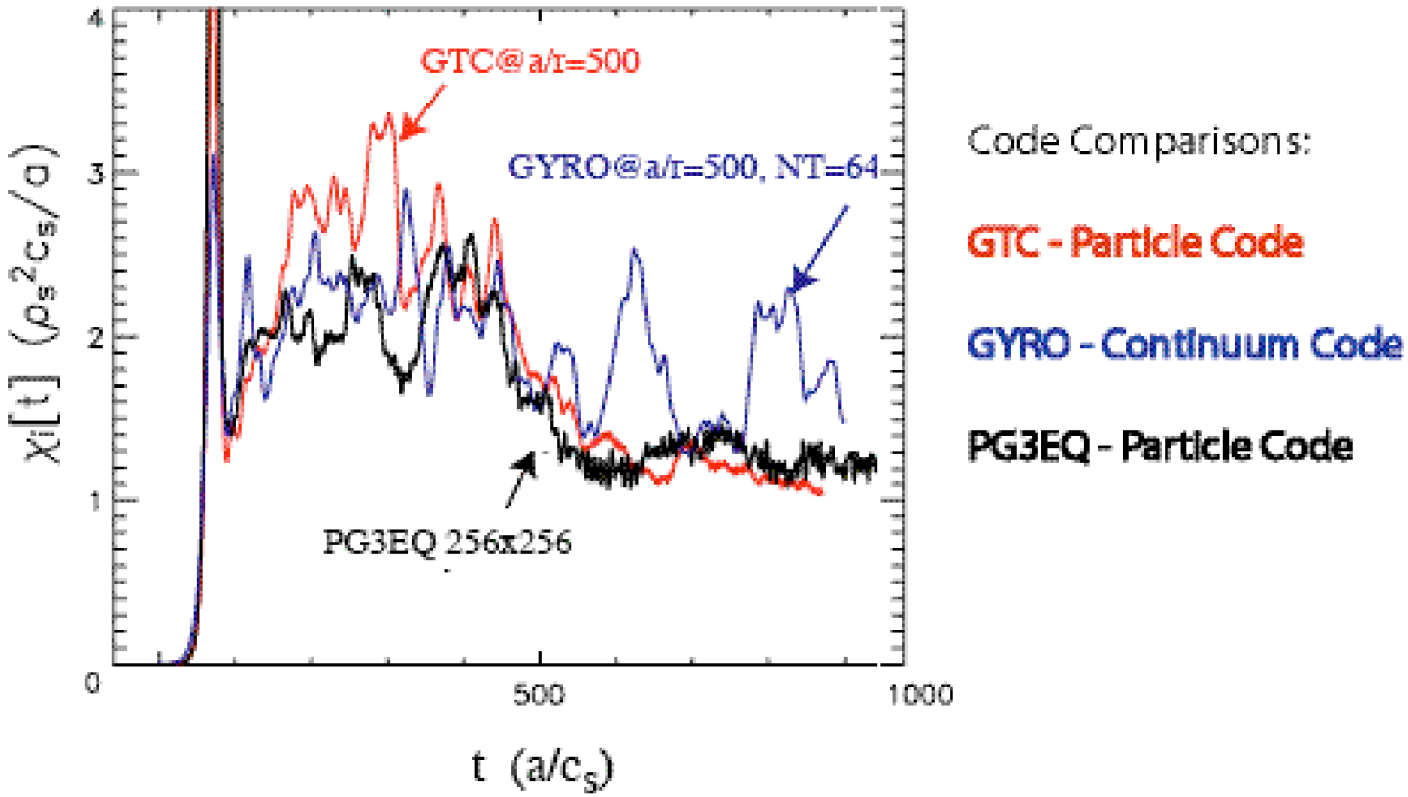
- Magnetic coordinates (ψ, θ, ζ) [Boozer, 1981]
- Guiding center Hamiltonian [Boozer, 1982; White and Chance, 1984]
- Non-spectral Poisson solver [Lin and Lee, 1995]
- Global field-line coordinates: $(\psi, \alpha, \zeta), \alpha = \theta - \zeta/q$
  - Microinstability wavelength: $\lambda_\perp \propto \rho_i$, $\lambda_\parallel \propto qR$
  - With field-line coordiantes: Grid # $N \propto a^2$, a: minor radius, $\triangle\zeta \propto R$
  - Without field-line coordinates: grid # $N \propto a^3$, $\triangle\zeta \propto \rho$
  - 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]





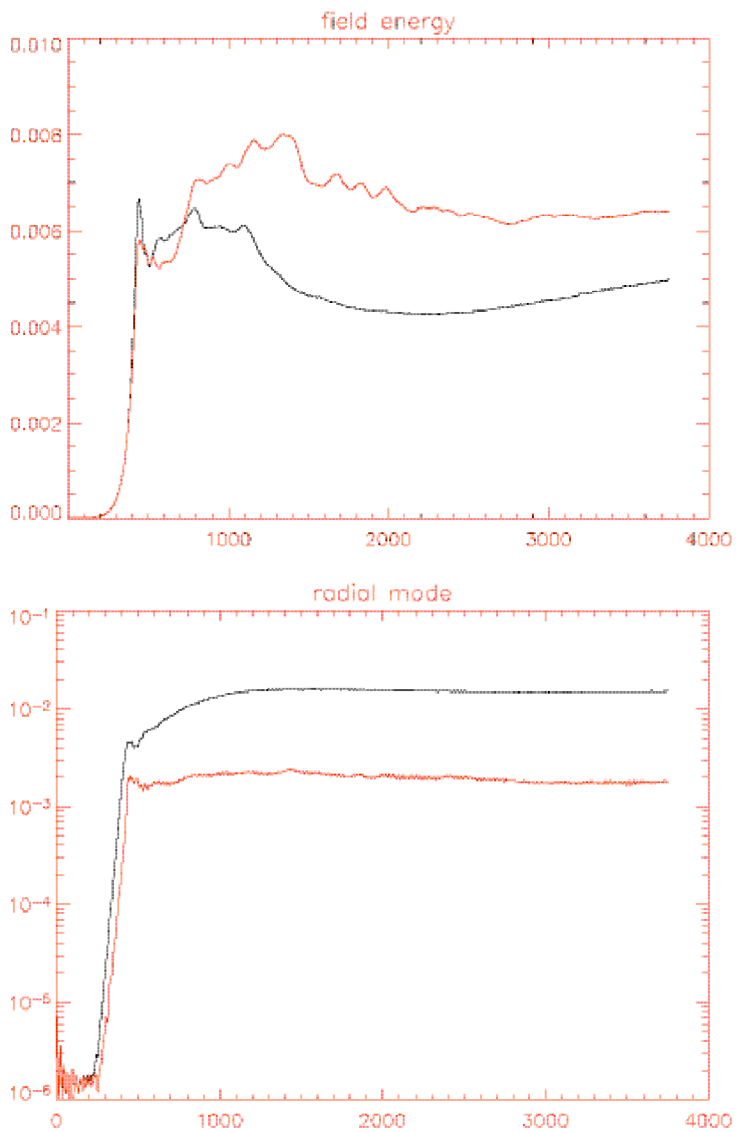
Recent PMP Code Comparisons and Controversies

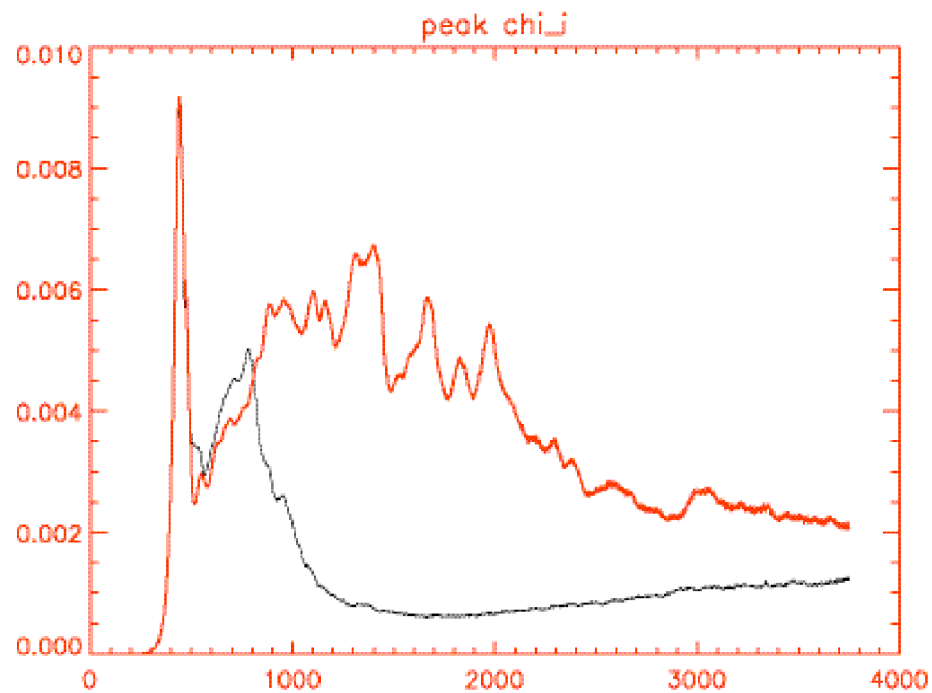
(W. M. Nevins, 04)



Velocity Space Nonlinearities on Toroidal ITG Modes

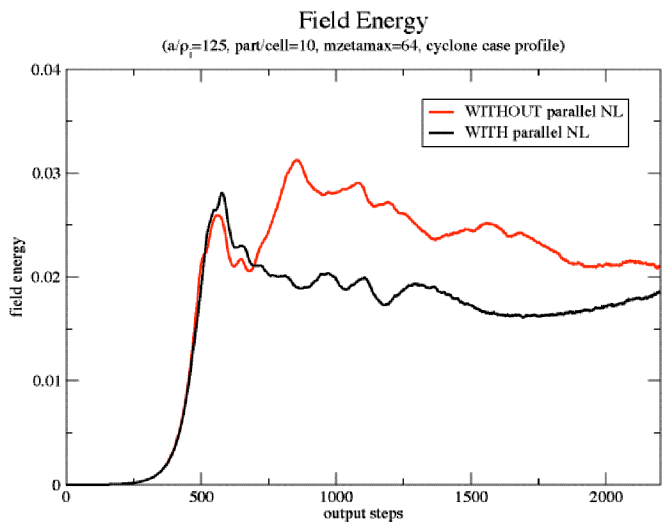
Cyclone parameters with $a/\rho = 500$ [W. W. Lee et al., Sherwood '04]

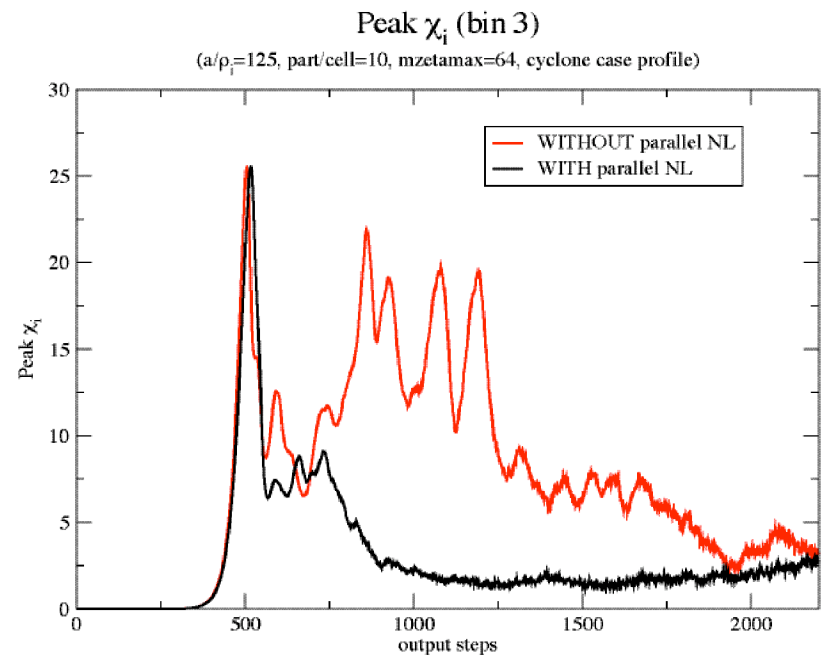


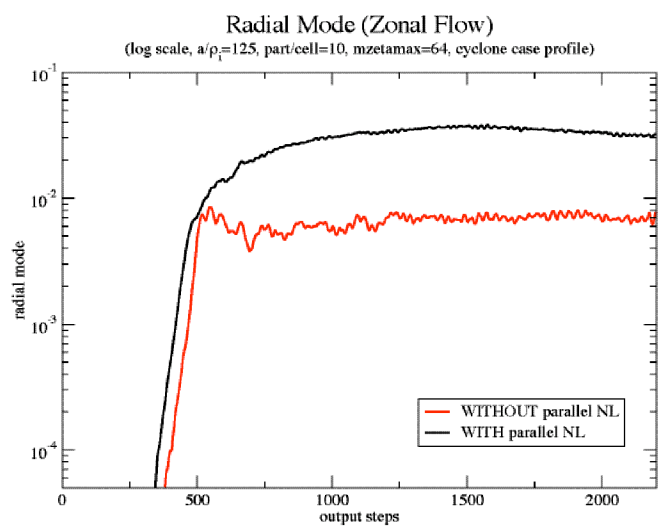


Velocity Space Nonlinearities on Toroidal ITG Modes (cont.)

Cyclone parameters with $a/\rho = 125$

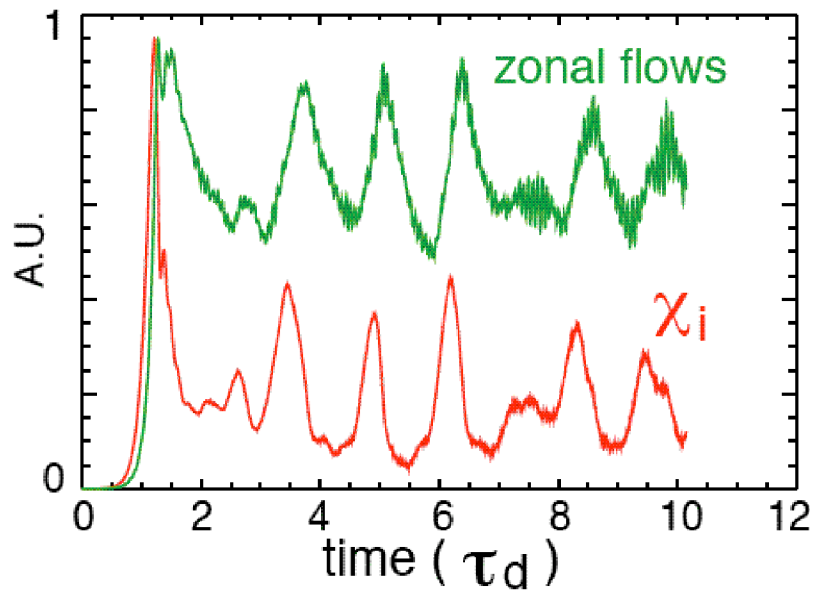






Collisional Effects on Toroidal ITG Modes

- Weak collisons have negiligible effects on linear growths. But, they can enhanced turbulent transport in the steady state.
- The bursting behavior is the result of the interplay between collisons, fluctuations and zonal flows.



[Lin, et al., 1999]

collisional damping of zonal flows causes bursts of turbulent transport in gyrokinetic simulations

PPPL PRINCETON PLASMA PHYSICS LABORATORY

Entropy Production - ITG modes

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

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

$$\tau \equiv T_e/T_i, \quad \kappa_{Ti} \equiv -dlnT_{0i}/dx, \quad \langle \ldots \rangle \equiv \frac{1}{V}\int d\mathbf{x}, \quad \phi \neq \phi_{00}$$

- 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,

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

- Energy balance: zonal flow plays no role here,

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

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

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

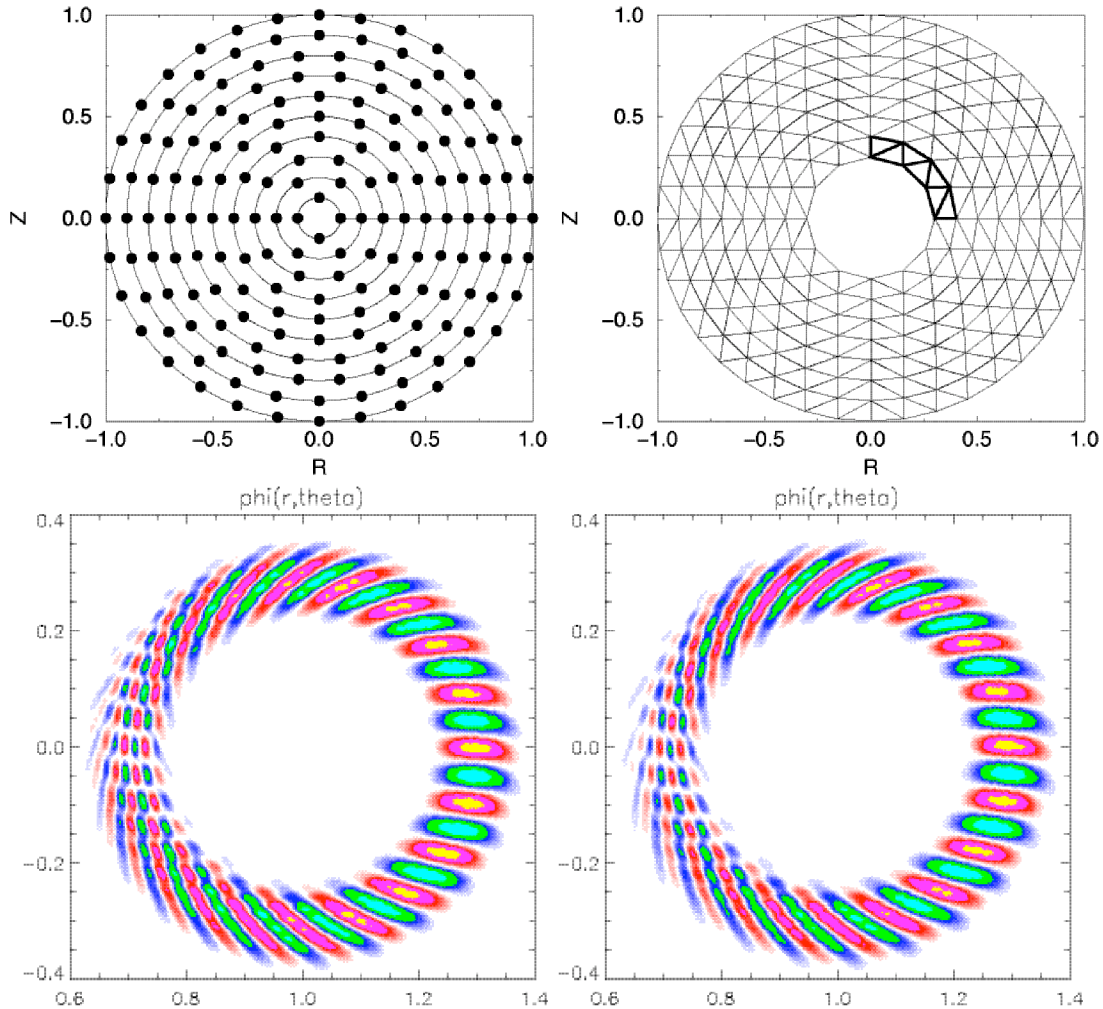
Velocity-Space nonlinearity reduces ion energy flux, but collisons enhance it.

PPPL PRINCETON PLASMA PHYSICS LABORATORY

Code Development - Finite Element Poisson Solver via PETSc

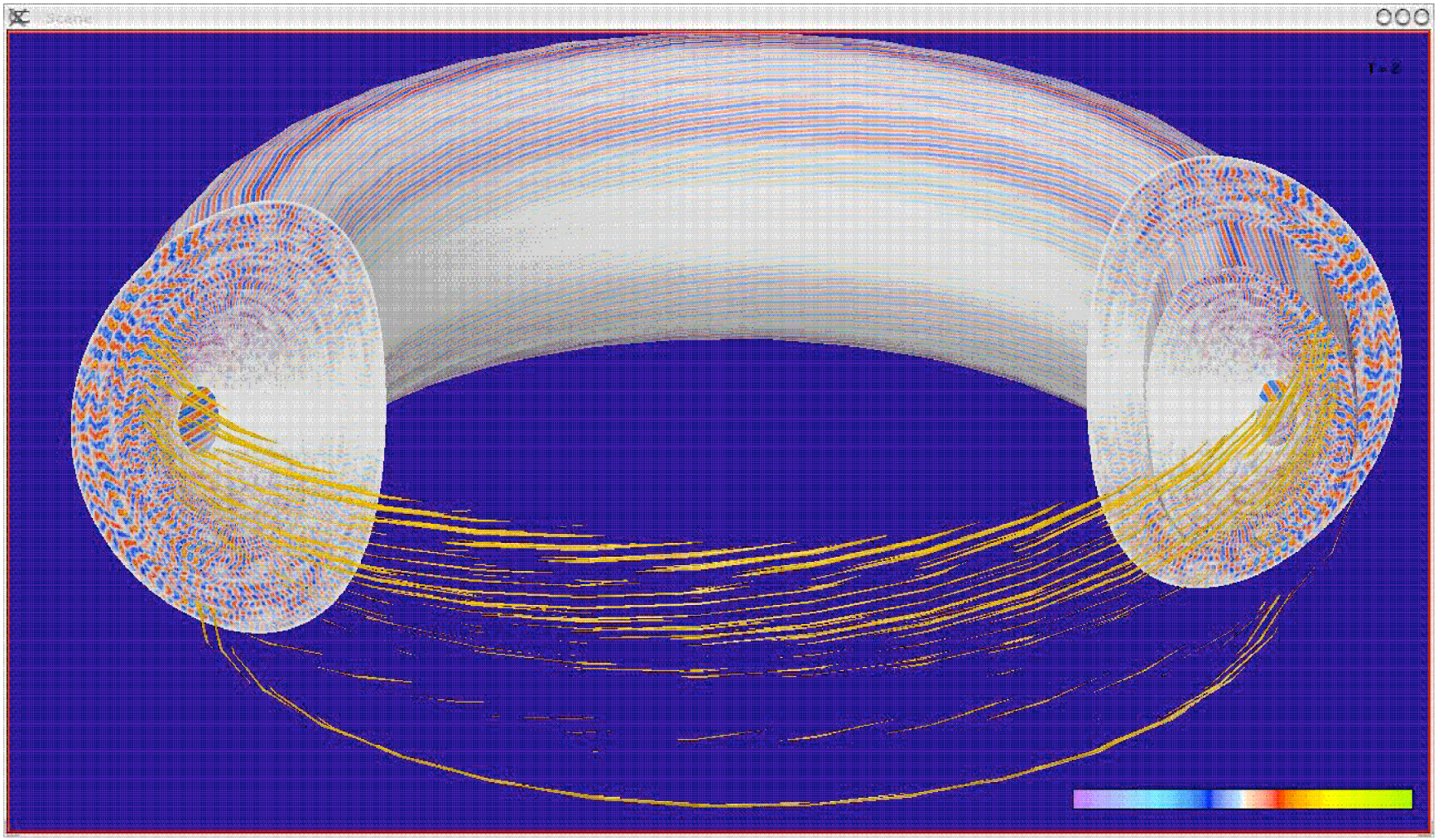
Old GTC solver vs. New GTC solver

[Nishimura et al., submitted to JCP]



Code Development - Shaped Plasmas

[Wang, Klasky and Ethier]



Code Development - Electron Dynamics and Finite-β effects

- Split-weight Scheme [Manuilskiy and Lee, PoP (2000); Lee et al., PoP (2002)]

$$F = F_0 + \psi F_0 + \delta h$$

- Electron Hybrid Scheme [Lin and Chen, PoP (2002)]

$$F \approx F_0 + \psi F_0 + \delta h (\propto \omega / k_{\|} v_{\|})$$

- Adiabatic response

$$\psi = \phi + \frac{1}{c} \int \frac{\partial A_{\|}}{\partial t} dx_{\|0}$$

- Time step restriction for the electrons is determined by zero-th order orbit along the field line not $k_{\|} v_{\|} \Delta t < 1$.

- Use electron subcycling to speed up the code

- Implementation to GTC by Lewandowski and Nishimura

PPPL
PRINCETON PLASMA PHYSICS LABORATORY

Core-Edge Simulations via GTC

- Basic requirements for the validity of gyrokinetic Vlasov-Maxwell equations are:

$$\rho/L_B \sim o(\epsilon),$$

$$\partial F/\partial \phi = 0,$$

$$d\mu_B/dt = 0.$$

- GTC already has Lorentz collision operators for e-i, and momentum and energy conserving collision operators for like species.

- The core uses the δf scheme of

$$\frac{D\delta f}{DT} = -\frac{DF_0}{Dt}.$$

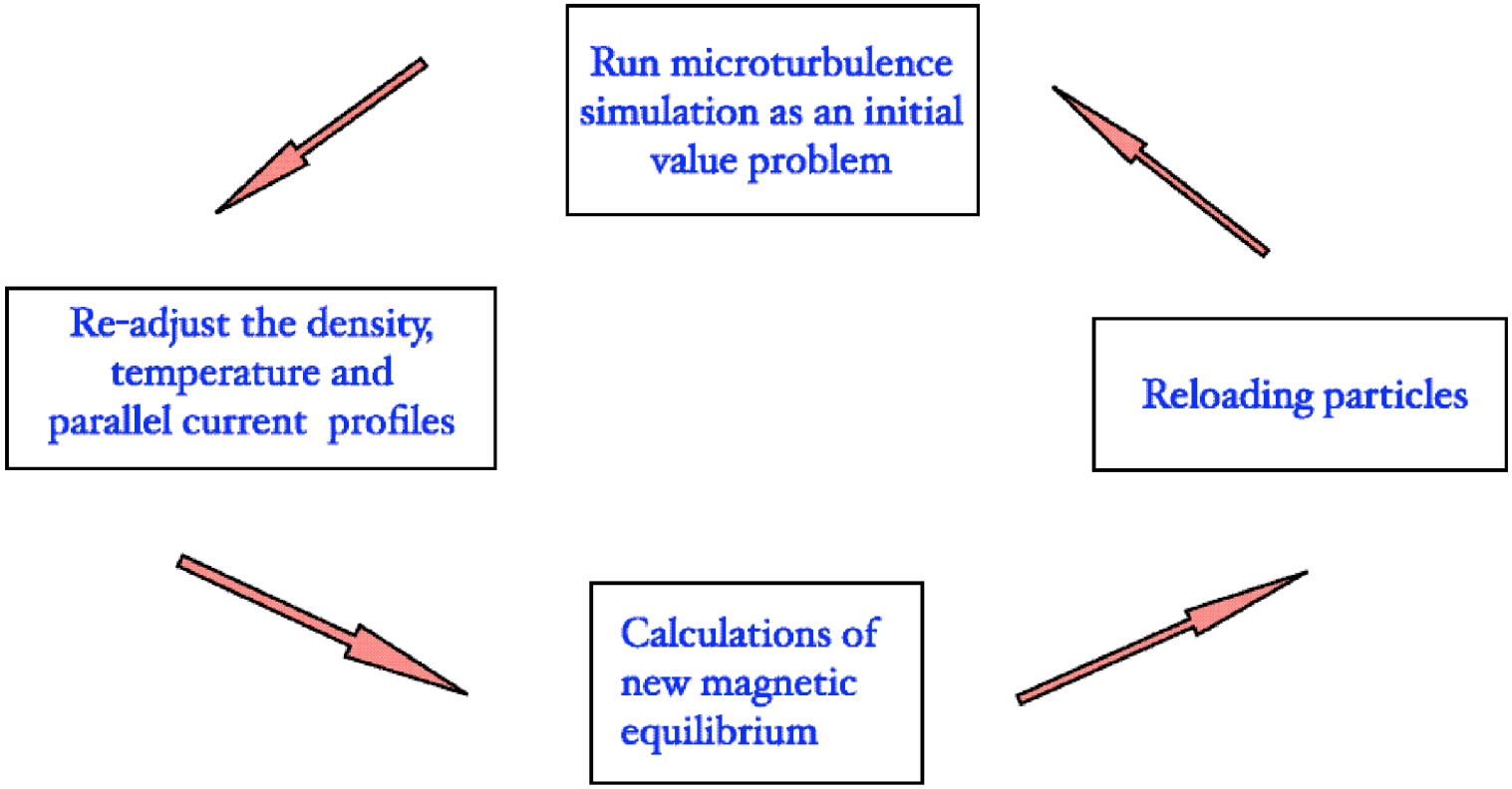
- The edge uses the δf scheme of

$$\delta f = F - F_0.$$

- Core-edge simulation inside the separatrix using GTC with electrons and multi-species ions is feasible.

PPPL PRINCETON PLASMA PHYSICS LABORATORY

Turbulence Simulation on Transport Time Scale



PPPL
PRINCETON PLASMA PHYSICS LABORATORY

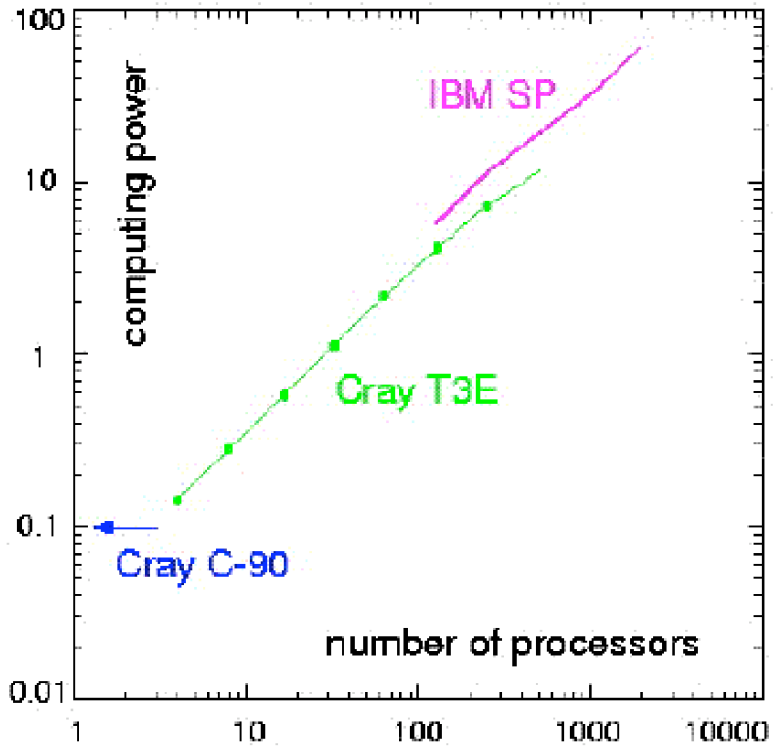
Global Turbulence Code (GTC)

Single Processor Performance

Processor	Max speed (Mflops)	GTC test (Mflops)	Efficiency (real/max)	Relative speed (user time)
Power3 (Seaborg)	1,500	173.6	12 %	1
Power4 (Cheetah)	5,200	304.5	6 %	1.9
SX6 (Rime)	8,000	715.7	9 %	5.2
Earth Simulator			18%	10

(S. Ethier)

GTC Scalable to a Large Number of processors

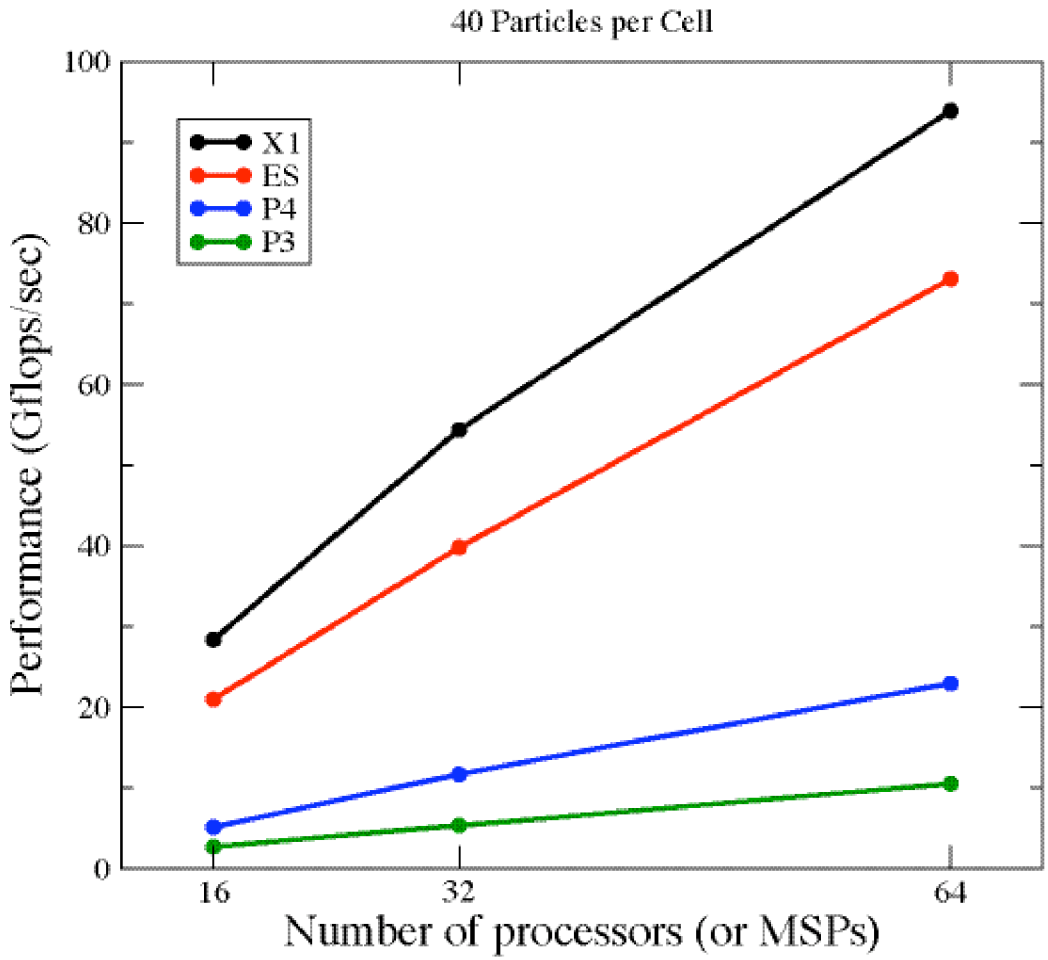


(Lin and Ethier)

Y-axis: the number of particles (in milions) which move 1 step in 1 second

More Recent GTC Performance on parallel platforms

[S. Ethier, '04]



Summary

- Thermodynamic properties of shear and compressional Alfvén waves in gyrokinetic plasmas and the related numerical algorithms for studying integrated plasma turbulence and kinetic-MHD physics on massively parallel computers are reported.
- The proposed schemes depend critically on the concept of steady state turbulent transport. As such, it calls for integrated simulation models that properly include velocity space nonlinearities and neoclassical effects.
- The possibility of integrated core-edge simulation is explored.
- The procedures for (1) utilizing the results from turbulence and kinetic-MHD simulations using GTC and (2) then modifying the GTC profiles interactively for the integrated simulations on the transport time scale are outlined.
- The possibilty of using high frequency gyrokinetics for wave heating integrating with microinstability and kinetic-MHD simulations will be explored.

PPPL
PRINCETON PLASMA PHYSICS LABORATORY