PPPL Theory Department
Five Year Plan Review

Turbulence and Transport Simulations

W. W. Lee

October 10-11, 2005

FESAC Priorities Panel Report (2005)

The PPPL turbulence and transport simulation group is engaging in multi-scale transport physics research to seek answers to the following questions asked by the panel :

T4) How does turbulence cause heat, particle and momentum to escape from plasmas?

T5) How are electromagnetic fields and mass flow generated in plasmas?

T6) How do magnetic fields in plasmas reconnect and dissipation their energy?

PPPL's Simulation Effort is Highly Leveraged through Extensive Collaborations Activities

- Theory Team at PPPL

- SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (GPSC)
  -- PPPL (lead), Columbia, Colorado, ORNL, UC-Irvine, UCLA, UC-Davis, UT-Knoxville

- FSP Center for Plasma Edge Simulation (CPES)
  -- NYU (lead), Caltech, GA, LBNL, Lehigh, UC-Irvine, Colorado, ORNL, MIT, Rutgers, PPPL, Utah, UT-Knoxvillle

- ASCR/MICS Project for Multi-Scale Gyrokinetic Particle Simulation of Magnetized Plasmas (MSG)
  -- PPPL (lead), Columbia

Roadmap for Turbulence and Transport Simulations at PPPL

Ion thermal transport and zone flow physics

- GTC studies on NSTX, DIII-D, JET, JT60U, NCSX, ... ITER and Benchmarking
- Benchmarking with GEM, PG3EQ, GS2, and GYRO
- General geometry, modularity, parallelization, parallel solvers, data management and visualization

Electron particle transport and thermal transport

- GTC studies on NSTX, DIII-D, JET, JT60U, NCSX, ... ITER and Benchmarking
- Kinetic electrons and magnetic fluttering models
- Gyrokinetic MHD models

Integrated simulation

- Edge simulation and code-edge coupling development
- Core-edge integration simulations and comparisons with experiments
- Algorithm design for transport time scale simulation
- Transport time scale simulation development
- Algorithm design for gyrokinetic wave heating
- Wave heating and gyrokinetic MHD coupling
- Integrated Simulation Applications

2006 2007 2008 2009 2010

Algorithm design | Code development | Simulation applications

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Governing Equations for Particle Pushing

- GK Vlasov equation - in gyrocenter coordinates

[Lee PF '83; Dubin et al. PF '83; Hahm et al. PF '88; Hahm PF '88; Brizard PF '88; Brizard J. Plas. Phys. '89; Qin et al. PoP '99; Qin et al. PoP '00; Qin et al., PoP '00; Lee and Qin PoP '03]

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

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

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

-- Velocity Space Nonlinearity

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

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

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

-- Coordinate Transformation

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

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Governing Equations for Particle Pushing (cont.)

- GK Poisson's equation - in laboratory coordinates

$$\boxed{\nabla^2\phi + \frac{\tau}{\lambda_D^2}[\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x})] = -4\pi\rho_{gc}(\mathbf{x})}$$

$(k_\perp\rho_i)^2 \ll 1$
==========>

$$\boxed{\frac{\rho_s^2}{\lambda_D^2}\nabla_\perp^2\phi(\mathbf{x}) = -4\pi\rho_{gc}(\mathbf{x})}$$

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

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

- GK Ampere's law -- in laboratory coordinates

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

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

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

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

Particle Noise in Particle Simulation

- "Kinetic theory for fluctuations and noise in computer simulation of plasmas," A. B. Langdon, Phys. Fluids **22**, 163 (1979)
  --- based on fluctuation-dissipation theorem (FDT) for linearly stable plasmas

- The studies on noise reduction in gyrokinetic particle simulation through the elimination of space charge waves and noise suppression of linear growths due to Resonant Broadening, $\Delta\omega$, through random walk were based on FDT [Lee, JCP '87]:

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

$$D \approx (\Delta x)^2/\Delta t$$

  --- delta f methods can alleviate the problem

- Particle noise in the steady state turbulence simulations may enhance (e.g., Parker and Lee '93) or suppress (e.g., Nevins *et al.* '05) particle and thermal diffusion.
- To resolve this issue,
  --- we are exploring the development of a modified FDT applicable to nonlinearly saturated plasmas
  --- we are undertaking convergence tests for ITG simulations using LCF at ORNL
  --- convergence tests of ETG simulations are ongoing by GPSC (Lin, Parker and Chen) then by broader community.
  --- if noise is indeed a issue, remedies such as re-gridding and collisions will be explored (long term memory vs. short term memory)

Perturbative Particle Simulation - noise reduction

- Delta-f simulation schemes:

-- [Dimits and Lee, JCP '93; Parker and Lee, PF '93]

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

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

Noise reduction: $|E|^2 \propto w^2$ [Hu and Krommes, PoP '94]

-- [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]

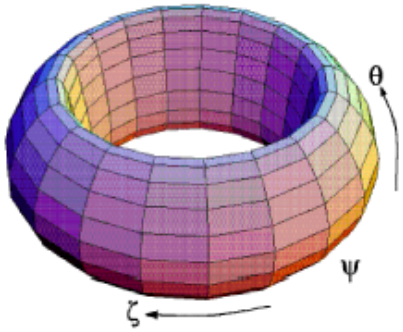
$$F = F_0 + \psi F_0 + \delta h \qquad \psi = \phi + \frac{1}{c}\int \frac{\partial A_\parallel}{\partial t} dx_{\parallel 0}$$

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

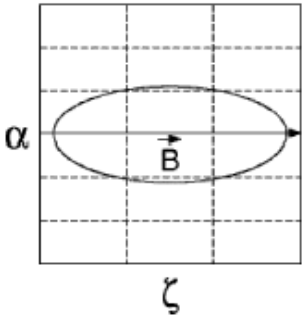
- CFL conditions can be violated without numerical instability.

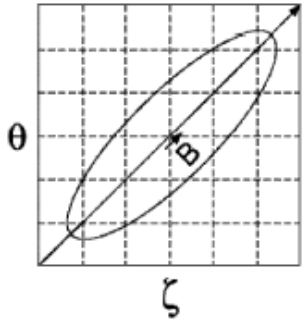
Global Gyrokinetic Toroidal Particle Simulation Code: GTC

[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]



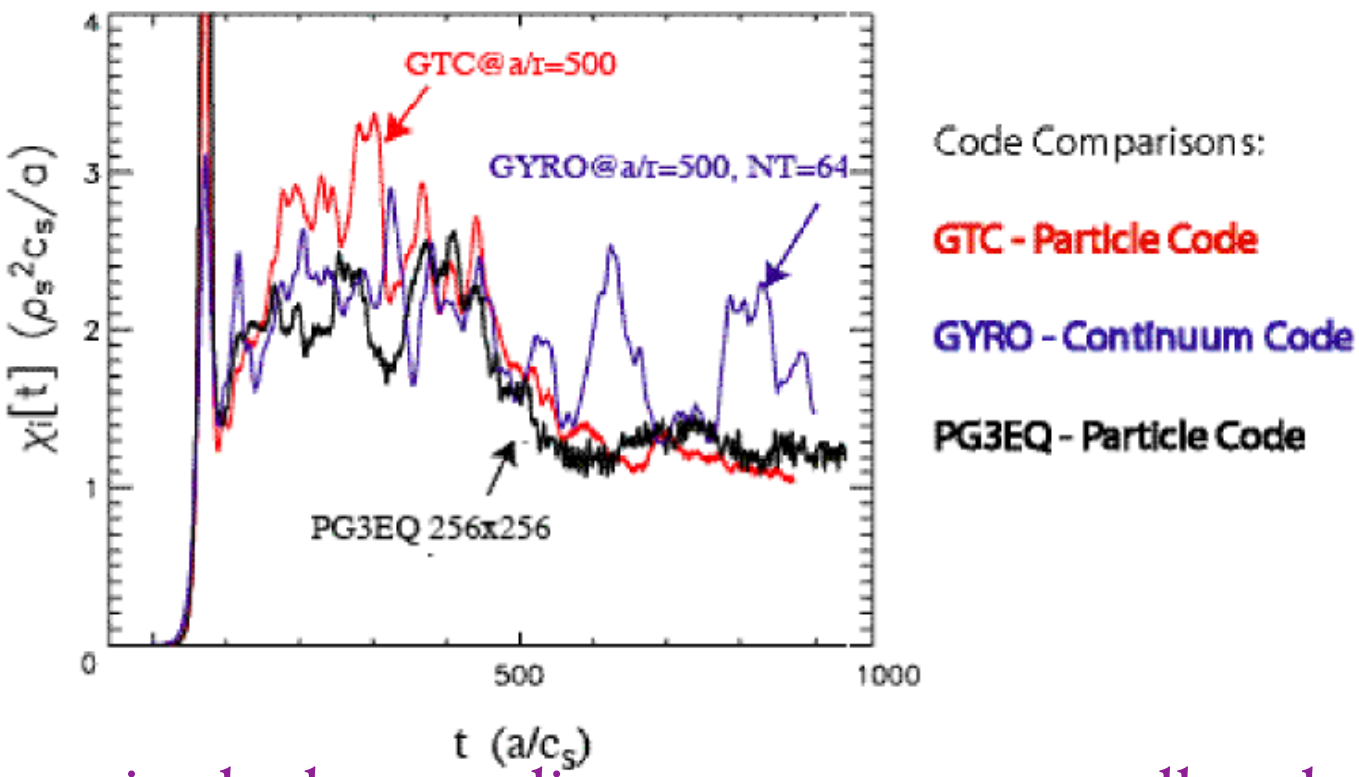


ITG simulations without velocity-space nonlinearity

PMP Code Comparisons

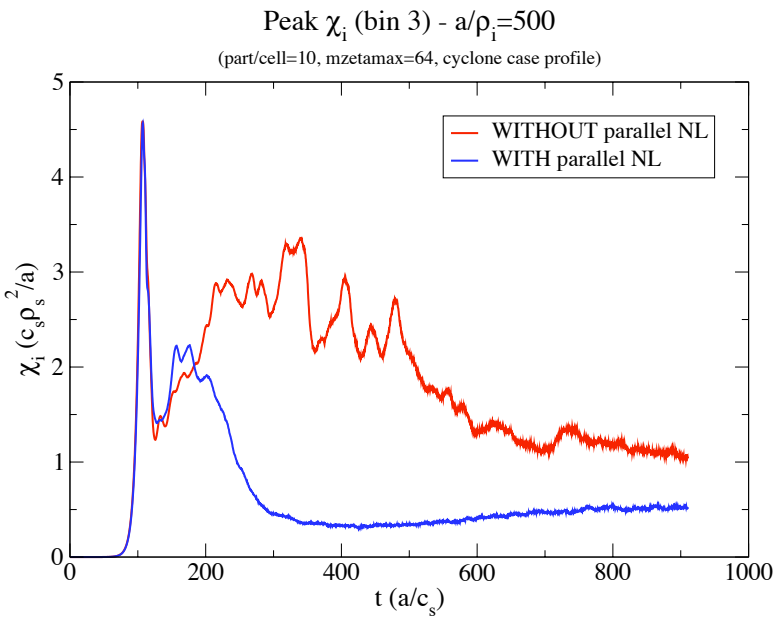
(W. M. Nevins, 04)

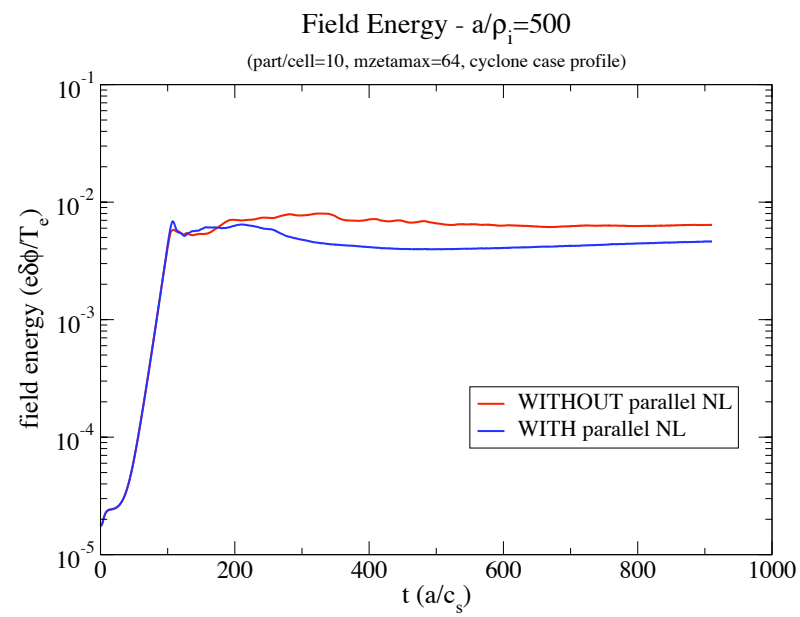
- Good agreement at linear and early nonlinear stages



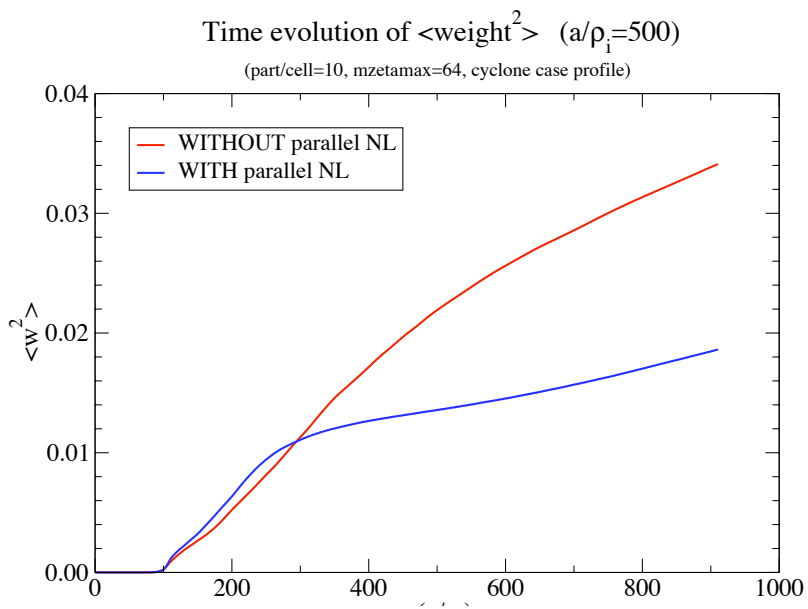
- Differences in the late nonlinear stage are not well understood: particle noise, poor velocity space resolution, geometry ...

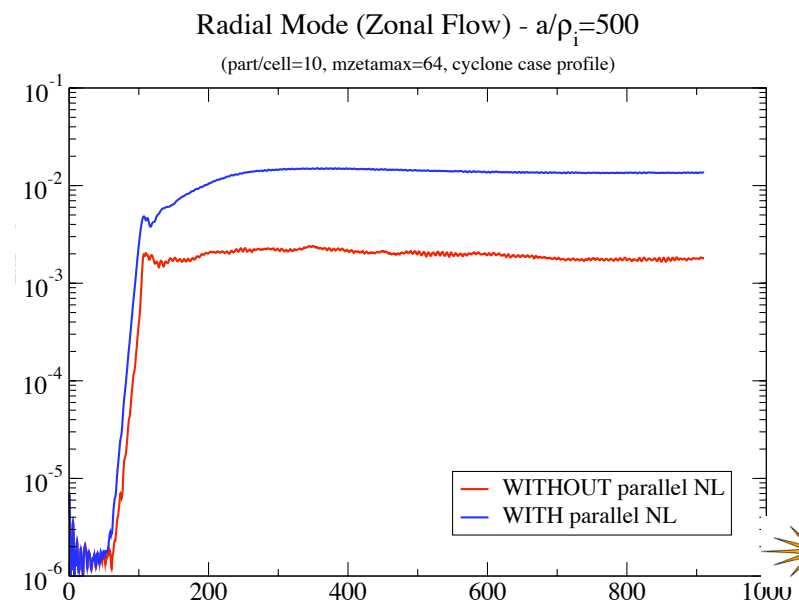
Steady State ITG simulations with velocity-space nonlinearity (Lee, Ethier et al.)





- Reaching steady state sooner but at lower level
- Lower field energy and enhanced zonal flow





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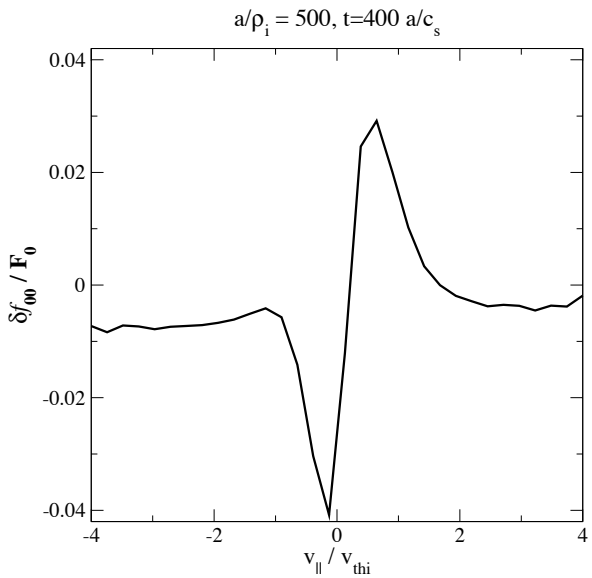
Steady State ITG simulations with velocity-space nonlinearity (cont.)

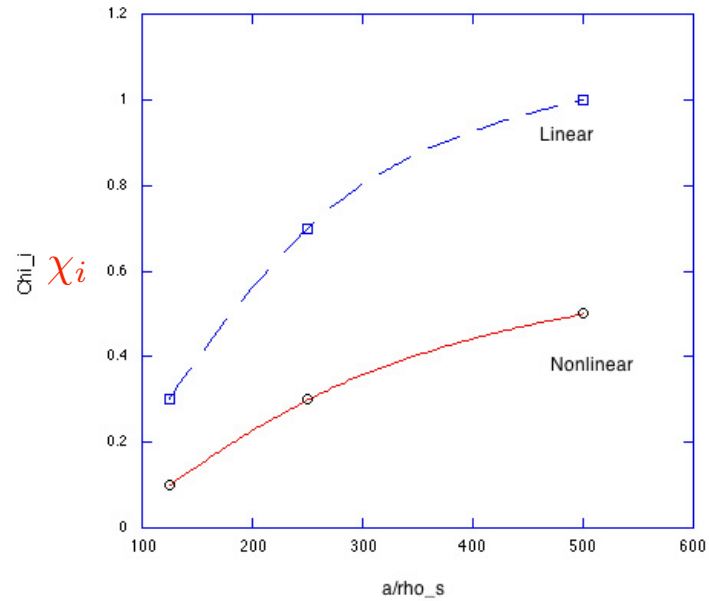
$< \delta f_i > / F_0$



$v_{||}/v_{ti}$

Nonlinear Change in Background Velocity Space Distribution
(a very large region is affected)

χ_i



a/ρ_s

Size Scaling
(transition from Bohm to GyroBohm is not affected by the velocity space nonlinearity)

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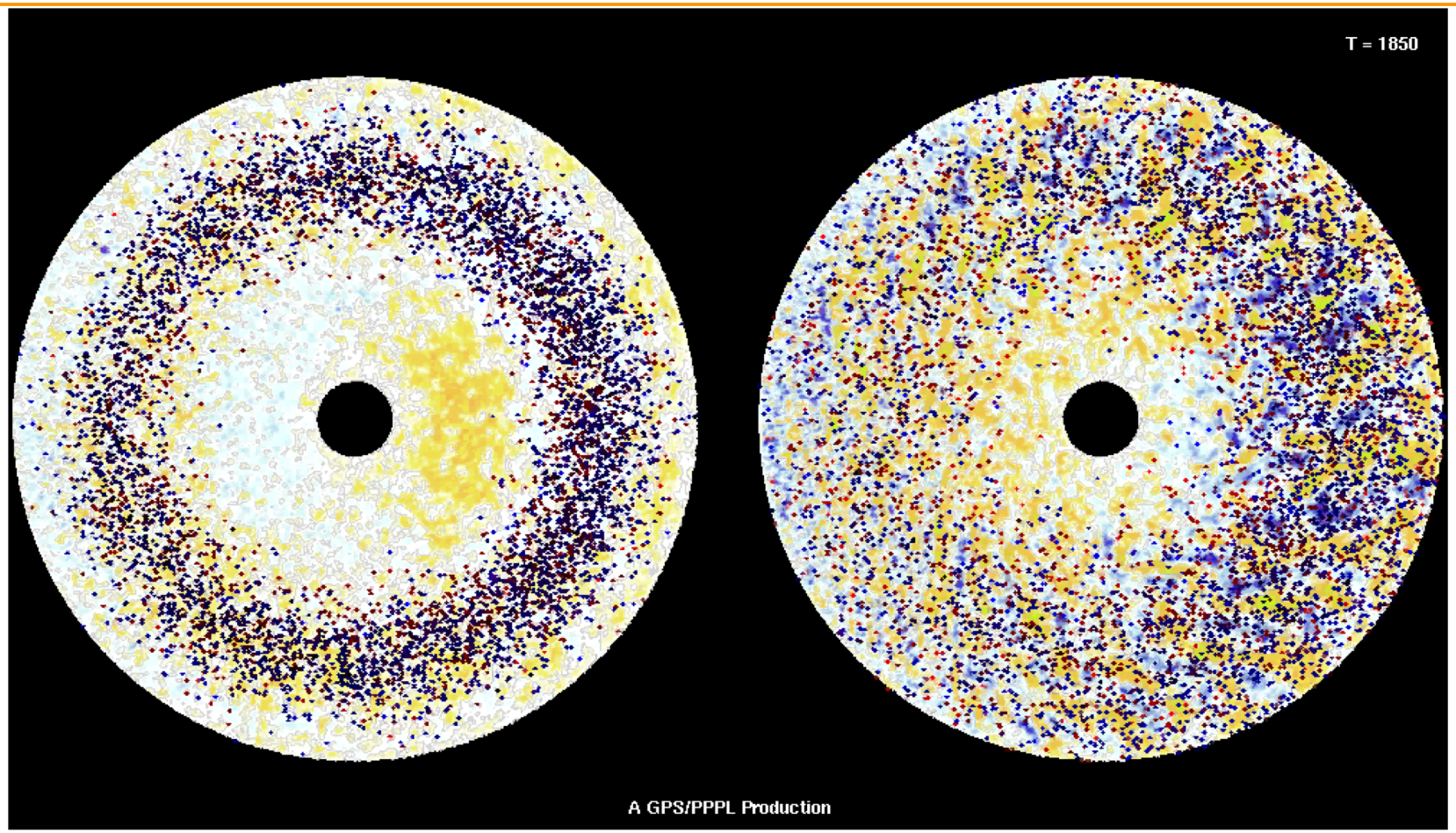
Time Evolution of ITG turbulence (GPSC)



With Without

Parallel Velocity-Space Nonlinearity

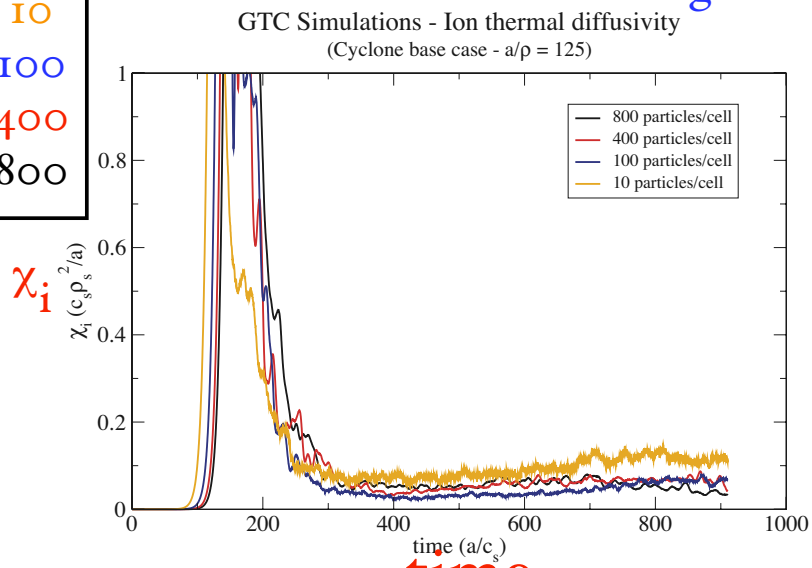
- different particle diffusion patterns
- different perturbed electrostatic potential patterns

Data Management and Visualization [Klasky, Ethier in collaboration with Beck, Ma Lee

Convergence tests of ITG simulations (LCF- ORNL)

Particle/cell scan: linear & nonlinear thermal fluxes seem to converge

10
100
400
800

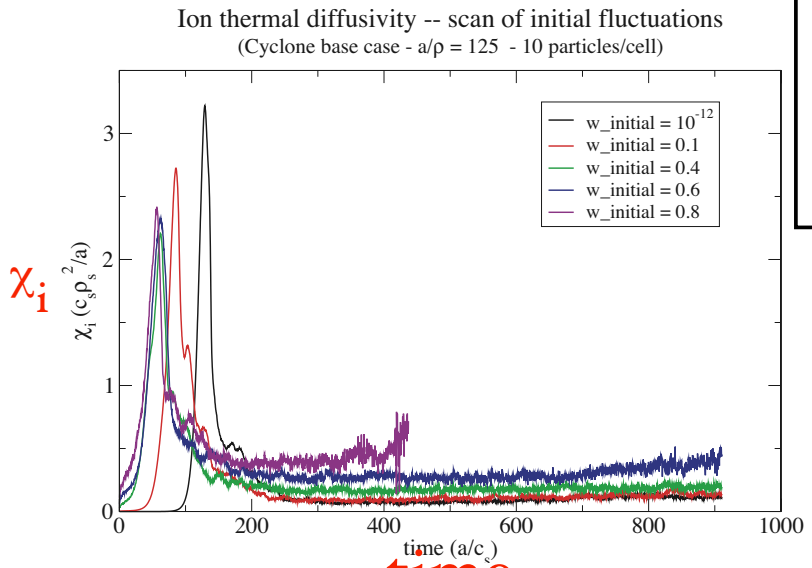


χ_i

time

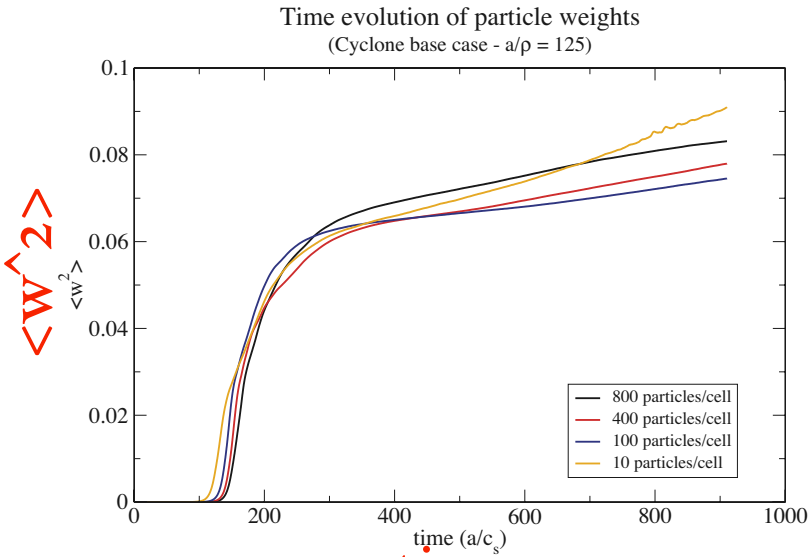
Initial particle weight scan: growing weights cause higher flux

10^-12
0.1
0.4
0.6
0.8



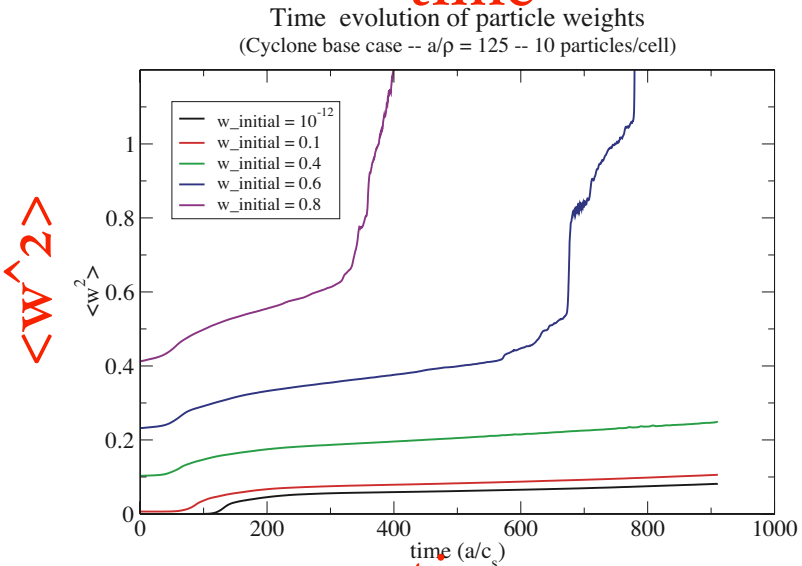
χ_i

time



<w^2>

time



<w^2>

time

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Theoretical Interpretations of the ITG Simulations

Entropy balance in ITG turbulence: velocity-space nonlinearity, collisions and numerical noise & dissipation in steady state

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

Monotonic increase in time | Vanishes in steady state | Velocity Space Nonlinearity | Collisional and/or numerical dissipation | Entropy production

[Lee and Tang, '88]

$\tau \equiv T_e/T_i$ $\qquad \kappa_{Ti} \equiv -dlnT_{0i}/dx$ $\qquad \langle \cdots \rangle \equiv \int d\mathbf{x}/V$

Let $w \equiv \frac{\delta f_i}{F_{0i}}$, we obtain

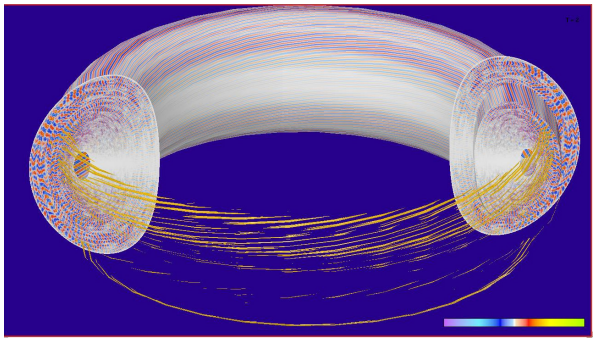
$$\boxed{\frac{\partial}{\partial t} \sum_{j=1}^{N} (1 - \alpha/4) w_j^2 + 2\nu\tau(1-\beta^2)\alpha \sum_{j=1}^{N} w_j^2 = \kappa_{Ti} \langle Q_{ix} \rangle}$$

$\alpha \approx 1, \beta << 1$ and N is number of simulation particles.

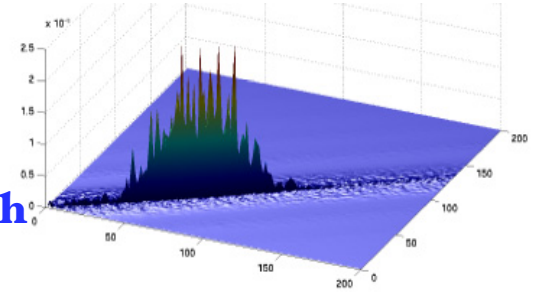
- Thus, without collisional or numerical dissipation and without velocity space nonlinearity effects, delta-f or particle weights will grow in time.
- Velocity space nonlinearity reduces ion energy flux, but collisions and numerical dissipation enhance it.

General Geometry Extension in GTC

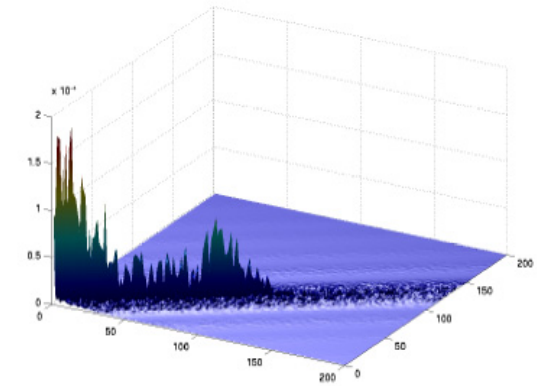
W. X. Wang



Energy Cascade to longer wavelength modes



t=1200



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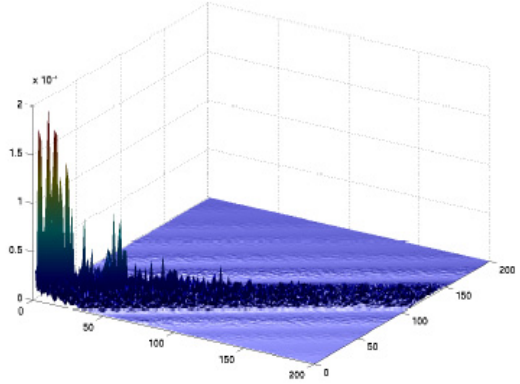

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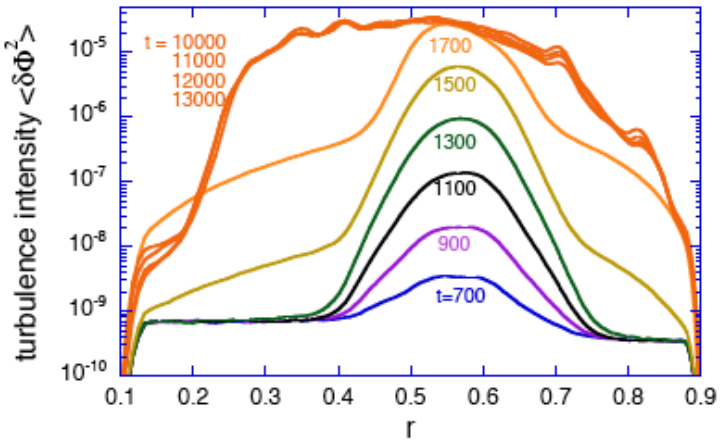
Turbulence Spreading



GTC-Neo Calculates Neoclassical fluxes with finite-orbit effects

- Global particle code GTC-Neo [W.X. Wang, *et al.,* Comp. Phys. Comm. **164**, 178 (2004)] calculates neoclassical fluxes of particles, momentum, and energy, as well as associated quantities such as radial electric field, bootstrap current, and poloidal velocity

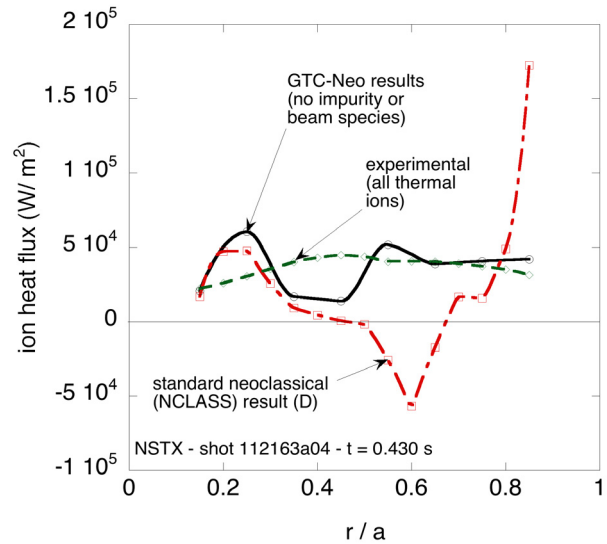
- Intrinsically non-local over the scale-length of the ion banana width due to included finite orbit effects (implies smoothing)

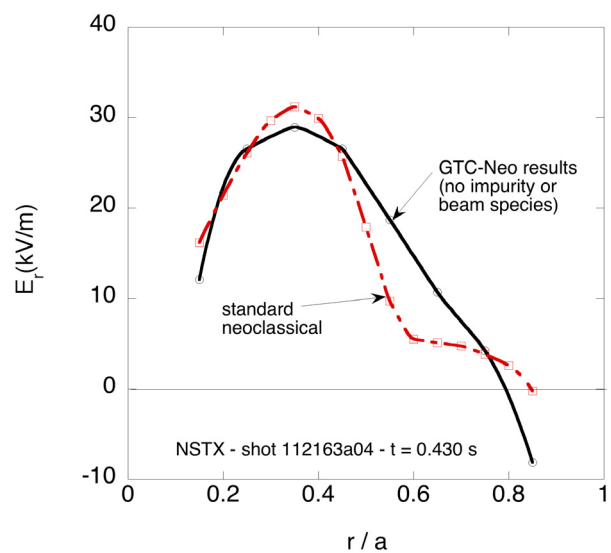
- Interfaced with MHD codes for the numerical MHD equilibrium and with TRANSP for experimental plasma profiles

- 9 cases have been run for NSTX

- Impurity and hot beam species to be added in future

Near-neoclassical(?) NSTX shot





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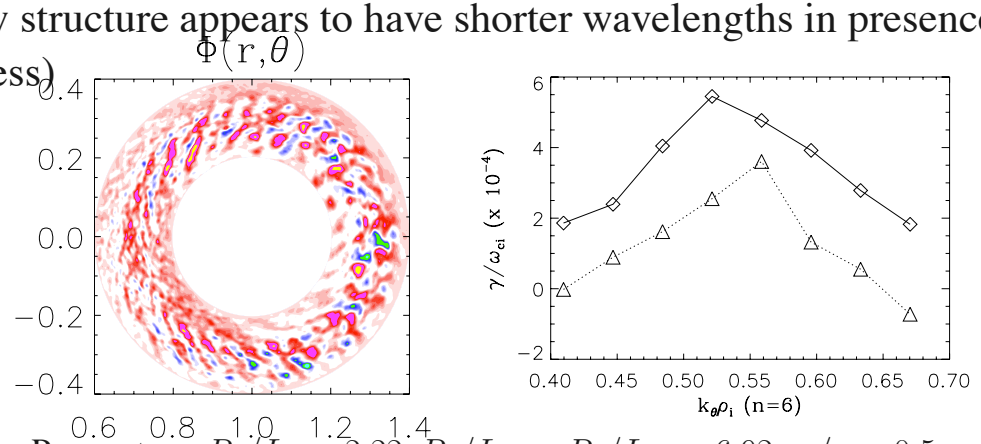
Electron Dynamics Extension in GTC

The split-weight scheme for toroidal, gyrokinetic particle-in-cell simulations with kinetic electrons

Motivation: remove the adiabatic electron response analytically and solve for non-adiabatic response numerically

- Split-weight scheme dynamically resolves non-adiabatic electron response only
- Good agreement with the FULL code [G. Rewoldt] for linear growth rate
- Numerical method is stable for large time step $\Delta t = 2 - 5\omega_{ci}^{-1}$
- Global finite element method coupled with PETSC standard solvers (Y. Nishimura *et al*, JCP 2005) used for inversion of global (toroidal) elliptic equations
- Steady-state χ_i in presence of trapped electrons increases when parallel velocity non-linearity is retained
- Zonal flow structure appears to have shorter wavelengths in presence of trapped electrons (in progress)



Parameters: $R_0/L_n = 2.22$, $R_0/L_{T_i} = R_0/L_{T_e} = 6.92$, $r/a = 0.5$.
[J.L.V. Lewandowski]

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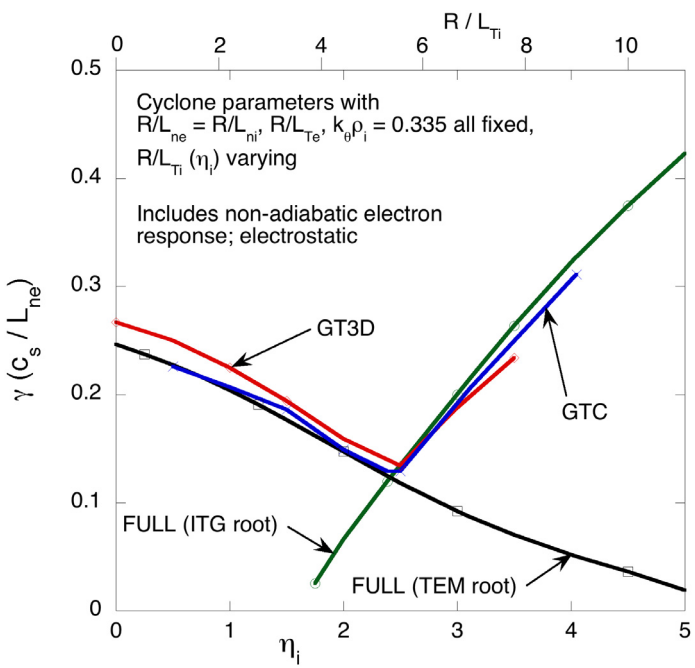
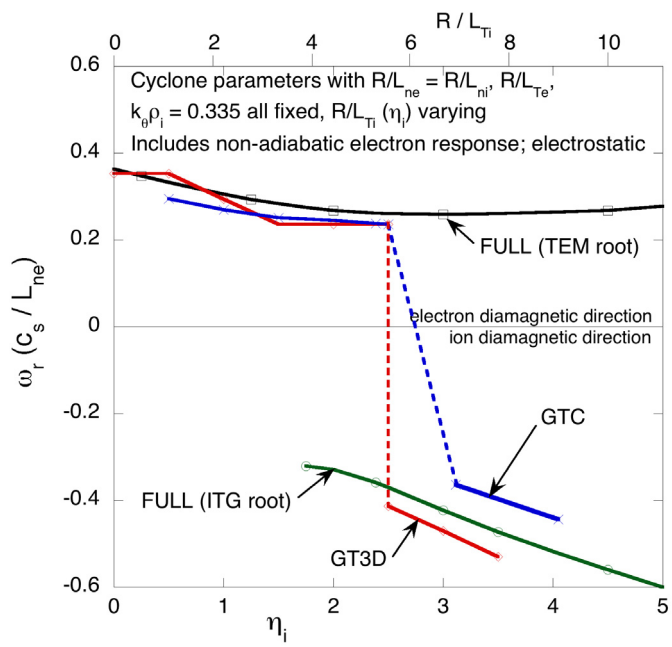
Ongoing GTC benchmarking studies

- Linear benchmarking, including the effects of trapped electrons, against global GT3D code (JAERI) and radially-local FULL code, for linear growth rates of ITG and TEM modes, carried out showing reasonably good agreement

- Nonlinear runs of GTC with trapped electrons, for convergence studies and for planned benchmarking, are now under way

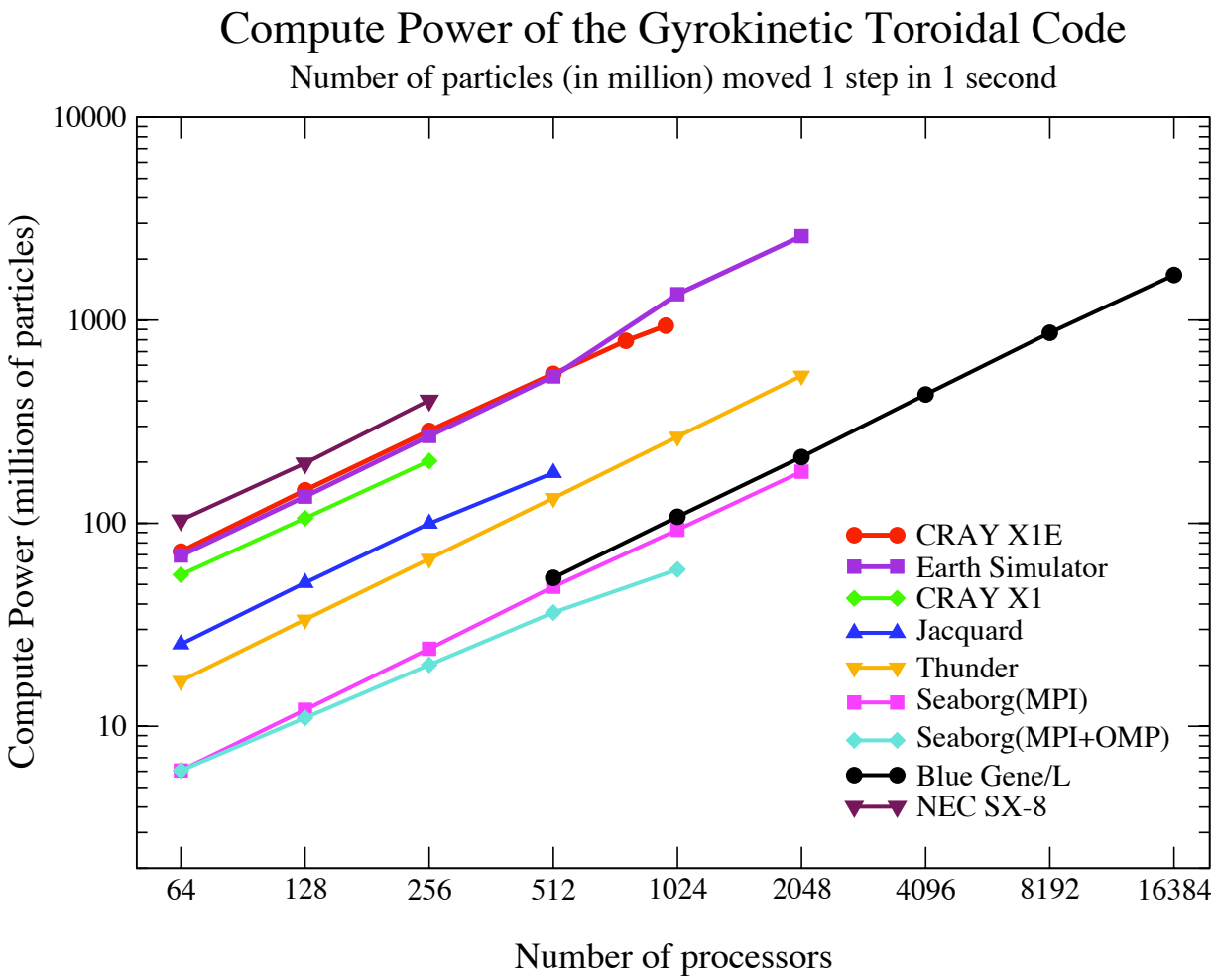




Y. Idomura (JAERI), Z. Lin (U.C. Irvine), G. Rewoldt

Enhancement of GTC performance on MPP platforms for ITER-size Plasmas (GPSC)

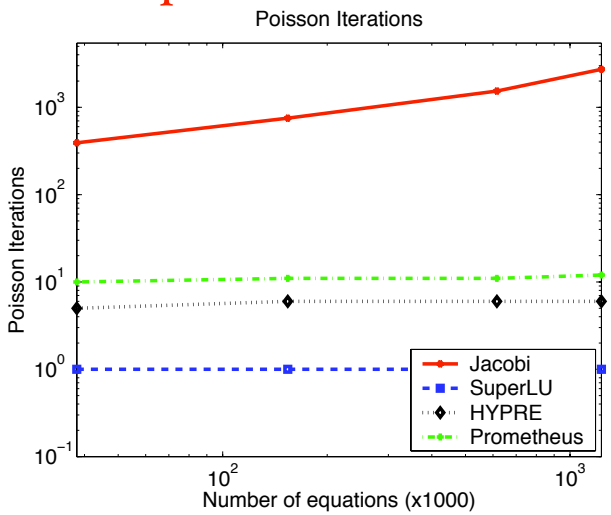
- Gyrokinetic particle codes are more portable, scalable and efficient on both cache-based and vector-parallel MPP platforms in comparisons with other fusion codes
- 3.7 teraflops achieved on the Earth Simulator with 2048 processors using 6.6 billion particles



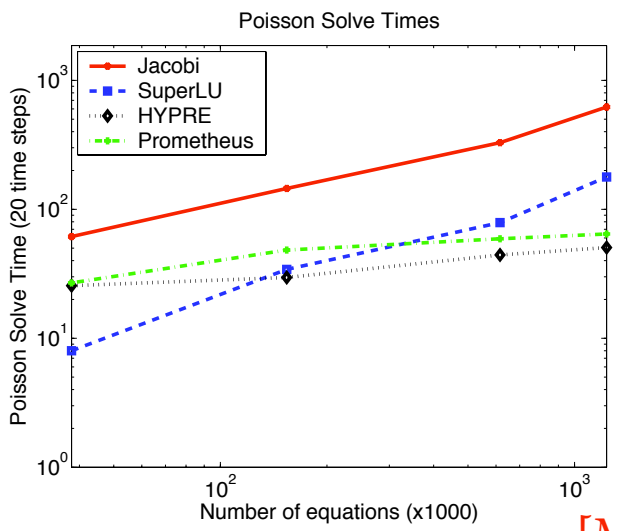
Ethier

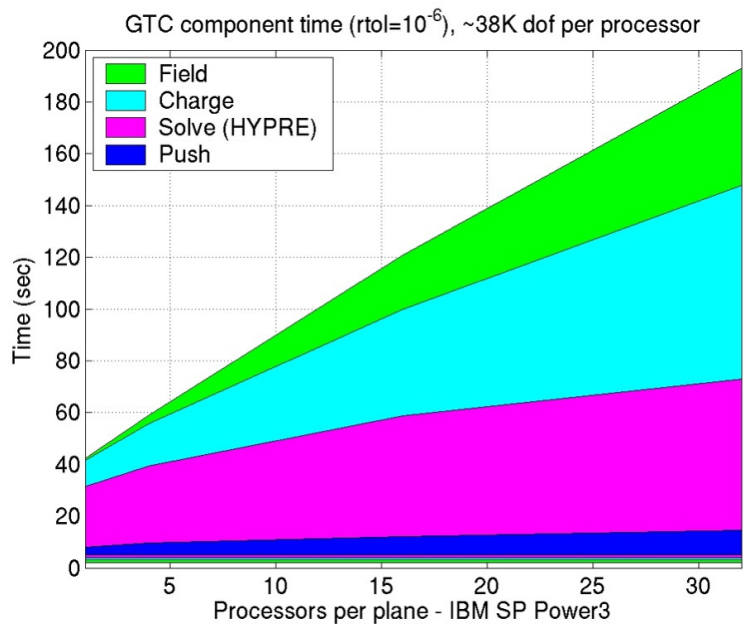
Enhancement of Poisson Solver Performance for ITER-size plasmas (GPSC in collaborations with TOPS-ISIC)

- Use modern solver techniques, we can efficiently solve our Poisson's equation and Ampere's law with realistic electron dynamics in large simulation systems



- Multigrid preconditioned Krylov solver
  - Prometheus (Columbia) & HYPRE (LLNL)
- Scaled speedup
  - ~38K dof per processor
  - 1 to 32 processors/plane
  - 8 planes, 20 time steps, 4 particles per cell





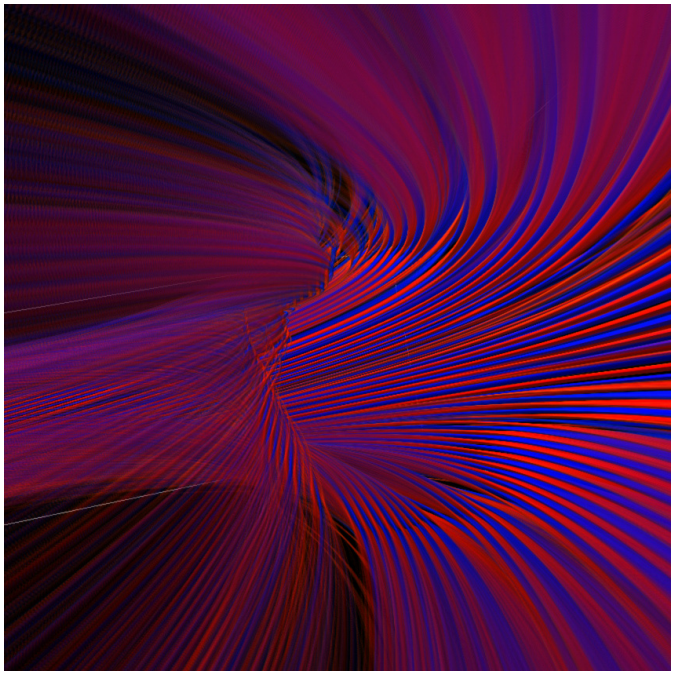
[M. Adams, Y. Nishimura, Ethier]

SciDAC collaborations: Data Management challenges (GPSC in collaboration with SDM-ISIC)

- GTC is producing TBs of data
  - Data rates: 80Mbs now, 1.6Gbs 5 years.
  - Need quality of service (QOS) to stream data.

- This data needs to be real-time processed and post-processed

- The post-processed data needs to be shared among collaborators
  -- Particle Data
  -- Field Data



Beck, Bhat, Klasky, Ma, Parashar

Plans for GTC

Near Term ('06 - '07)

- Implementing the split-weight scheme for electrons to study finite-beta physics in general geometry using GTC is the top priority

- Benchmarking with other simulation codes and carrying out NSTX and DIIID simulations will follow

Longer Term ('08 and beyond)

- NCSX simulation studies

- ITER simulation studies

- Integrated simulation studies

Plans for
Core-Edge Simulations via GTC
(GPSC & CPES)

- 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.

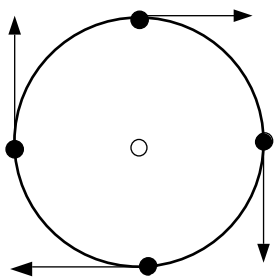
Extending Gyrokinetic Simulation to MHD Regime (MSG)

- For given zeroth-order field and density, parallel current and temperature profiles

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

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

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



- Ampere's law

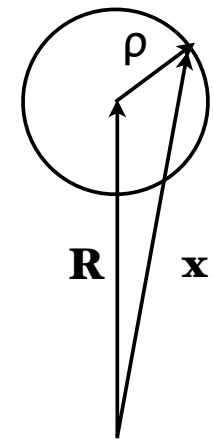
$$\nabla^2 \mathbf{A} = -\frac{4\pi}{c} \mathbf{J}_{gc}$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

- FLR effects are taken into accounted in gyrocenter-space and electron inertia is also accounted for.
- Implement these calculations in GTC, we will have temporal integration between turbulence and gyrokinetic-MHD

Extending Gyrokinetic Simulation to Wave Heating (MSG)

High-Frequency Gyrokinetics



- Gyrokinetic equation in slab geometry ($\rho/L \to 0$) as

$$\frac{\partial F}{\partial t} + (U\hat{\mathbf{b}} + \frac{cE \times \hat{\mathbf{b}}}{B}) \cdot \frac{\partial F}{\partial \mathbf{R}} + \frac{q}{m}\mathbf{E} \cdot \hat{\mathbf{b}}\frac{\partial F}{\partial U} - \Omega\frac{\partial}{\partial \varphi}(F - \frac{q}{m}\frac{\Phi}{B}\frac{\partial F}{\partial \mu}) - \Omega\frac{\partial}{\partial \mu}(\frac{q}{m}\frac{\Phi}{B}\frac{\partial F}{\partial \varphi}) = 0.$$

- For $F = F_0 + \delta f$ and $\partial F_0/\partial\varphi = 0$,

$$\frac{\partial \delta f}{\partial t} + (U\hat{\mathbf{b}} + \frac{cE \times \hat{\mathbf{b}}}{B}) \cdot \frac{\partial (F_0 + \delta f)}{\partial \mathbf{R}} + \frac{q}{m}\mathbf{E} \cdot \hat{\mathbf{b}}\frac{\partial (F_0 + \delta f)}{\partial U} - \Omega\frac{\partial}{\partial \varphi}(\delta f - \frac{q}{m}\frac{\Phi}{B}\frac{\partial F_0}{\partial \mu}) = 0,$$

- Separate gyrocenter motion from gyromotion: $\delta f = \delta f_g(\mathbf{R}) + g(\varphi)$,

$$\frac{dg}{dt} \equiv \frac{\partial g}{\partial t} - \Omega\frac{\partial g}{\partial \varphi} = -\Omega\frac{\partial}{\partial \varphi}(\frac{q}{m}\frac{\Phi}{B}\frac{\partial F_0}{\partial \mu}) \to \frac{dg}{dt} = -\mathbf{v}_\perp \cdot \mathbf{E}\frac{q}{mB}\frac{\partial F_0}{\partial \mu}.$$

- To the next order, we have

$$\frac{df_g}{dt} \equiv \frac{\partial \delta f_g}{\partial t} + (U\hat{\mathbf{b}} + \frac{c\mathbf{E} \times \hat{\mathbf{b}}}{B}) \cdot \frac{\partial \delta f_g}{\partial \mathbf{R}} + \frac{q}{m}\mathbf{E} \cdot \hat{\mathbf{b}}\frac{\partial \delta f_g}{\partial U} = -\frac{c\mathbf{E} \times \hat{\mathbf{b}}}{B} \cdot \frac{\partial F_0}{\partial \mathbf{R}} - \frac{q}{m}\mathbf{E} \cdot \hat{\mathbf{b}}\frac{\partial F_0}{\partial U},$$

- Dispersion Relation: [Qin et al. PoP, 1999.]

$$1 = \sum_j \frac{1}{k^2\lambda_D^2}\sum_{n=1}^{\infty}\frac{2n^2}{(\omega/\Omega)^2 - n^2}exp(-\frac{k^2T}{\Omega^2 m})I_n(\frac{k^2T}{\Omega^2 m})$$

- Need efficient numerical schemes for wave heating.

Plans for Integrated Gyrokinetic Particle Simulation

- Microturbulence simulation including electron dynamics and finite-β physics:
  - Time step set by electron zeroth-order orbit, e.g., 0.1 μsec.
    FL-coord. + Split-weight + Adiabatic field pusher
  - Simulation time to reach steady-state turbulence: e.g. 1 msec.
  - Transport time scale: e.g. 1 sec.

- Wave Heating
  - Time step to resolve Bernstein harmonics: 0.01 μsec

- Gyrokinetic MHD
  - FLR effects electron inertia and compressional Alfven effects

- Disparate spatial scales: $c/\omega_{pe} \approx 0.05$ cm, $\rho_i = 0.5$ cm, a = 1 m.

Transport time scale simulation: combinations of gyrokinetic turbulence and MHD simulations with reduced models

Integrated simulations of gyrokinetic MHD and wave-heating

PPPL PRINCETON PLASMA PHYSICS LABORATORY

Summary and Conclusions

- Ours is a joint endeavor of fusion, applied mathematics and computer sciences communities
- OFES provide crucial support, which is well leveraged through SciDAC and MICS
- We have made excellent use of computing resources and will benefit from more
- Our activities are enabled by collaboration and support from our fusion colleagues in and out of PPPL
- We plan to train young computational physicists through summer school courses (MSG)
- We have made substantial progress in ITG global simulations and will focus our attentions to ETG and the associated noise issues, if any, in the near future
- We are progressing towards incorporating electron dynamics and finite-beta effects in shaped plasmas in preparation for code comparisons with our simulation colleagues and, in collaboration with our theoretical and experimental colleagues, for realistic DIIID, NSTX, NCSX and, eventually, ITER simulations
- Integrated simulations of fusion plasmas, in both space and time, based on solid physics principles and efficient numerical schemes, that are most suitable for MPP platforms, are our ultimate goal.

Recent Related Publications and Talks

Z. Lin and L. Chen, “A fluid-kinetic hybrid electron model for electromagnetic simulations”, Phys. Plasmas **8**, 1447 (2001).

W. W. Lee *et al.*, “Shear-Alfven waves in gyrokinetic plasmas”, Phys. Plasmas **8**, 4435 (2001).

J. L. V. Lewandowski *et al.*, “Gyrokinetic calculations of the neoclassical radial electric field in stellarator plasmas,” Phys. Plasmas 8, 2849 (2001).

Z. Lin, *et al.*, “Size scaling of turbulent transport in magnetically confined plasmas”, Phys. Rev. Lett. **88**, 195004 (2002).

Z. Lin *et al*., “Size Scaling of Turbulent Transport in Tokamak Plasmas,” invited talk, IAEA (2002).

W. W. Lee and H. Qin, “Alfven waves in gyrokinetic plasmas”, Phys. Plasmas **10**, 3196 (2003).

W. W. Lee, “Theoretical and numerical properties of a gyrokinetic plasma: implications on transport scale simulation” Comput. Phys. Comm. 164, 244 (2004).

Z. Lin and T. S. Hahm, “Turbulence spreading and transport scaling in global gyrokinetic particle simulations”, Phys. Plasmas **11**, 1099 (2004).

Z. Lin *et al.*, “Electron Thermal Transport in Tokamaks: ETG or TEM Turbulence?,” invited talk, IAEA (2004).

W. X. Wang, *et al*., "Global delta-f particle simulation of neoclassical transport and ambipolar electric field in general geometry", Comput. Phys. Comm. **164**, 178 (2004).

S. Ethier and Z. Lin, “ Porting the 3D gyrokinetic particle-in-cell code GTC to the NEC SX-6 vector architecture: perspectives and challenges,” Comp. Phys. Comm. 164, 456 (2004).

W. W. Lee, “Steady State Global Simulations of Microturbulence ,” invited talk, APS/DPP (2004).

J. L. V. Lewandowski, “Low-noise Collision operators for particle-in-cell simulations,” Phys. Plasmas **12**, 052322 (2005).

S. Ethier, “Gyrokinetic Particle-in-Cell Simulations of Plasma Microturbulence on Advanced Computing Platforms,” keynote talk, SciDAC Conference (2005).

G. Rewoldt, “Particle-In-Cell simulations of electron transport,” invited talk, SciDAC Conference (2005).

S. Klasky, “Data Management on the Fusion Computational Pipeline,” invited talk, SciDAC Conference (2005).

J. L. V. Lewandowski, “Global particle-in-cell simulations of microturbulence with kinetic electrons,” invited talk, APS/DPP (2005).

W. X. Wang, “Neoclassical and turbulent transport in shaped toroidal plasmas,” invited talk, APS/DPP (2005).

Outline

- Collaborative activities
- Past and recent accomplishments
- Gyrokinetic particle simulation and particle noise
- Microturbulence simulation
  - Global Turbulence Code (GTC)
  - ITG simulations and convergence tests
  - Code comparisons
  - Performance on MPP platforms
  - Associated computer sciences issues
- Neoclassical simulation
- Future plans
  - Finite-β physics and gyrokinetic MHD
  - Core-edge simulation
  - Transport time scale simulation
  - Wave heating
- Conclusions

Enhancement of GTC performance on MPP platforms

(S. Ethier)

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!!

PPPL PRINCETON PLASMA PHYSICS LABORATORY

Highlights of Turbulence and Transport Simulations at PPPL

We have

- Laid the foundations of nonlinear gyrokinetic theory
- Developed the methodology of gyrokinetic particle (PIC) simulation and the associated numerical schemes
- Confirmed ITG modes as possible candidate for turbulent transport in tokamaks
- Studied the paradigm of global zonal flow physics

We are working on

- Relating turbulence spreading to scaling trends
- Exploring the connection of turbulence & steady state transport
- Implementing electron dynamics, finite-beta effects and general geometry in the GTC code
- Demonstrating the efficiency and scalability of PIC codes on MPP platforms

Extending Gyrokinetic Simulation to MHD Regime

- GK Three-field Equations for $k_\perp \rho_i \ll 1$ w/o geometric simplification [Lee and Qin PP '03]

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

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

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

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} - \frac{c}{B}\nabla\bar{\phi}\times\hat{\mathbf{b}}_0\cdot\nabla$$

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

- Reduced High-ß Three-Field MHD Equations [Strauss PF '78]

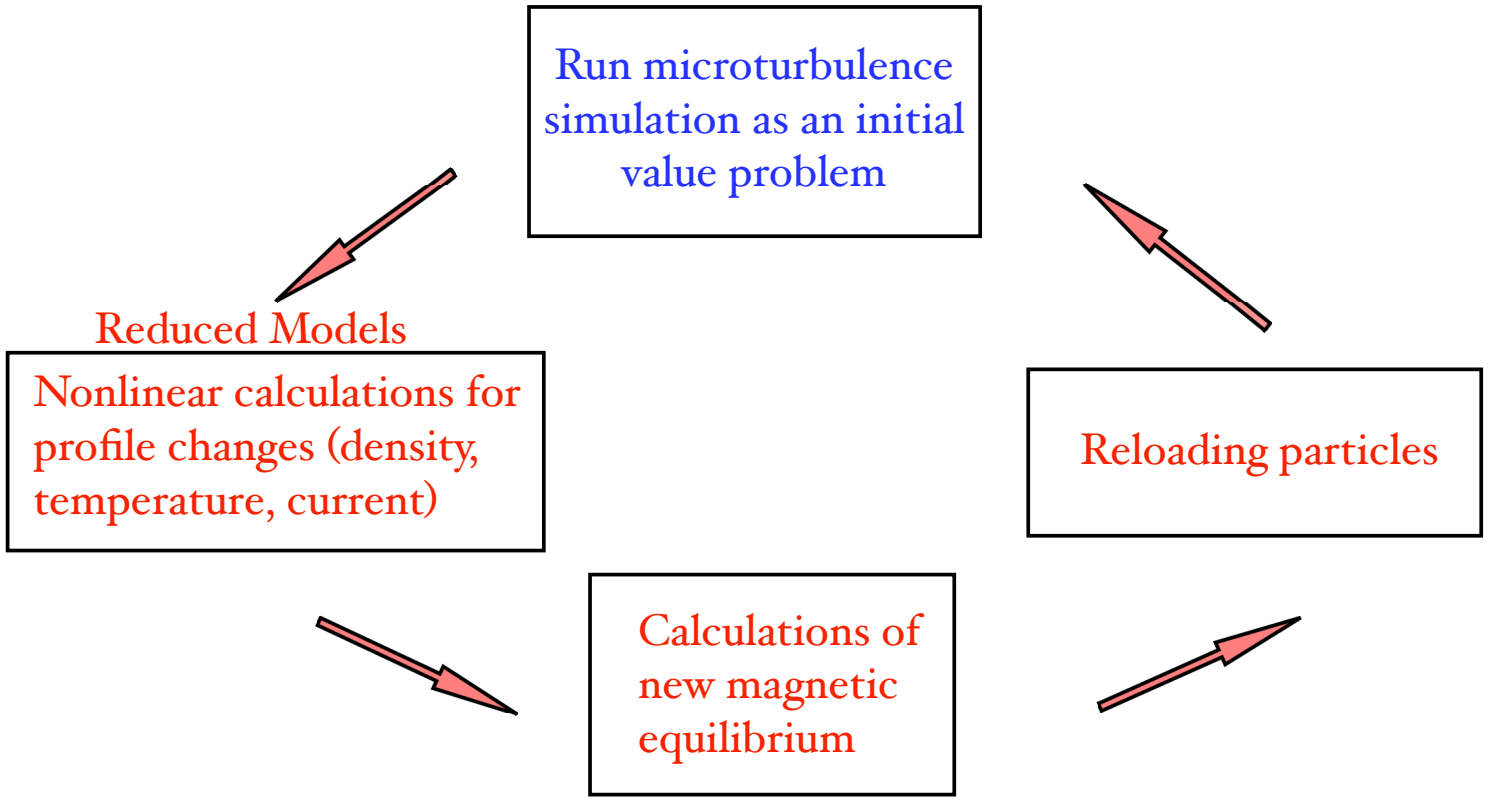
$$\frac{d\nabla_\perp^2\phi}{dt} + \frac{v_A^2}{c}(\hat{\mathbf{b}}\cdot\nabla)\nabla_\perp^2 A_\parallel - \boxed{\frac{2}{R_0}\frac{\partial p}{\partial y}} = 0$$

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

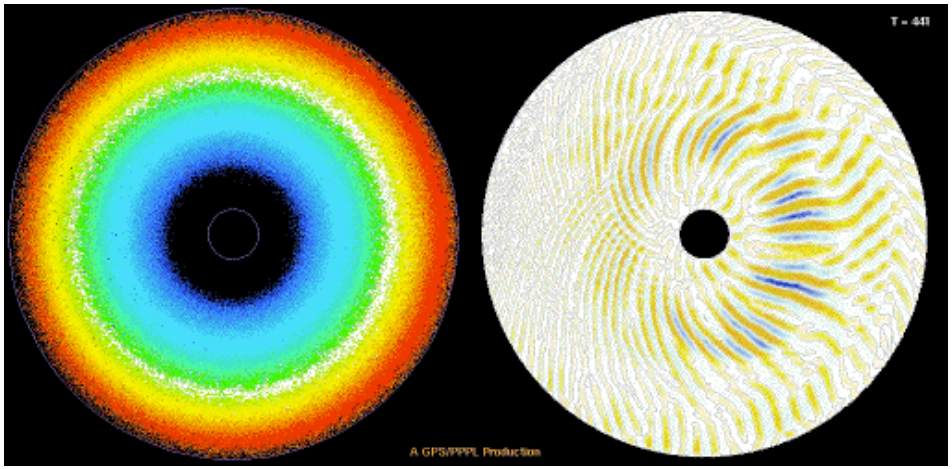
$$\frac{dp}{dt} = 0$$

Lee

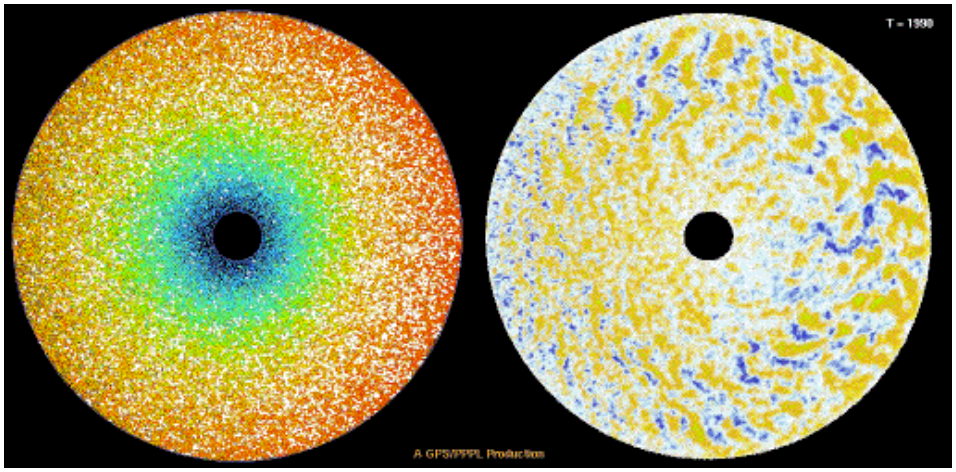
Future Plan
Turbulence Simulation in Transport Time Scale (MSG)



Visualization of ITG simulations [Klasky and Ethier]



TracerParticles Perturbed Potentials



Diffusion is a global phenomenon
(Net particle diffusion is zero, but thermal diffusion is nonzero)