First Year Status
on
SciDAC Center for Gyrokinetic Particle Simulation of Turbulence Transport in Burning Plasmas

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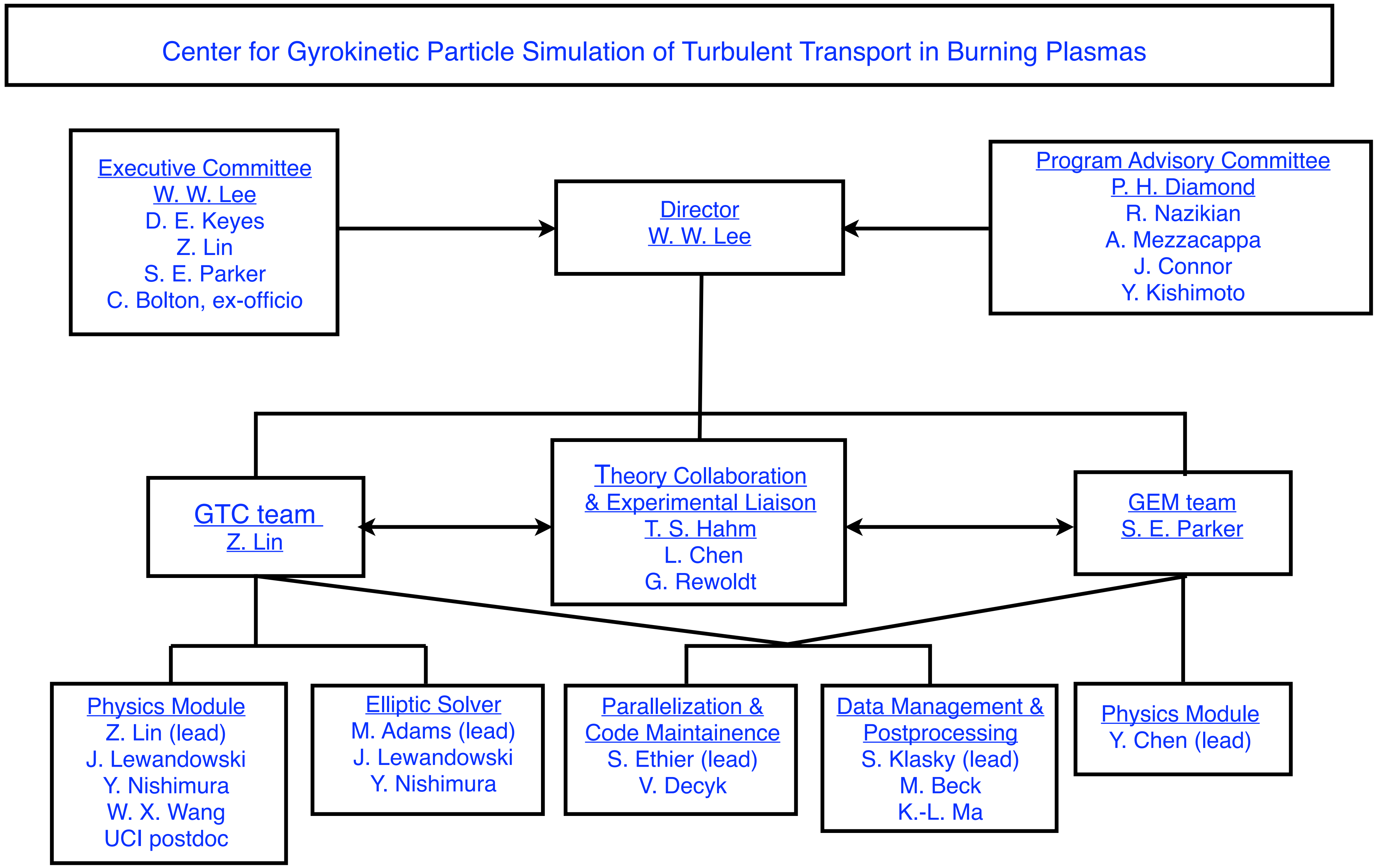
Presented at
PSACI PAC Meeting
June 2005

GPSC Organization



Activities

- Invited talks (12): One at IAEA conference in Vilamoura, Portugal, one at Varenna, Itatly, two at the APS/DPP Conference in Savannah, GA, one at the IEEE ICOPS Meeting, four more at the upcoming 2005 SciDAC Conference in San Francisco, CA, one more at 2005 EPS, Spain, two more at 2005 ICNSP, Japan.

- Publications (8) and submissions(5+): Four in PoP, one in Plasma Phys. Contr. Fusion, one in SC2004 Conference Proceedings, one in VIZ2004 Conference Proceedings and one more in GRID2004 Conference Proceedings; one on ETG to PRL, one on edge-core coupling to PoP, one to CPC, two more to JCP, and several more manuscripts ready for submission shortly.

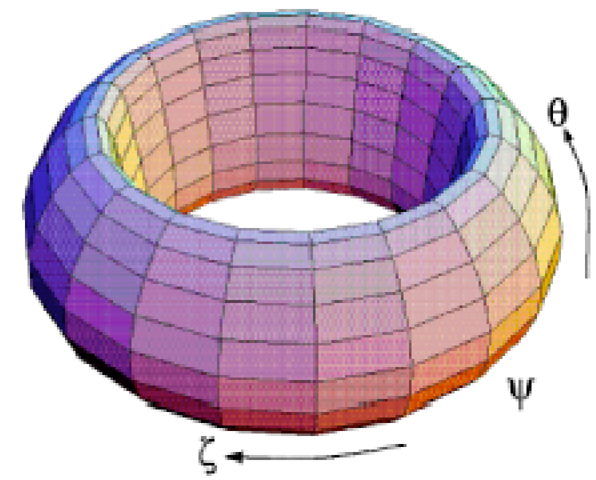
- Meetings sponsored by GPSC (2) : Evening session at APS/DPP, Savannah, GA (18 attendants), 2 day workshop, Laguna Beach, CA (50+ attendants), 2 day working sessions, Irvine, CA (15+ attendants).
- Many video/telephone conferences and onsite visits among GPSC personnel.

Outline

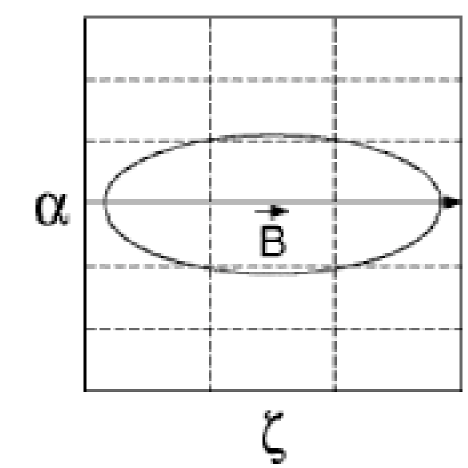
- Organization and Activities
- GTC team
  - ETG physics: transport and saturation
  - ITG physics: steady state transport, shaped plasmas, non-adiabatic electrons
  - Alfven waves
- Theory/Experimental Liaison team
  - Turbulence spreading of ITG
  - Toroidal mode coupling of ETG
  - Neoclassical transport: GTC-neo vs. NSTX
  - GTC benchmarking and convergence studies
- GEM team
  - Flux tube > full cross section > shaped plasmas
  - Finite-β physics
  - Tearing mode simulations
- SAPP team
  - Code performance studies
  - Poisson solver
  - Team coding
  - Data management and Visualization
- Controversy on particle noise in gyrokinetic particle codes
- Conclusions

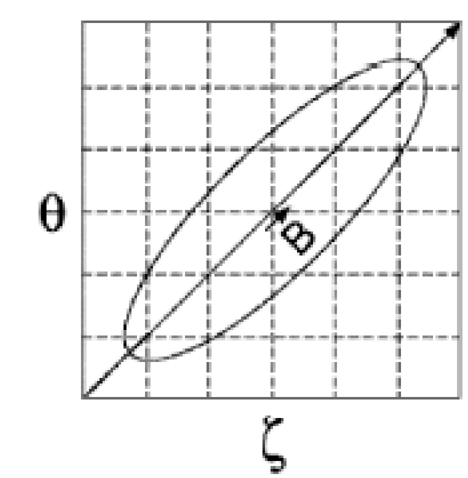
Global Gyrokinetic Toroidal Particle Simulation Code: GTC

[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]

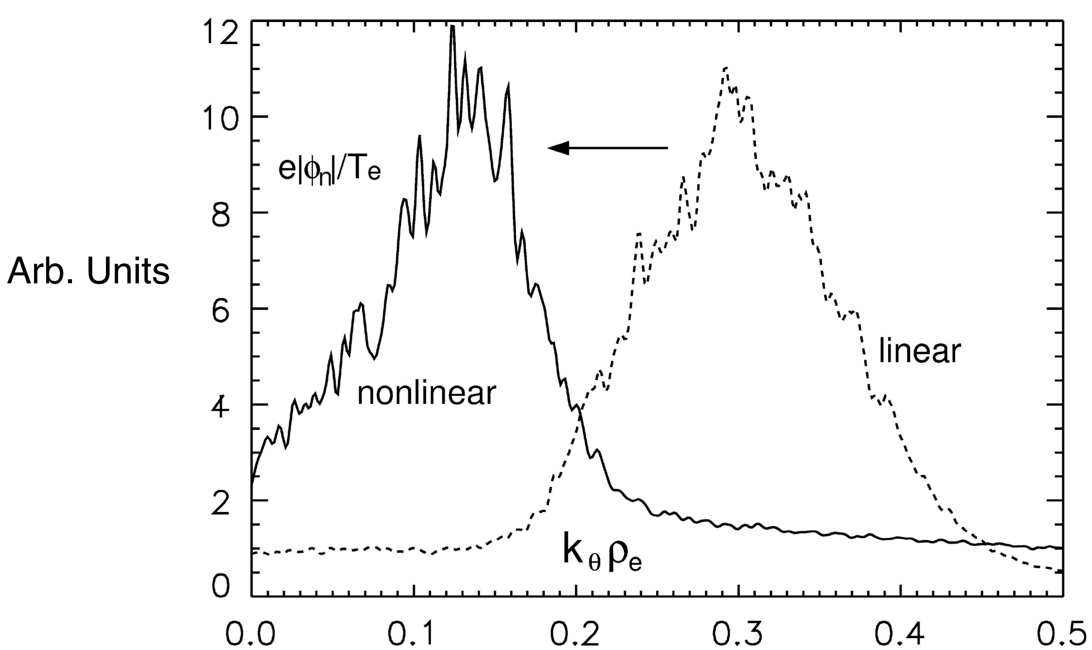


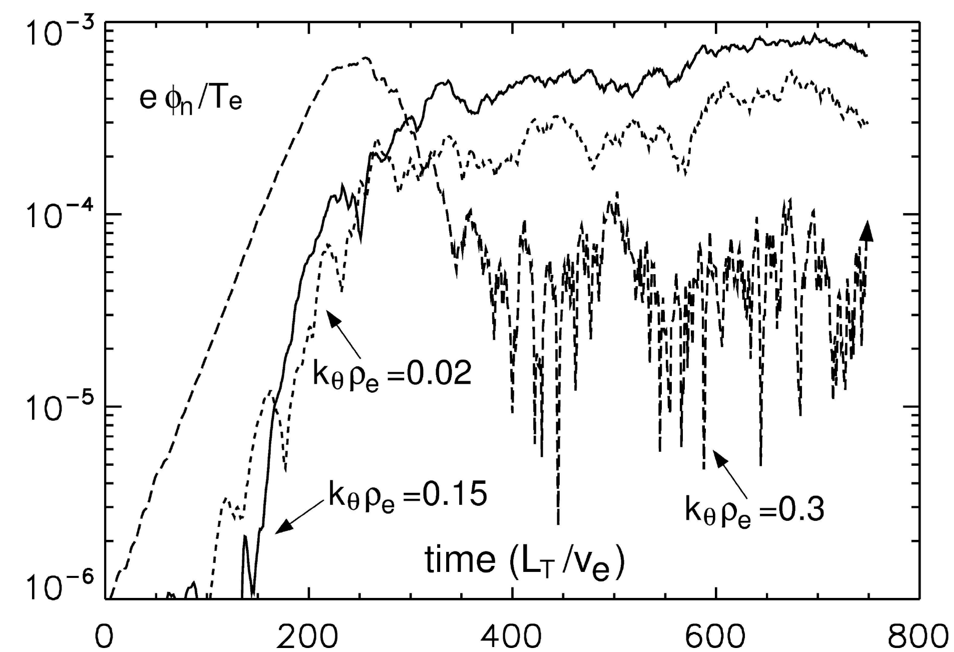


ETG Turbulence Structure Nonlinearly Generated

Lin et al.

- Poloidal spectrum down shifts from linear $k_\theta\rho_e$~*0.3* to nonlinear $k_\theta\rho_e$~*0.12*
  - Over 10 linear growth times
- Energy containing modes grow faster than linearly most unstable modes
  - Saturation via nonlinear mode coupling
  - Streamers nonlinearly generated
- Low-*n* modes driven up first before energy containing modes
  - Nonlocal interaction in *k*-space: not inverse cascade *[Hasegawa & Mima, PRL1977]*





ETG Saturates via Nonlinear Toroidal Coupling

- Generation of low-*n* quasi-mode

$$(n_1, m_1) + (n_2, m_2) \rightarrow (\Delta n, \Delta m) = (n_2 - n_1, m_2 - m_1)$$

- Energy transfer to nonlinear mode

$$(n_1, m_1) + (\Delta n, \Delta m) \rightarrow (n_1 - \Delta n, m_1 - \Delta m)$$

  - Streamers nonlinearly generated

- Cascade facilitated by low-*n* quasi-mode

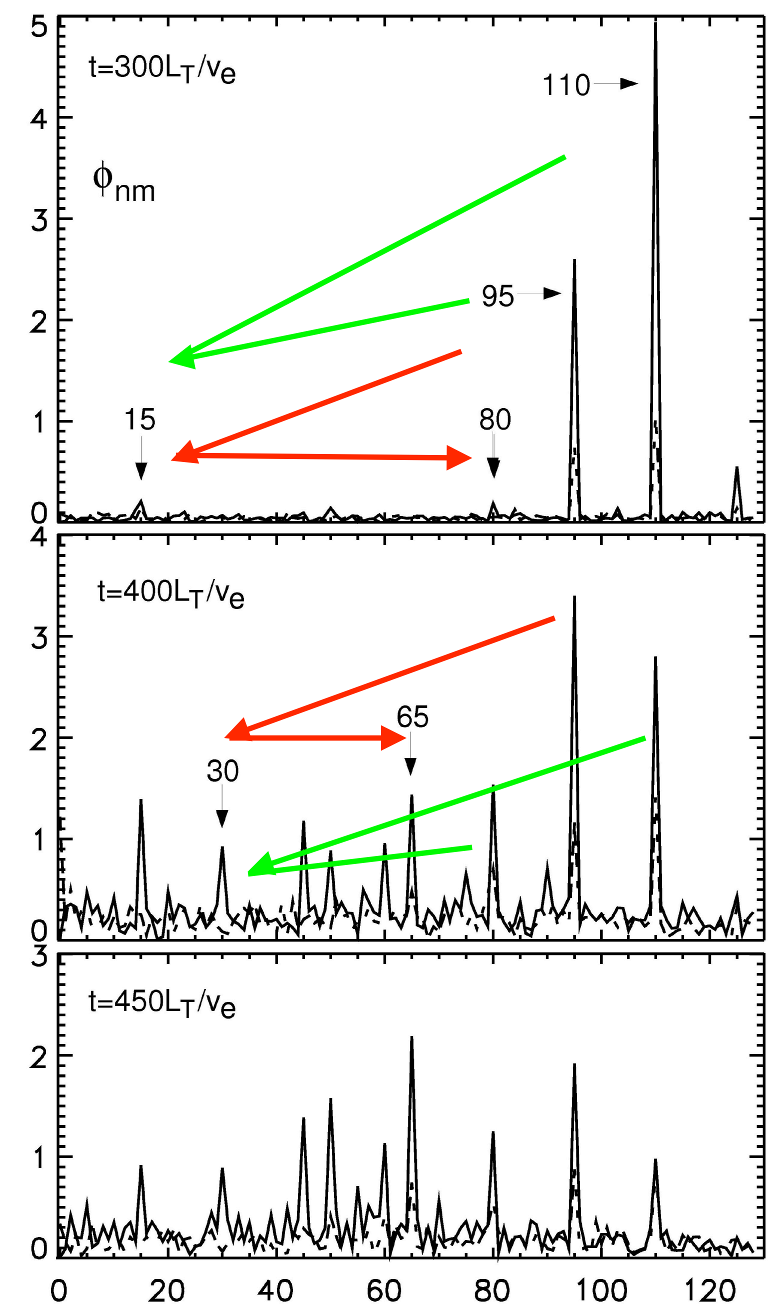
  - Nonlocal in *k*-space: "Compton Scattering"

  - *[Similon & Diamond, PF1984; Hahm & Tang, PF1991]*

- Saturation via nonlinear toroidal coupling before onset of Kelvin-Helmholtz instability

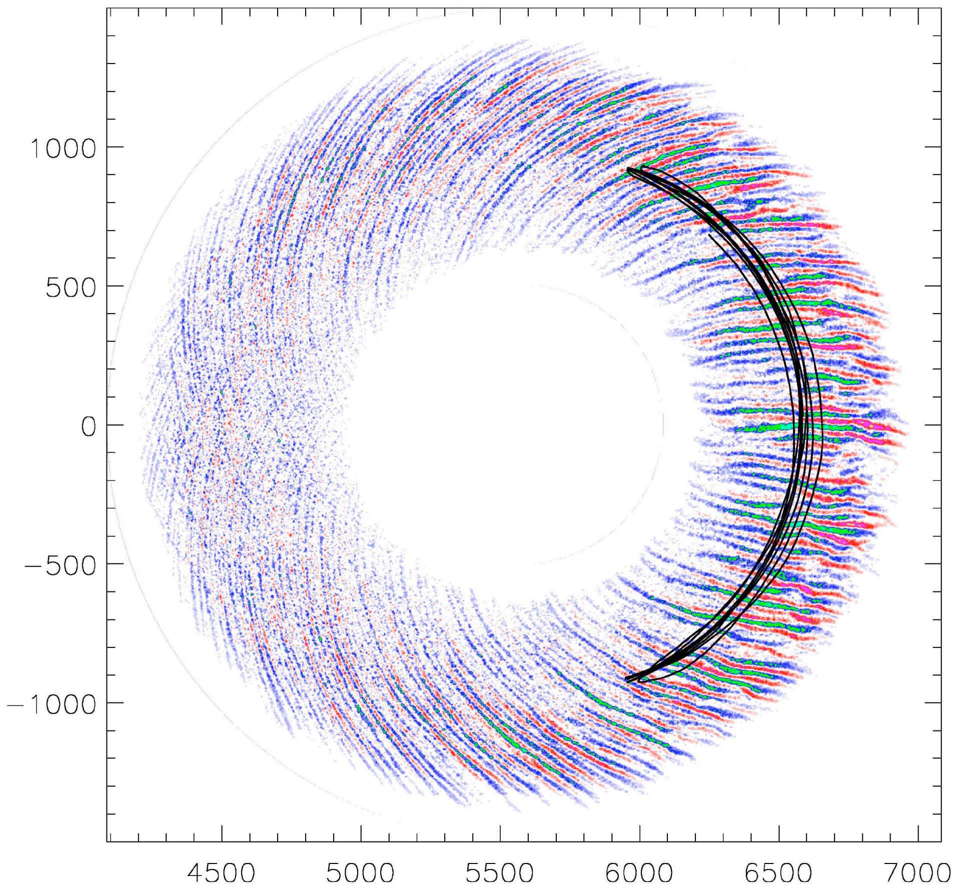
- Consistent with nonlinear gyrokinetic theory

Lin, Chen, & Zonca, PoP2005



Saturation Amplitude Insensitive to Streamer Length

- Streamer length scales with device size
- At saturation *I* & χ_e insensitive to streamer length
- Electrons do not rotate with radial streamers
- Eddy turnover time >> linear growth time
  - *Suppressed by sheared flows?*
  - $\omega_{EXB} > \gamma_{nl}\, k_r/k_\theta$ *[Biglari et al, PF1990]*
- Need further studies for steady state ETG transport
  - Controversy on saturation & transport mechanisms
  - Incomplete physics: sheared flows, coupling to ITG/TEM, etc
  - Profile relaxation
  - Numerical convergence

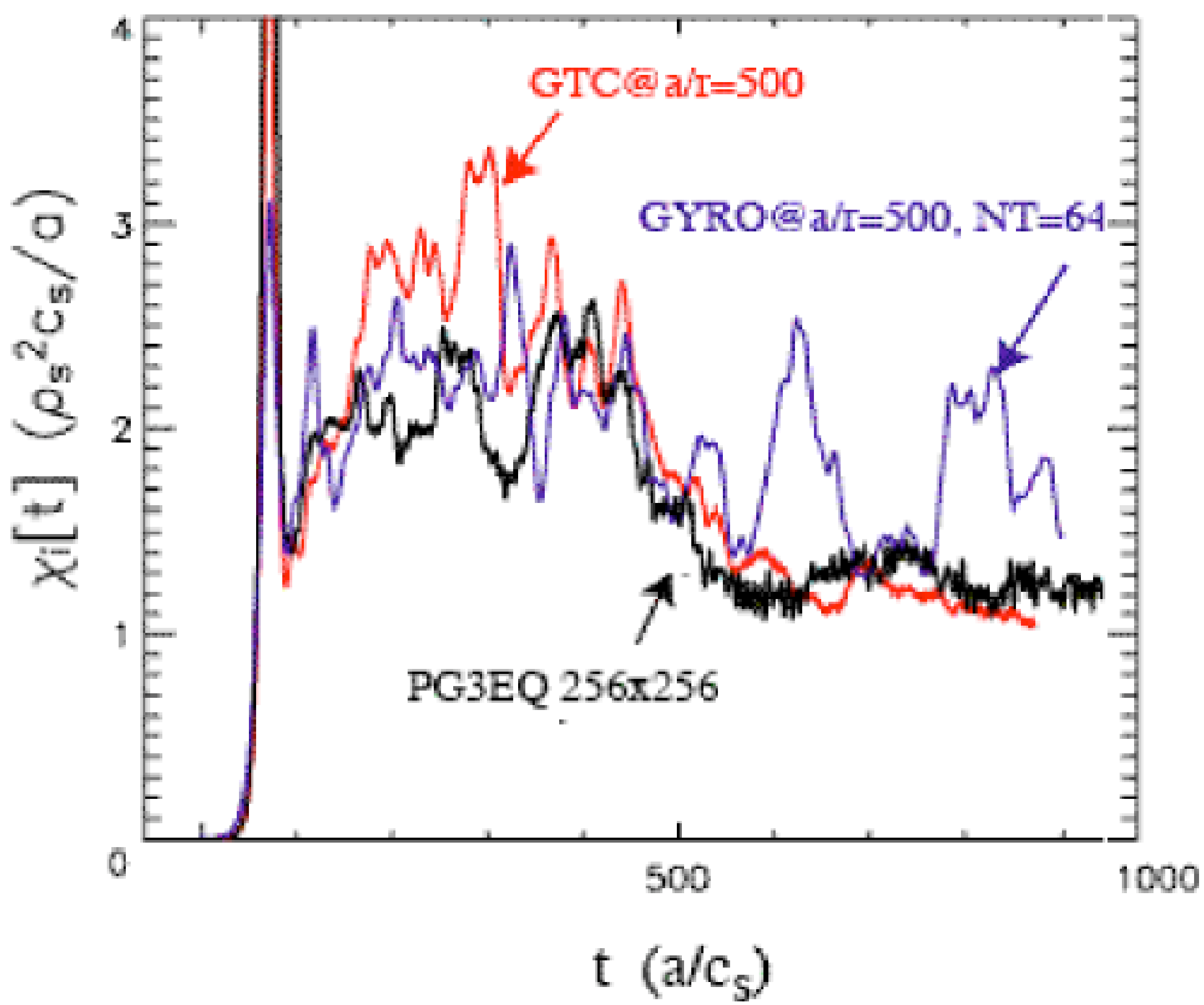


Lin, Chen, & Zonca, PoP2005

Recent PMP Code Comparisons and Controversies

(W. M. Nevins, 04)

Cyclone-based ITG Simulations



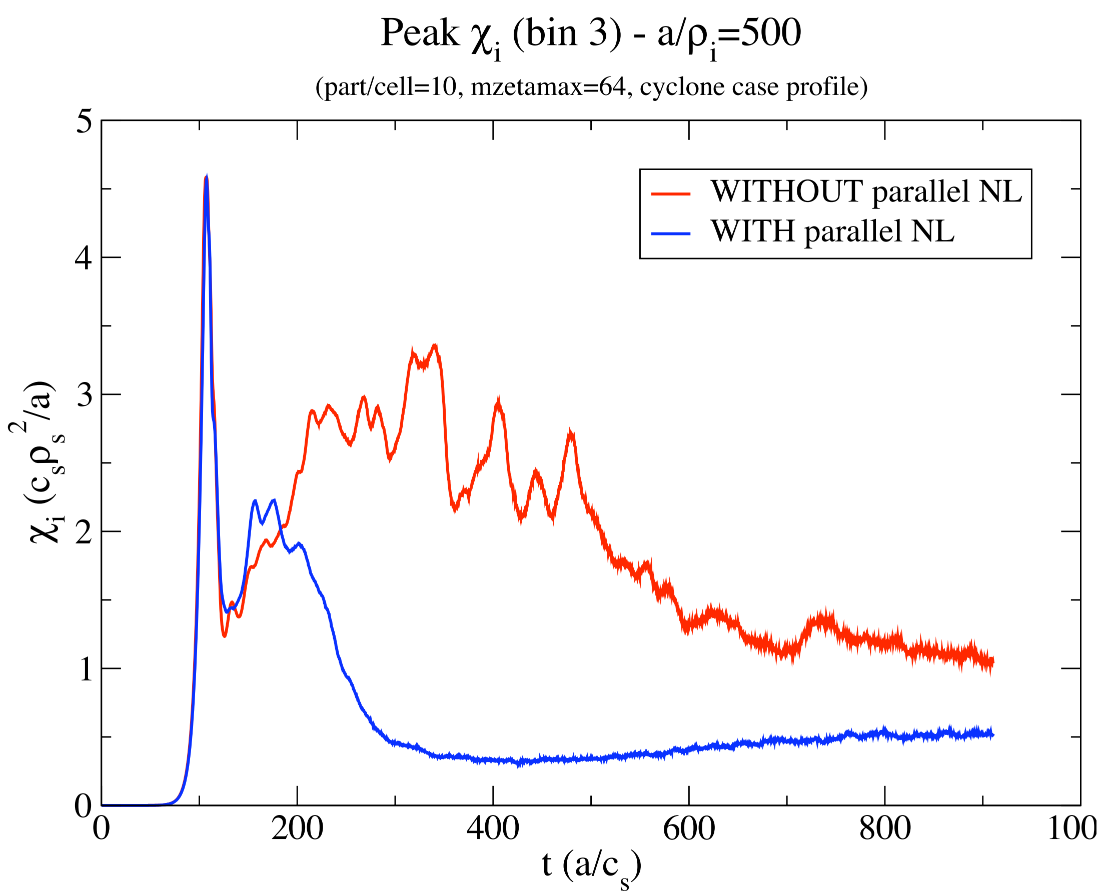
Code Comparisons:

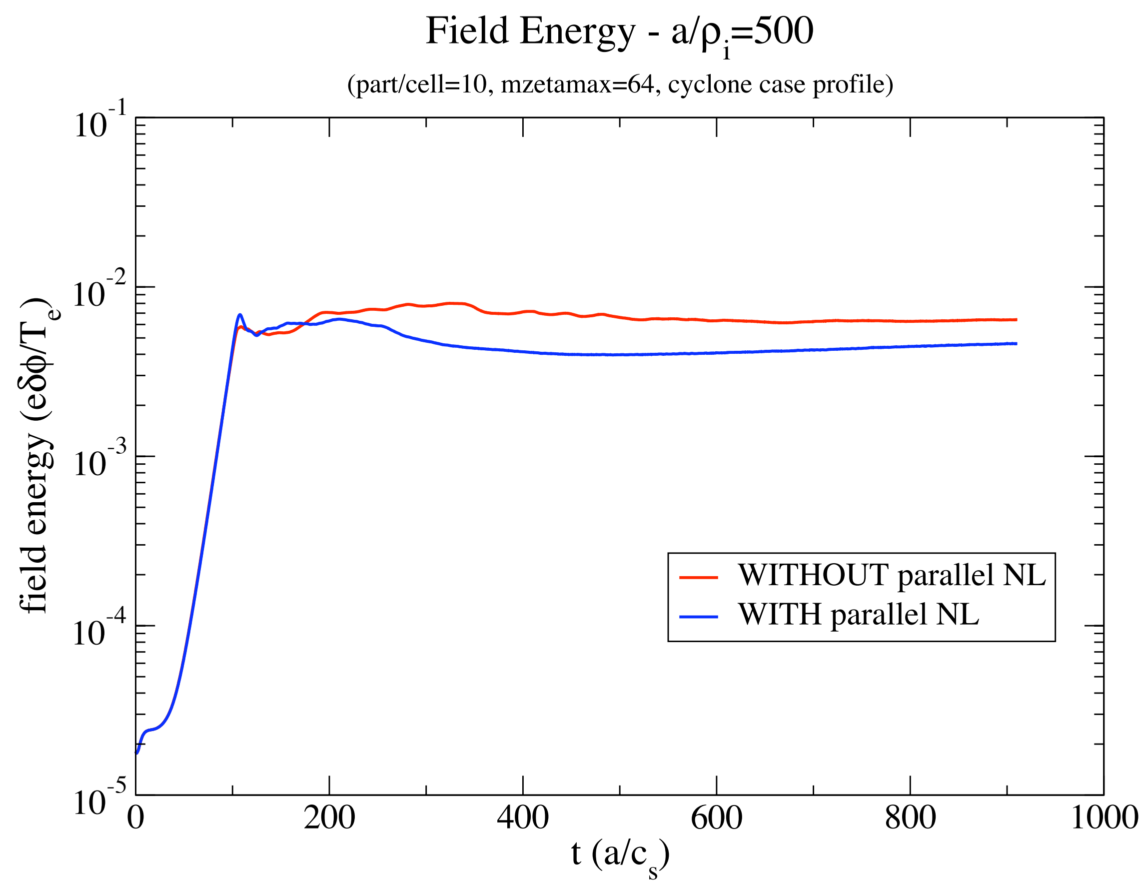
GTC - Particle Code

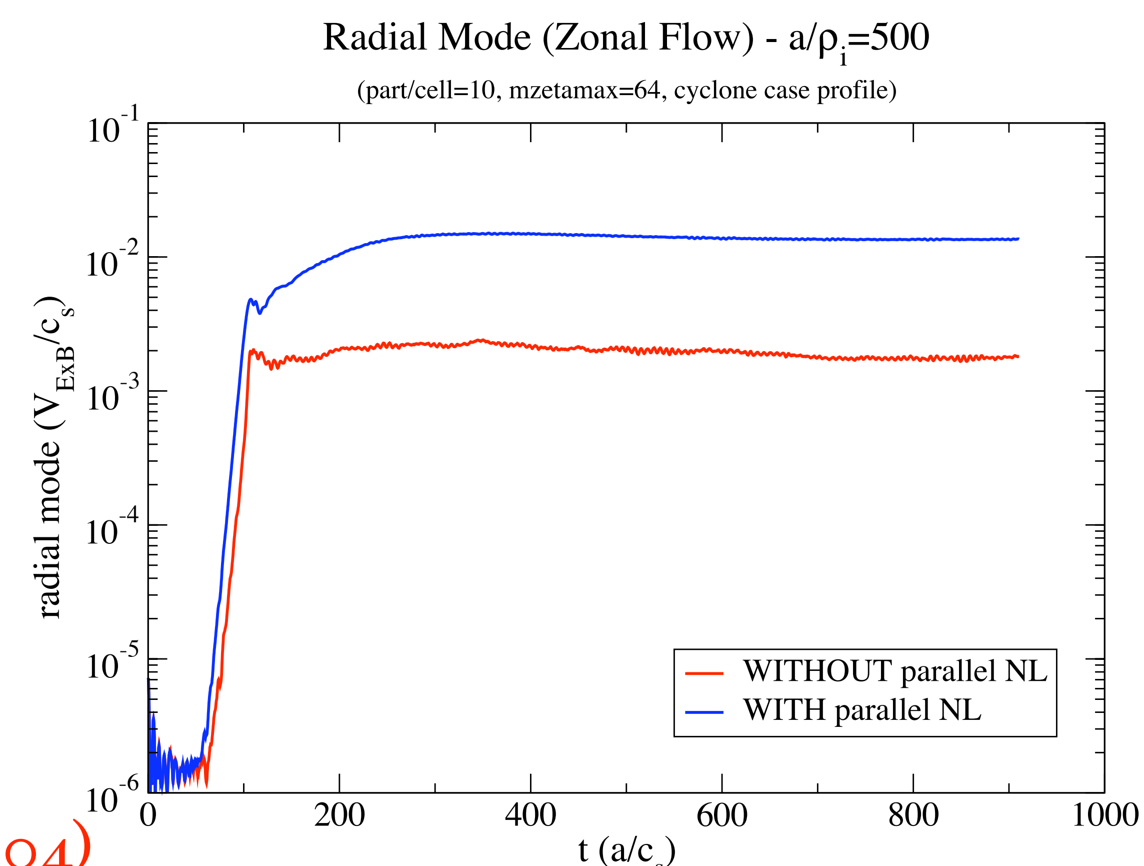
GYRO - Continuum Code

PG3EQ - Particle Code

Steady State ITG simulations with and without velocity-space nonlinearity



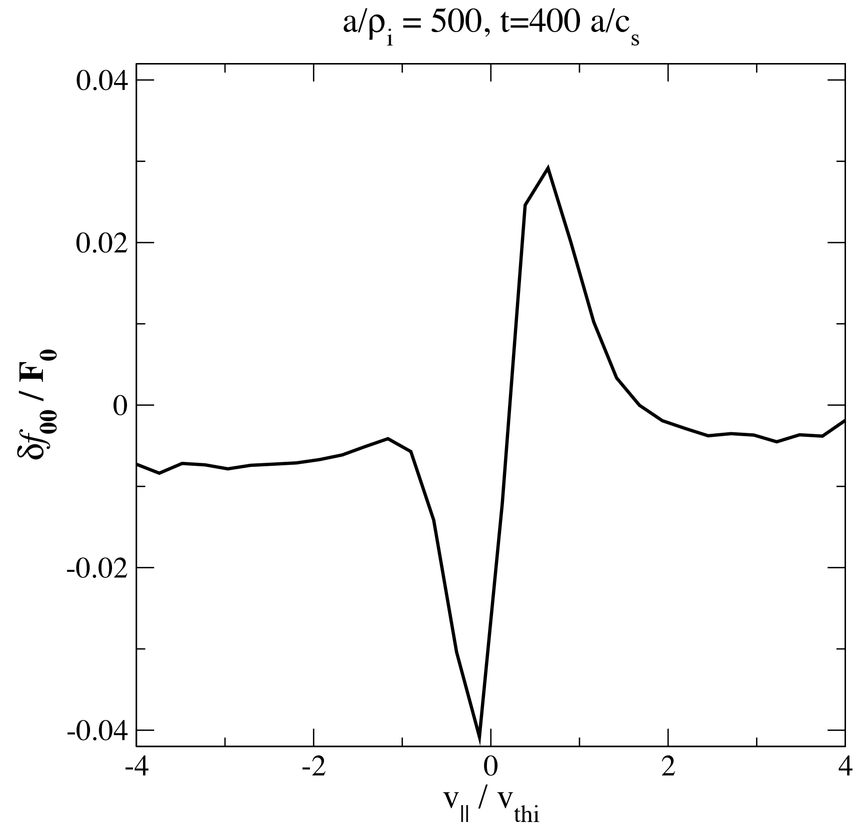


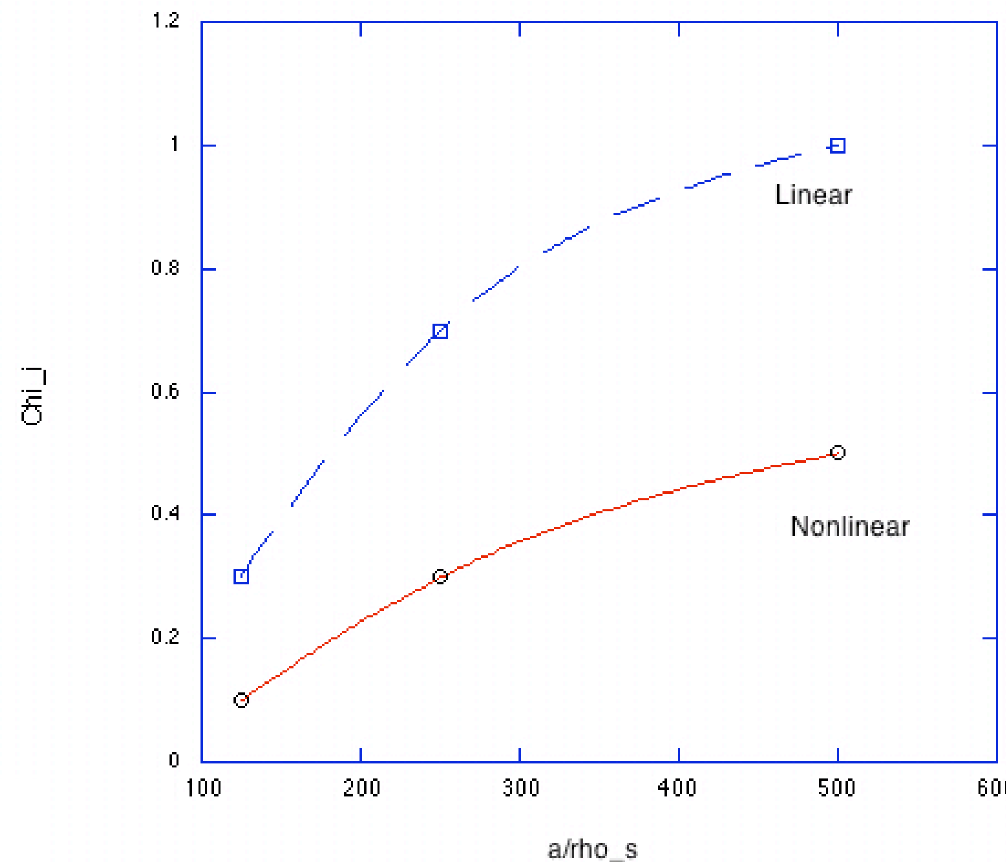


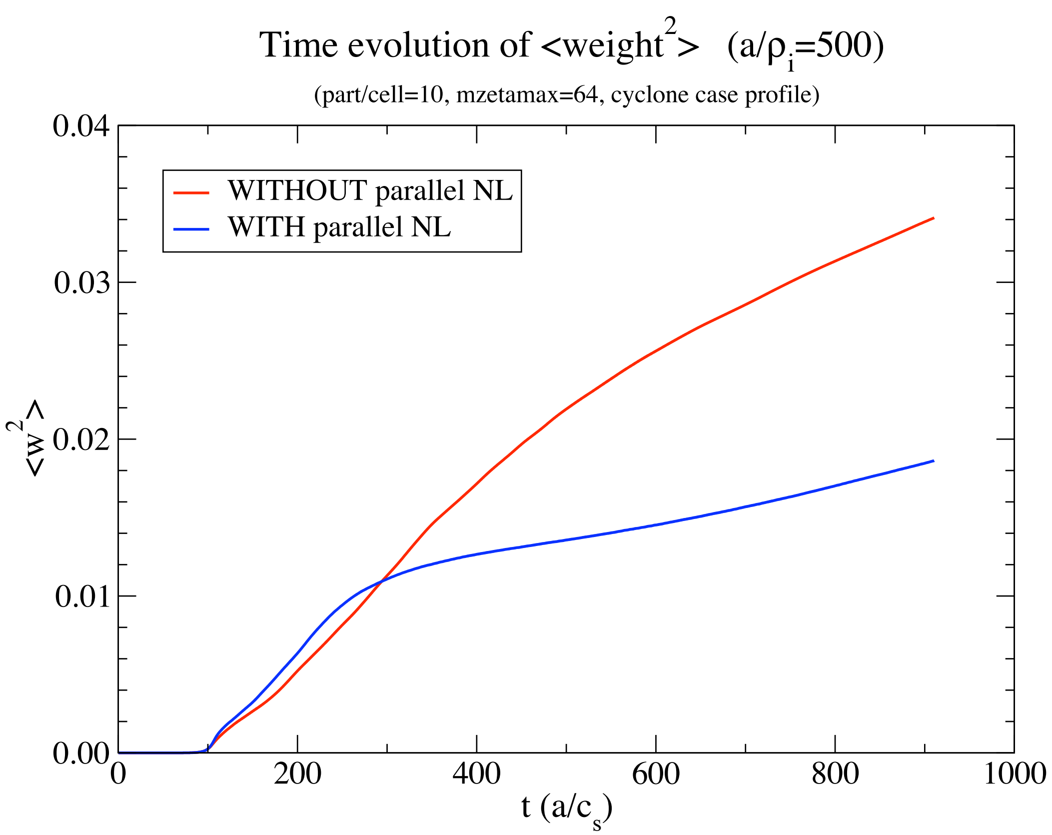
- Steady state turbulence can be achieved at much faster rate with velocity space nonlinearity, and with a lower level of thermal diffusivity and a much higher level of zonal flow

Lee. Ethier et al., ASP/DPP invited talk (2004)

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







Size Scaling (Bohm > GyroBohm)

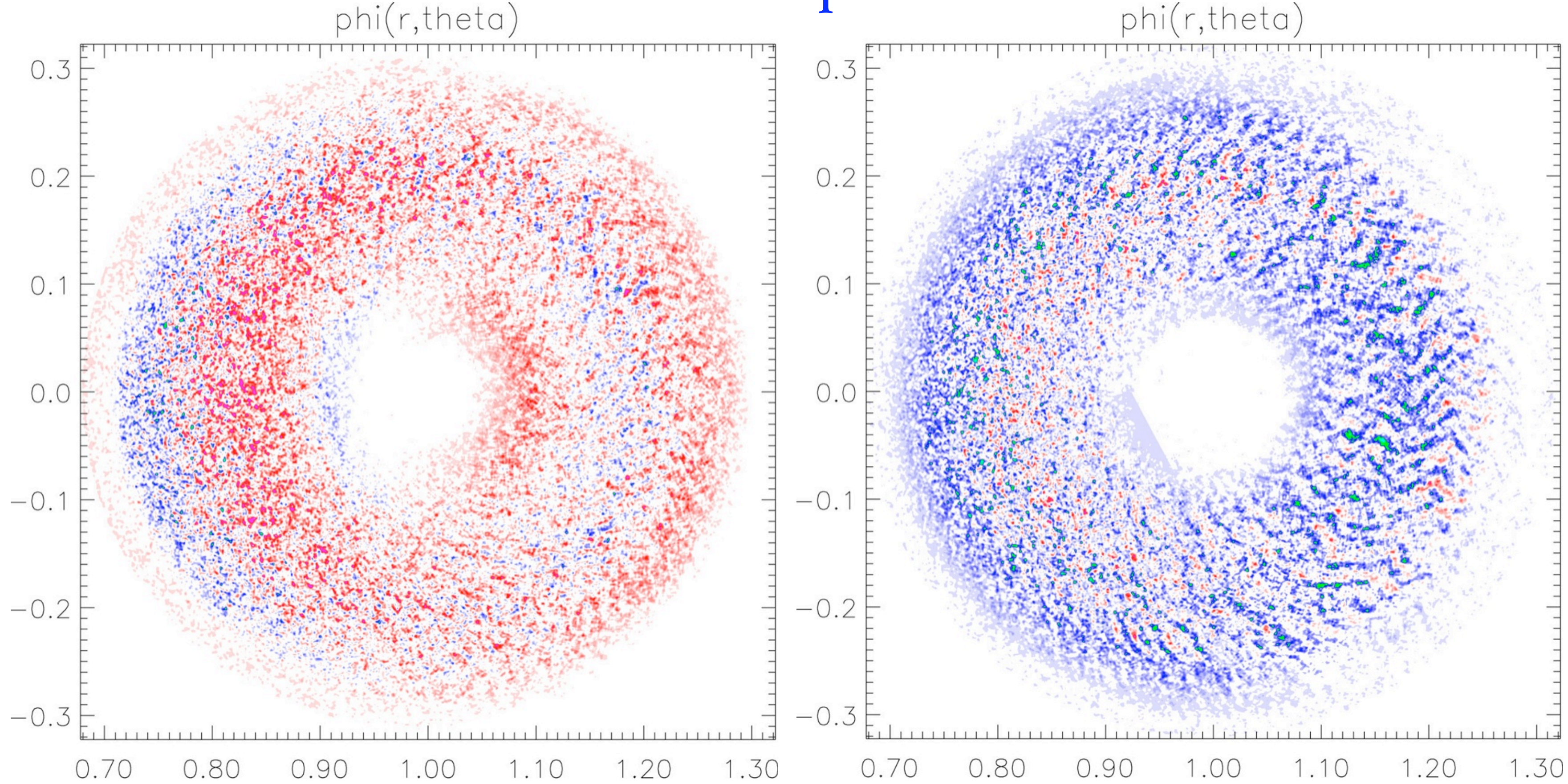
$$\frac{\partial}{\partial t}\sum_{j=1}^{N}(1-\frac{\alpha}{4})w_j^2 = \kappa_{Ti} < Q_r^i >$$

$\alpha \approx 1$ is associated with velocity-space nonlinearity

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

Perturbed potentials

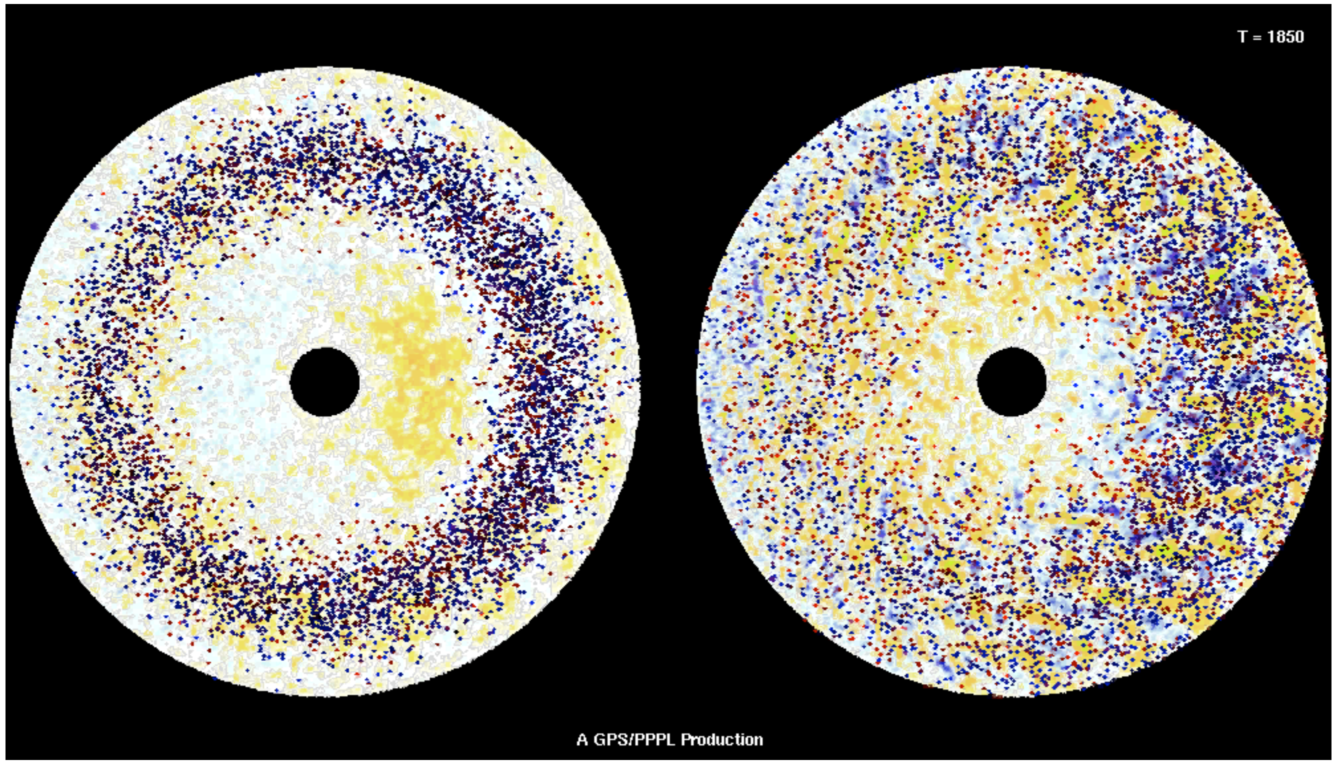
m=1 mode



Streamers

with

without

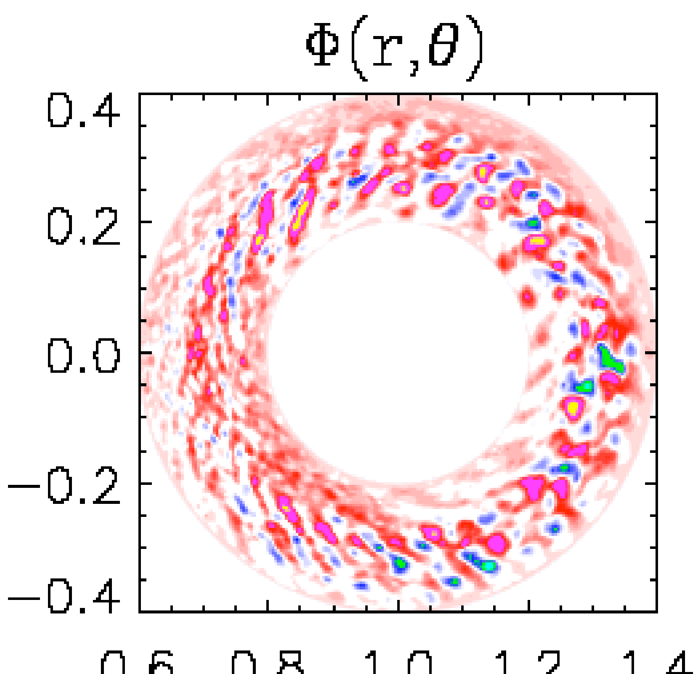


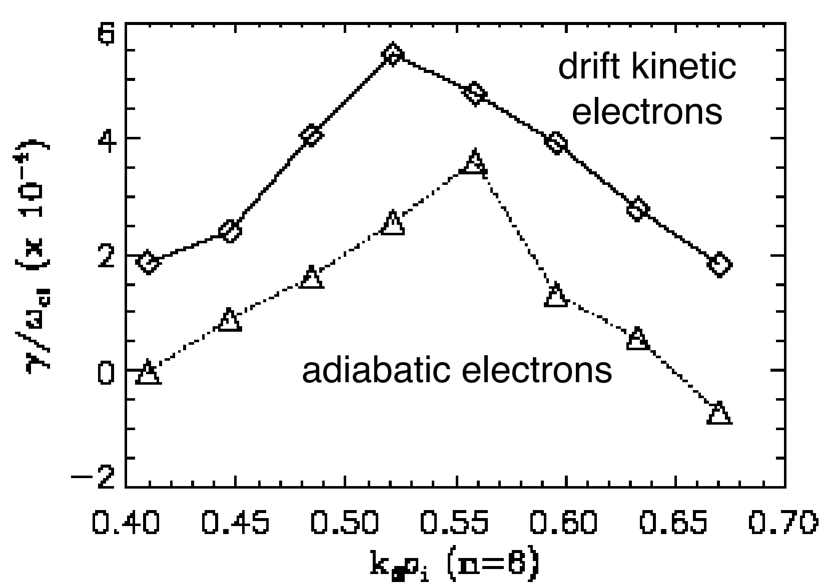
Particle diffusion pattern

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

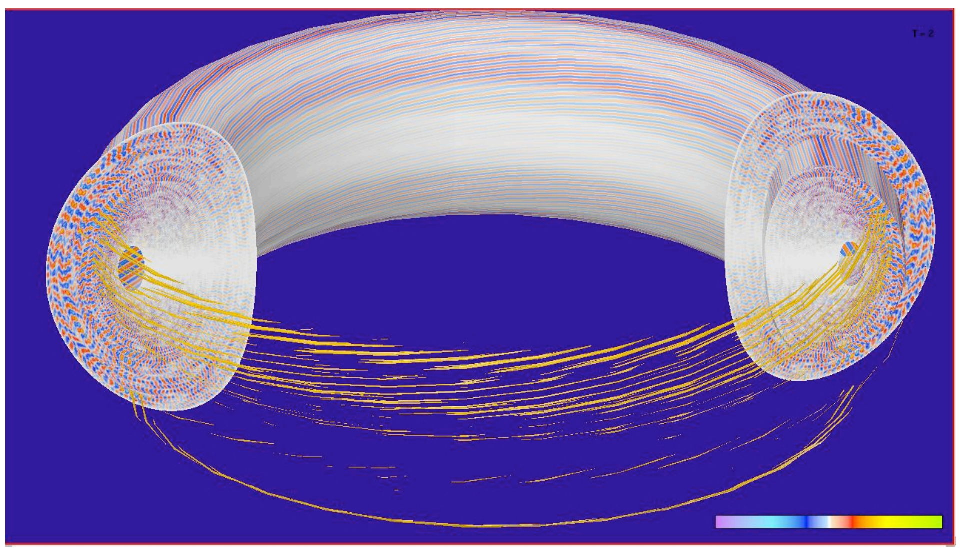
- Numerical method is stable for large time step $\Delta t = 5 - 10\omega_{ci}^{-1}$
- Global finite element method coupled with PETSC standard solvers (Y. Nishimura *et al*, JCP 2005) used for inversion of global (toroidal) elliptic equations
- Steady-state χ_i in presence of trapped electrons increases when parallel velocity non-linearity is retained
- Zonal flow structure appears to have shorter wavelengths in presence of trapped electrons





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]

GTC General Geometry

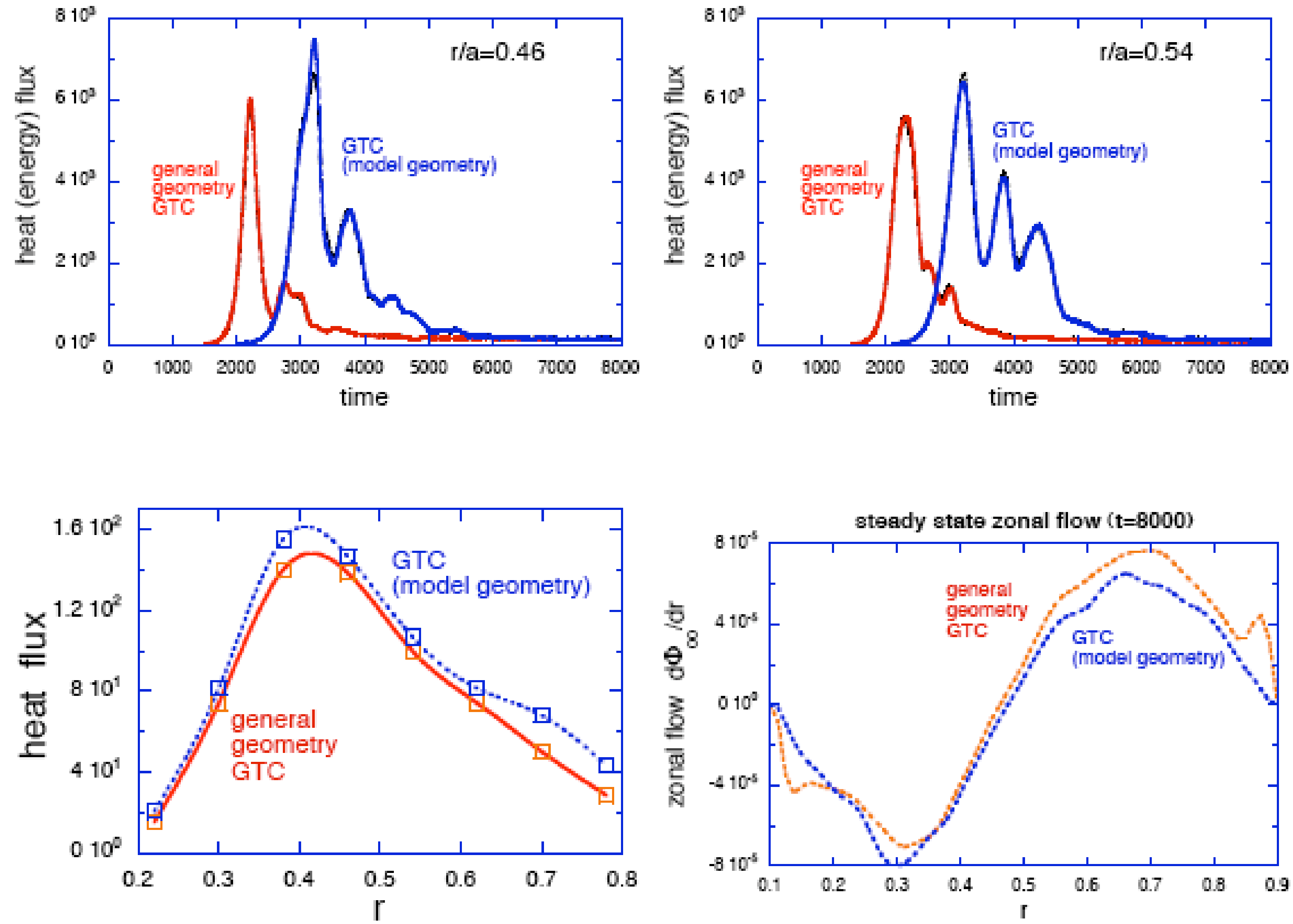


W. X. Wang

Nonlinear Benchmark with Original GTC

(Model Circular Geometry with Cyclone Parameters)

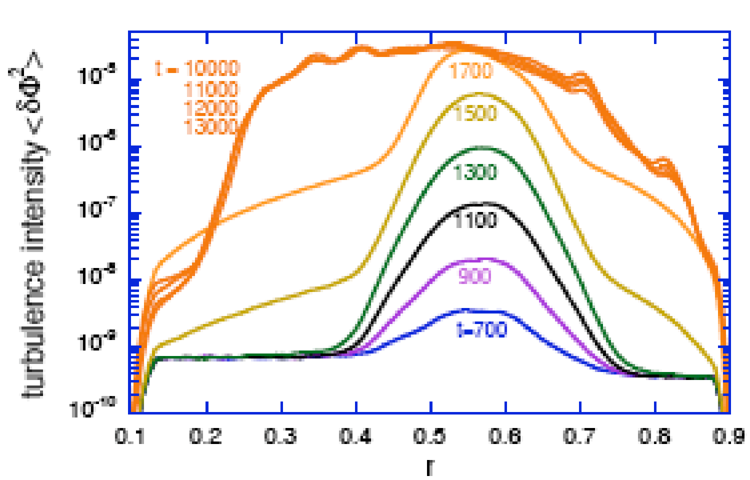
- $R_0/L_T = 6.9 \exp\{-[(r-0.5)/0.28]^6\}$, • flat T_i and n,
- with velocity nonlinearity

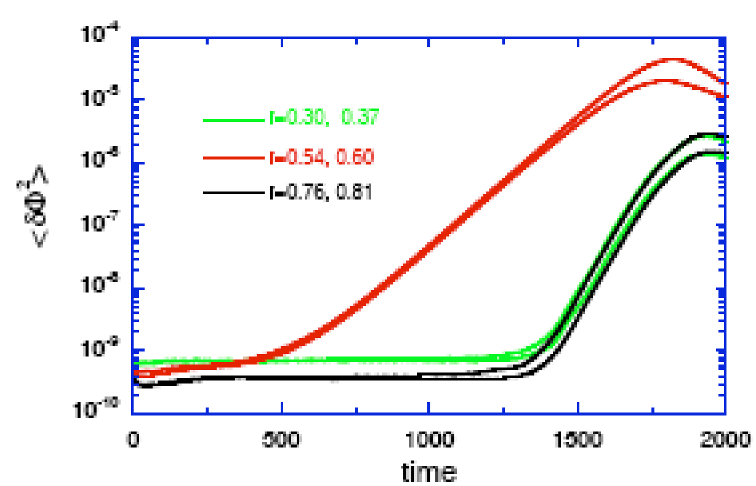


- good agreement in steady state heat flux and zonal flow (some difference in linear stage and dynamics approach to steady state)
- zonal flow shows global scale of minor radius
- heat flux = energy flux indicates no particles flux is produced in adiabatic electron ITG (an interesting test for simulation)

ITG Turbulence Spreading

- DIIID sized shaped plasma with radial variation in T_i and n profiles consistent with their gradient profiles
- Turbulence spreads both inward and outward into linearly stable regions, leading to radially global turbulence and transport nonlocality
- A significant nonlinear spreading is observed to occur before the satuation of initially linear instibility
- Nonlinearly driven turbulence in the stable regions grows even faster





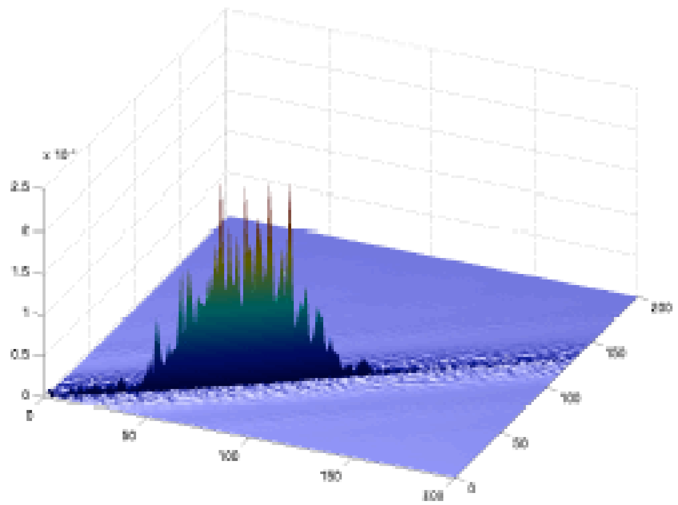
W. X. Wang

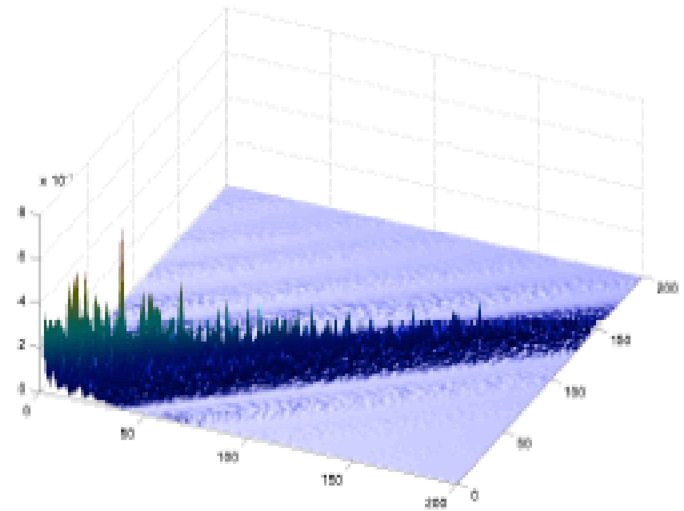
Turbulence Energy Cascading Dynamics

- Interesting difference in turbulence spectra between stable and unstable region
- Turbulence energy transfer to lower-n modes along $m/n \approx q$

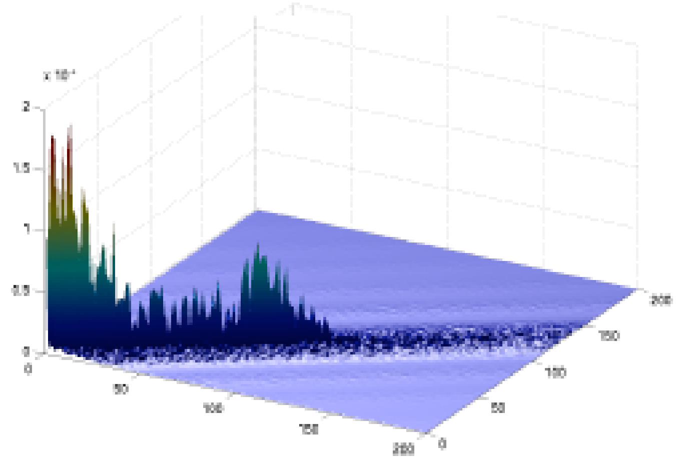
unstable region (r/a=0.5)

stable region (r/a=0.26)

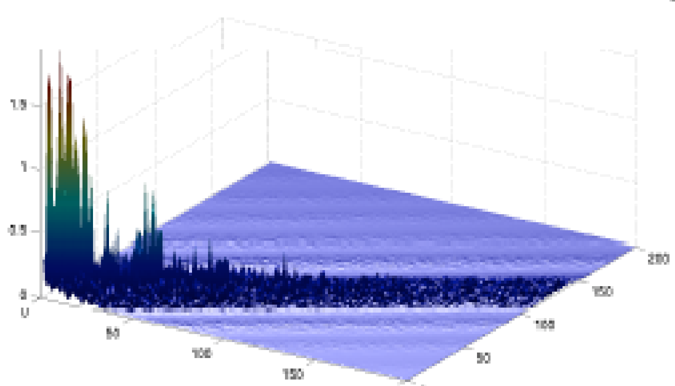


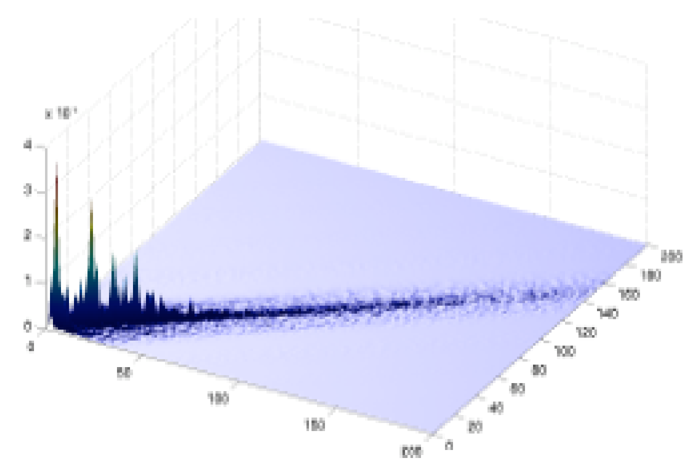


t=1200



t=2000





t=12400

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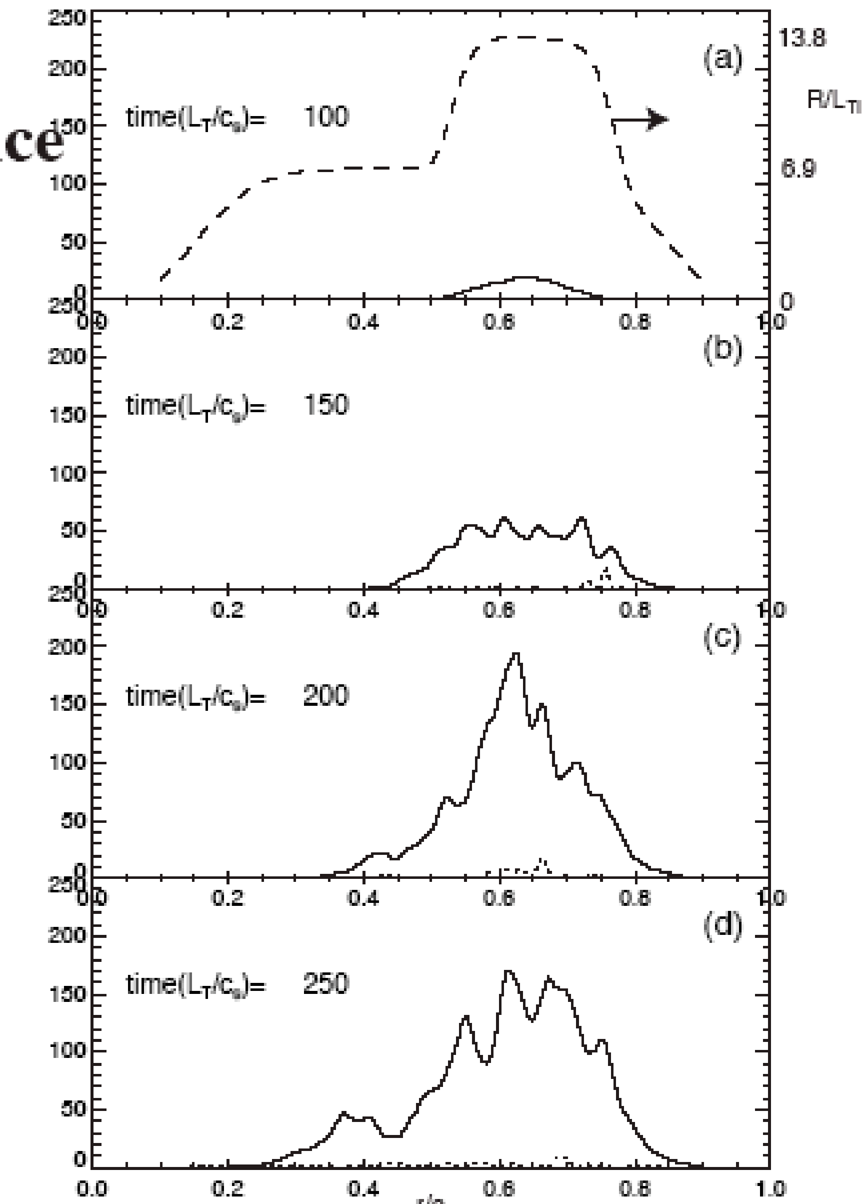
Turbulence Spreading from Edge to Core *PPPL*

[**Hahm, Diamond, Lin et al.,** *submitted, PoP '05*]

Nonlinear Gyrokinetic Simulation of Ion Temperature Gradient Turbulence



$\frac{R}{L_T} = 6.9$ at core (Cyclone value)
$\frac{R}{L_T} = 13.8$ at edge:

Initial Growth at Edge followed by Ballistic **Front Propagation** into Core

Saturation Level at Core
$\sim \mathbf{2}\times$ Core (only) Simulation

From Simulation, U_x increases with $\frac{R}{L_T}$
Scaling suggests Nonlinear Mechanism
e.g., [Gurcan,Diamond,Hahm, and Lin, PoP '04] dominant,
than Toroidal Linear Coupling [Garbet,Laurent,Samain et al., NF '94]

Turbulence Spreading from Edge to Stable Core

PPPL

[**Hahm, Diamond, Lin et al.,** *submitted, PoP '05*]

Nonlinear GTC Simulation
of Ion Temperature Gradient Turbulence

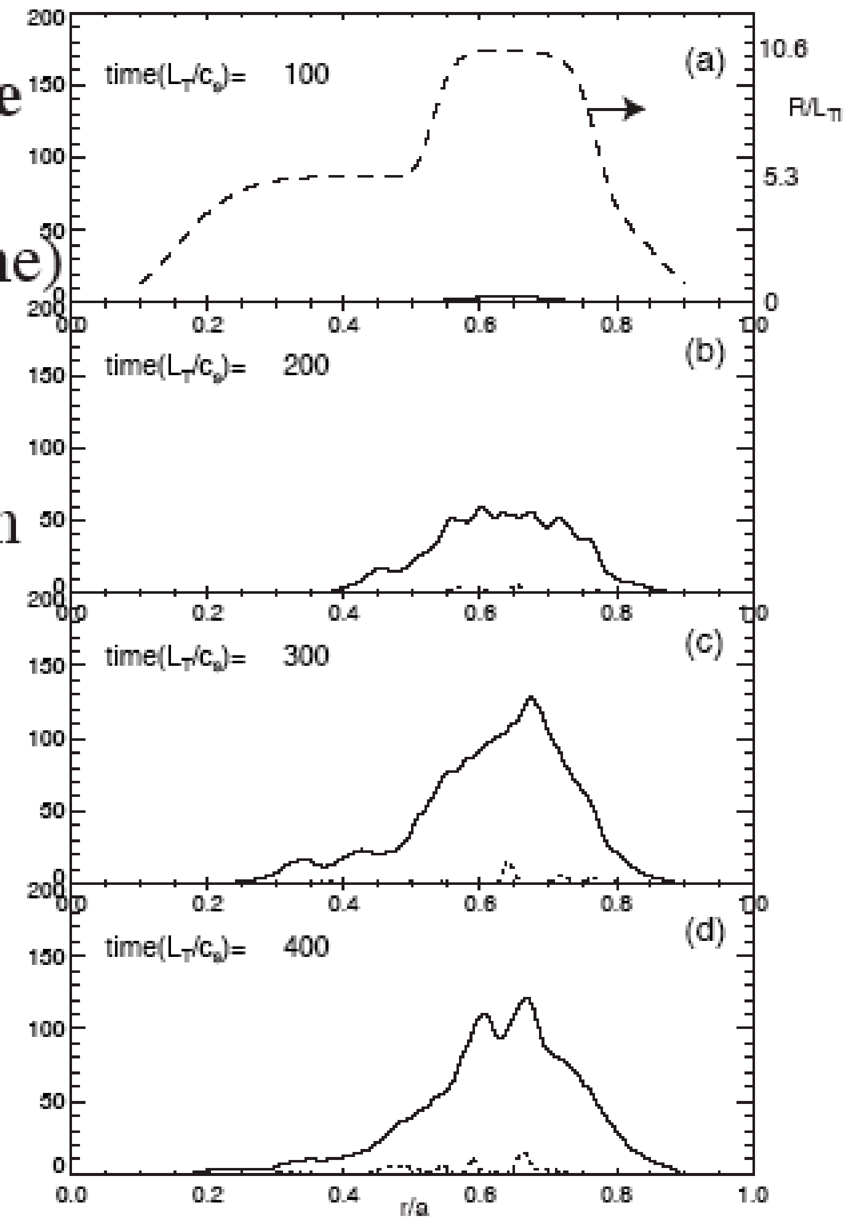
$\frac{R}{L_T} = 5.3$ at core (within Dimits shift regime)
$\frac{R}{L_T} = 10.6$ at edge:

Initial Growth at Edge and Local Saturation
$\rightarrow$ Penetration into *stable* Core:
Lin,Hahm,Diamond,... PRL '02, PPCF '04

Saturation Level at Core:

$\frac{e\delta\phi}{T_e} \sim 3.6\frac{\rho_i}{a}$

$\rightarrow$ sometimes $\nabla \cdot \Gamma_{\mathrm{spreading}} >> \gamma_{local}$



GTC-Neo for 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)

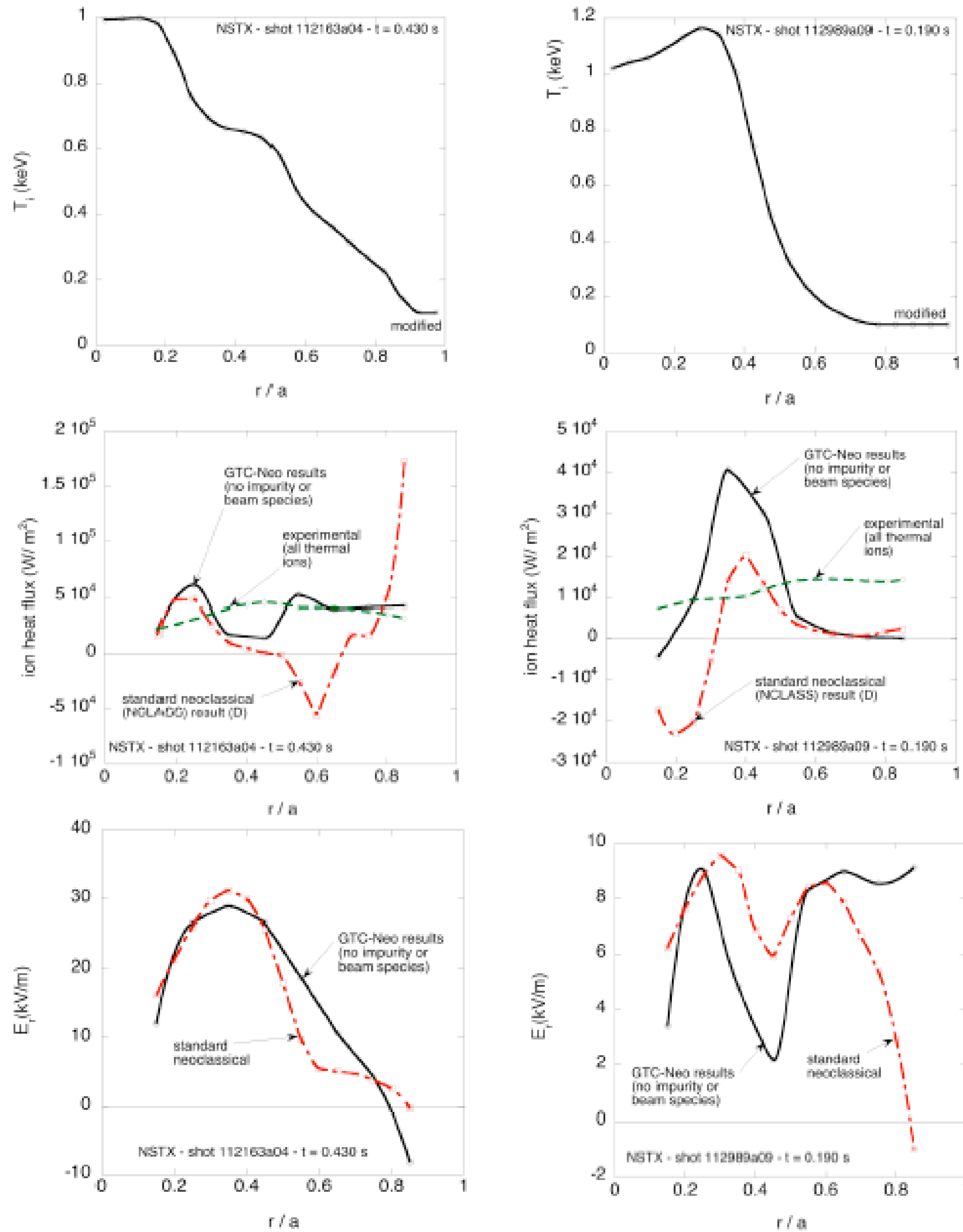
- Interfaced with MHD codes for the numerical MHD equilibrium and with TRANSP for experimental plasma profiles

- Runs currently on the massively-parallel IBM-SP computer at NERSC - 9 cases run for NSTX now

- Impurity and hot beam species to be added in future

Near-neoclassical(?) shot

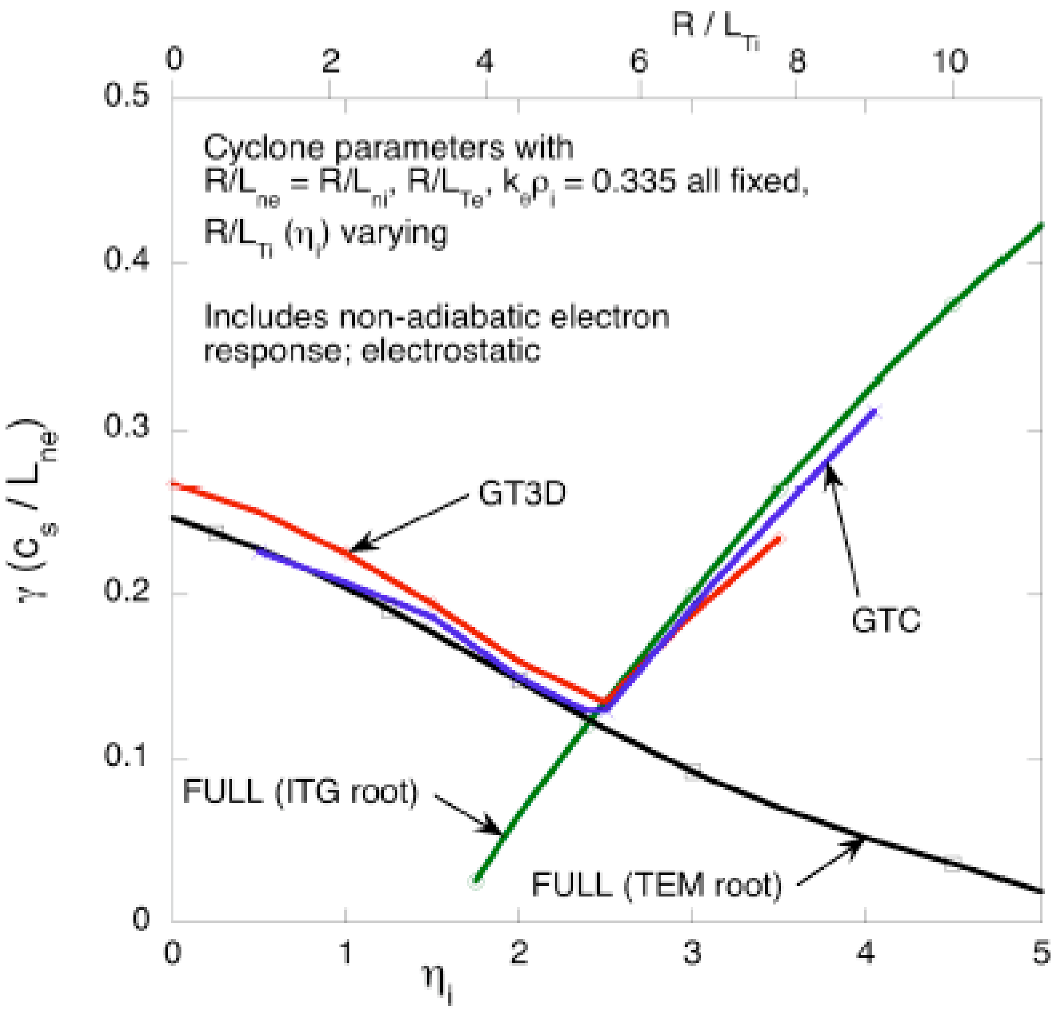
ITB shot

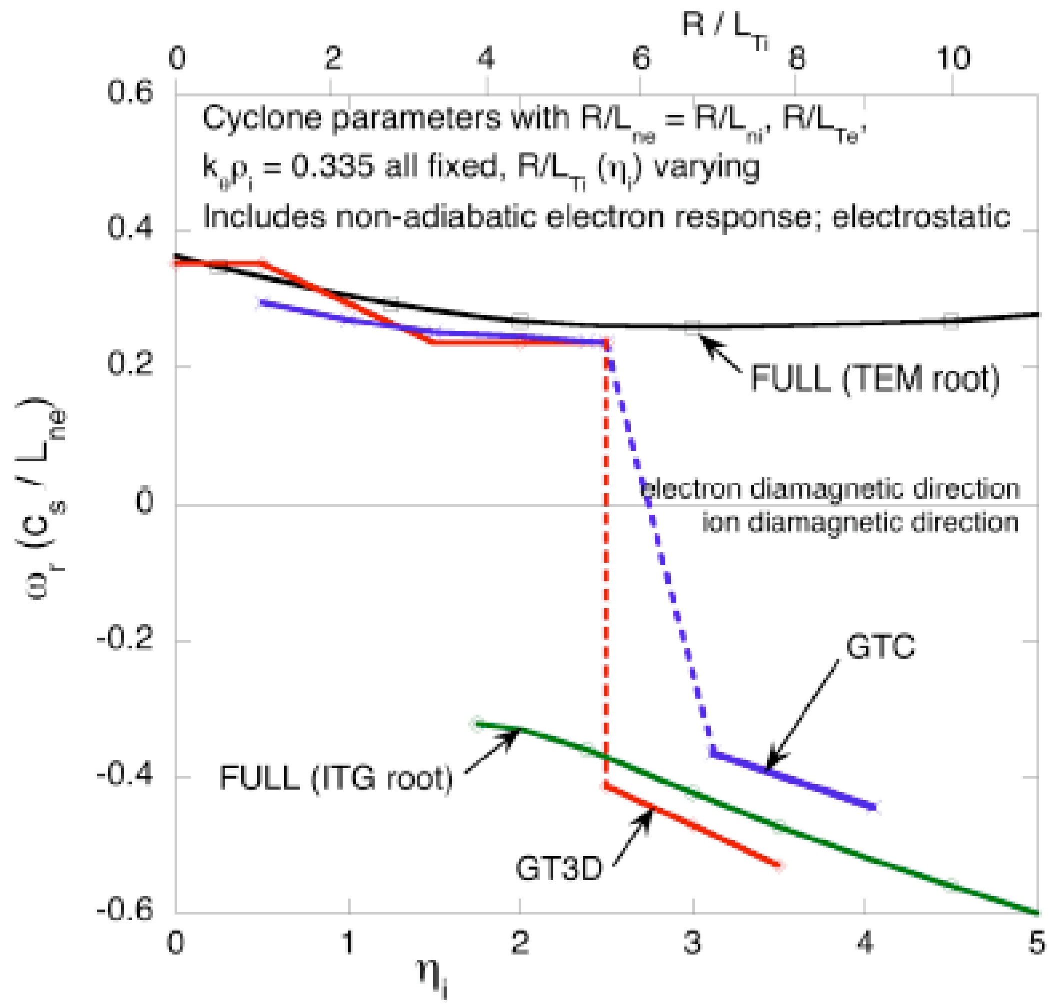


W.X. Wang, G. Rewoldt

Ongoing GTC benchmarking and convergence studies

- Linear benchmarking, including the effects of trapped electrons, against global GT3D code of Dr. Y. Idomura of JAERI in Japan, and radially-local FULL code, for linear growth rates of ITG and TEM modes, carried out showing reasonably good agreement, with expected increase in ITG mode linear growth rates due to kinetic electron effects
- Vary R/L_{Ti} (and η_i) at fixed R/L_{Te} = 6.92, R/L_n = 2.22, and $k_\theta \rho_i$ = 0.335 (on reference surface) including trapped electrons
- Nonlinear runs of GTC with trapped electrons, for convergence studies and for planned benchmarking against GT3D, are now under way

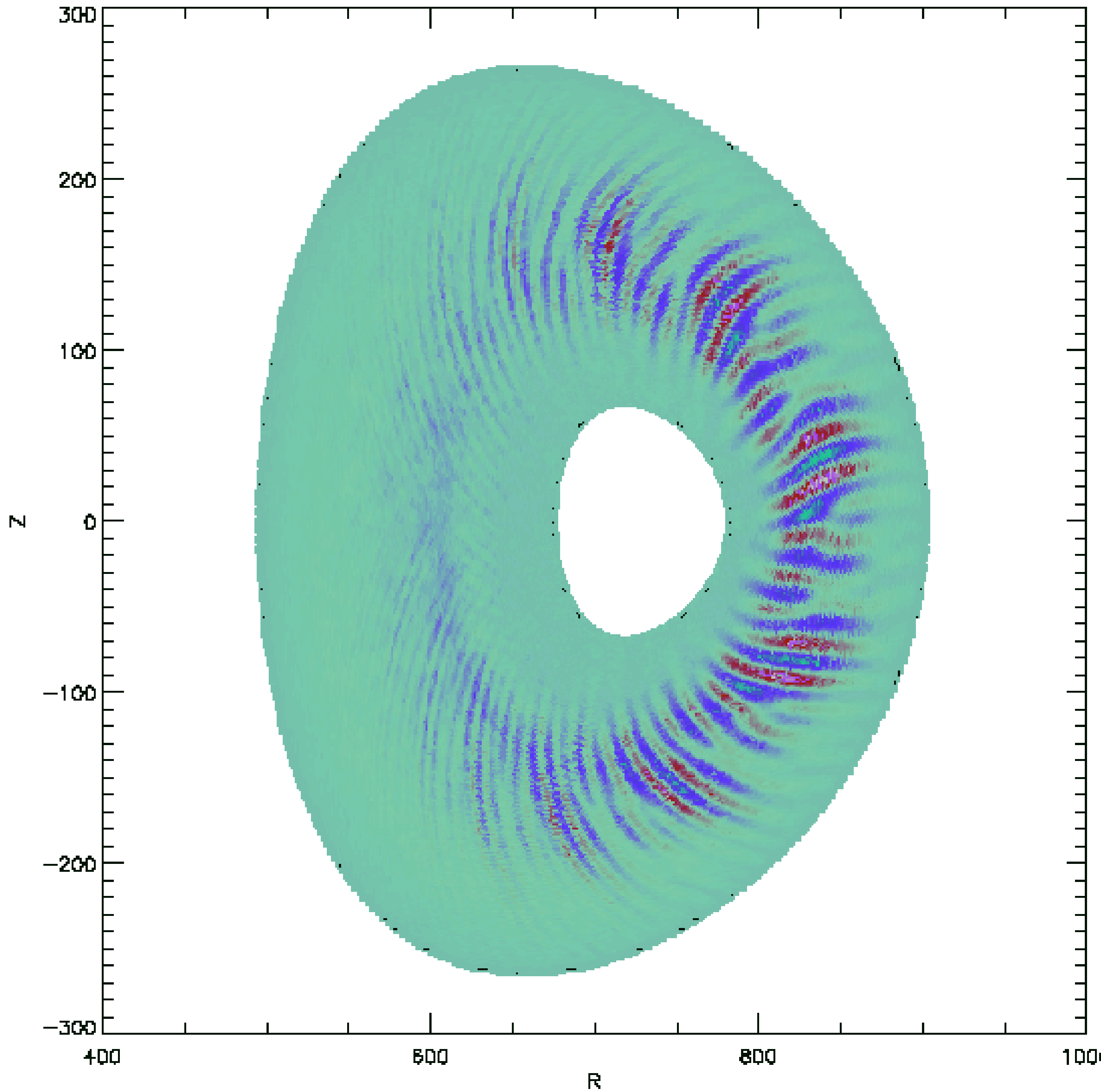




Y. Idomura(JAERI), Z. Lin (U.C. Irvine), G. Rewoldt

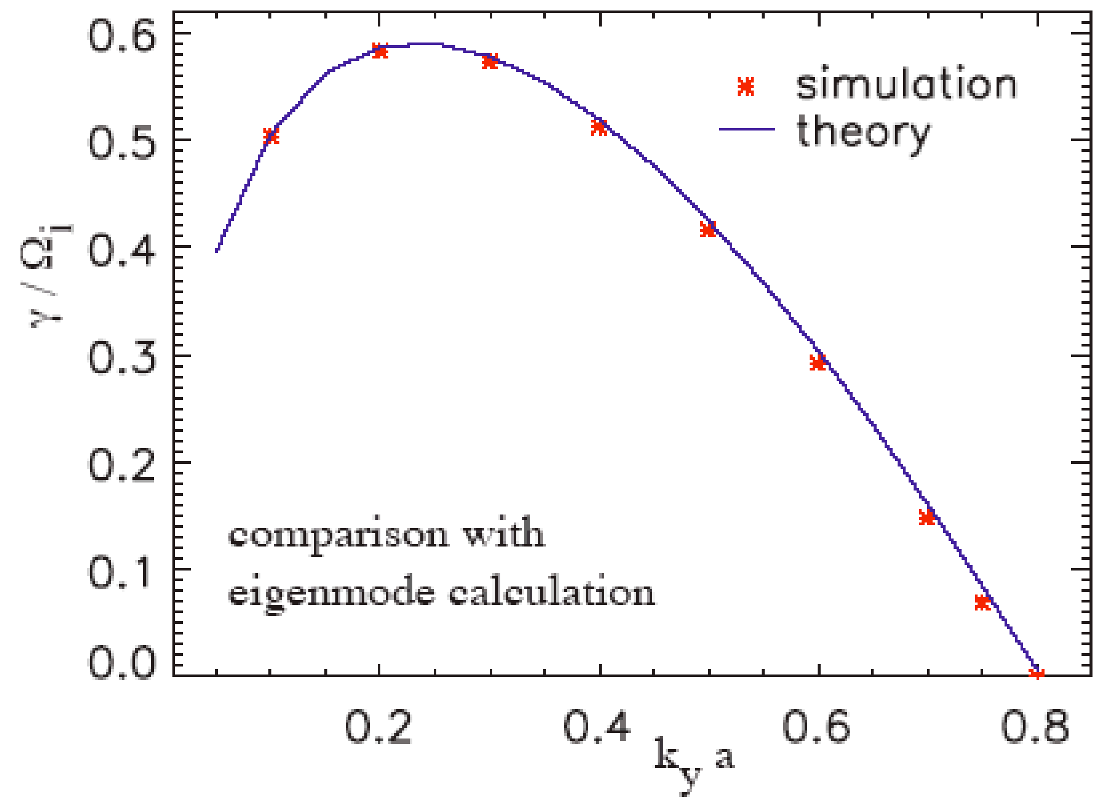
The GEM Code

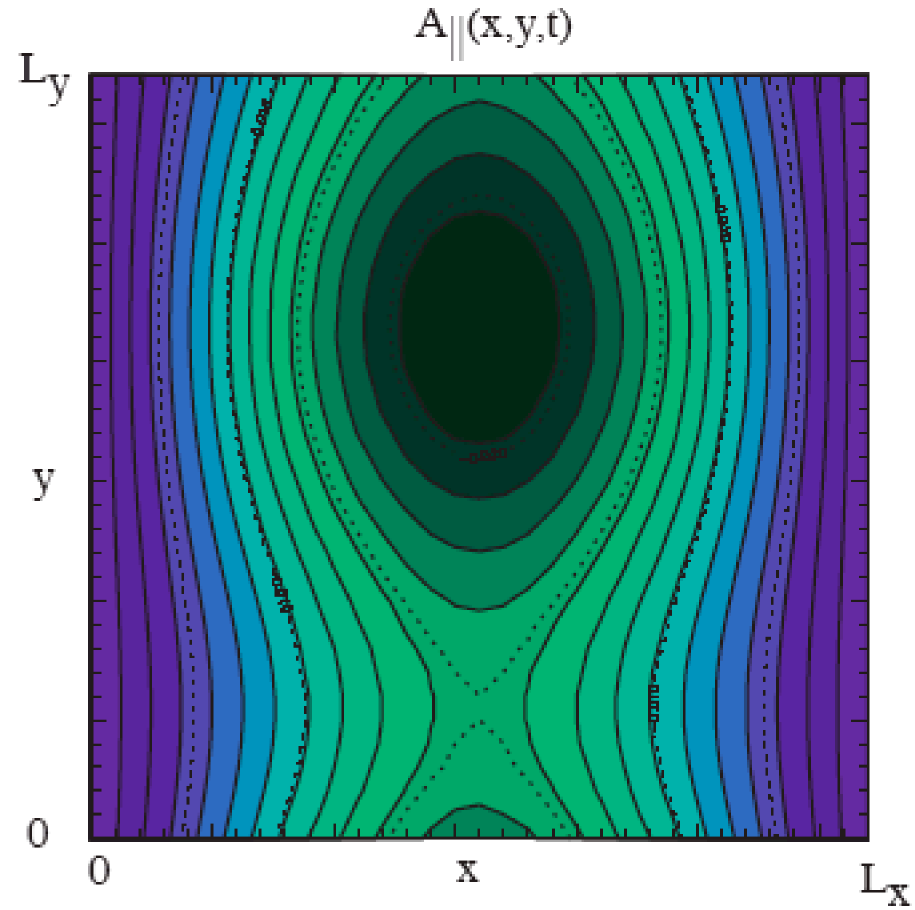
- $p_\parallel$ formulation, δf, split-weight
- Use field-line-following coordinates
  - Cover $0 \leq \theta \leq 2\pi$
  - Radially global
  - Arbitrary size toroidal section
- Passing and trapped electrons
- Collisions
- Magnetic perturbations
- $E_\parallel$ nonlinearity
- Arbitrary shape tokamak equilibrium and equilibrium flow

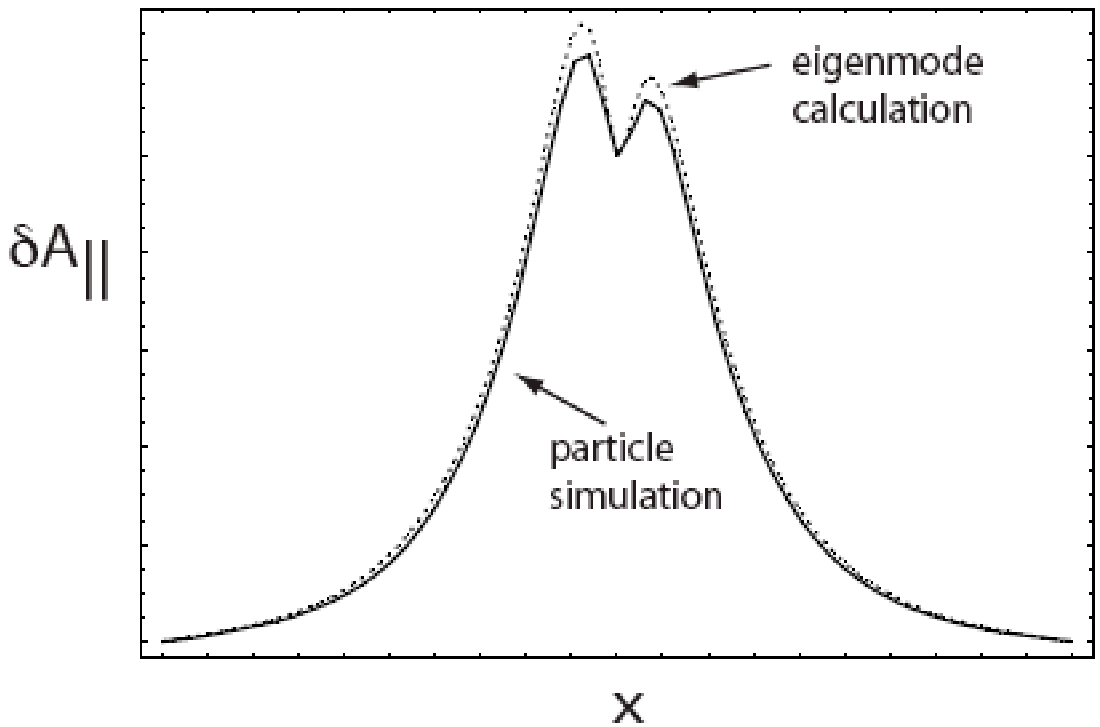


Chen and Parker, JCP <189>, 463 (2005).

Gyrokinetic Simulation of Tearing Modes





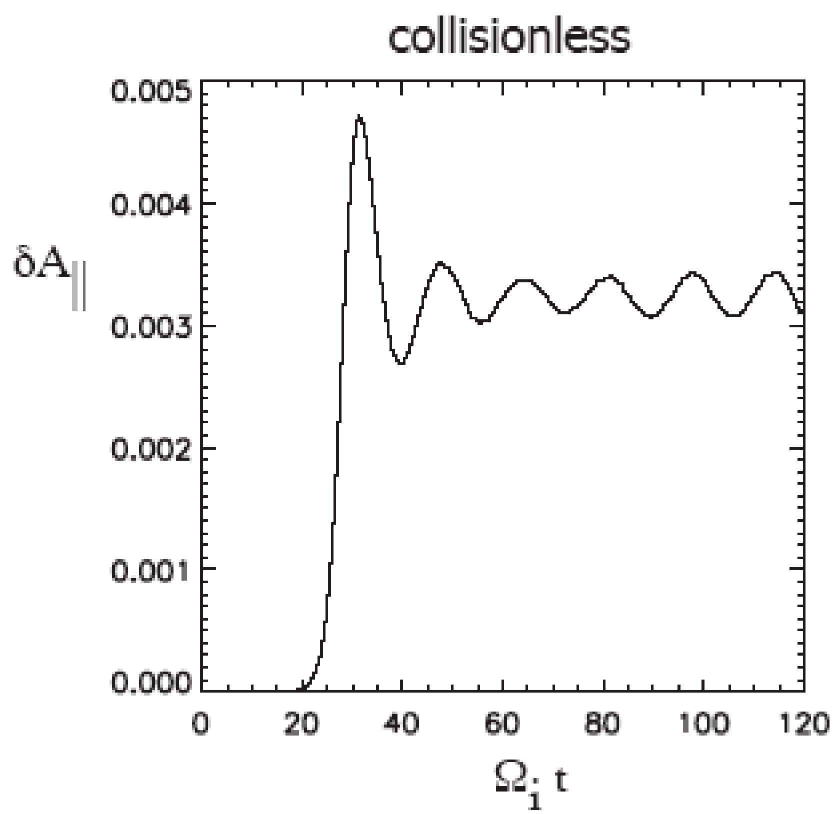


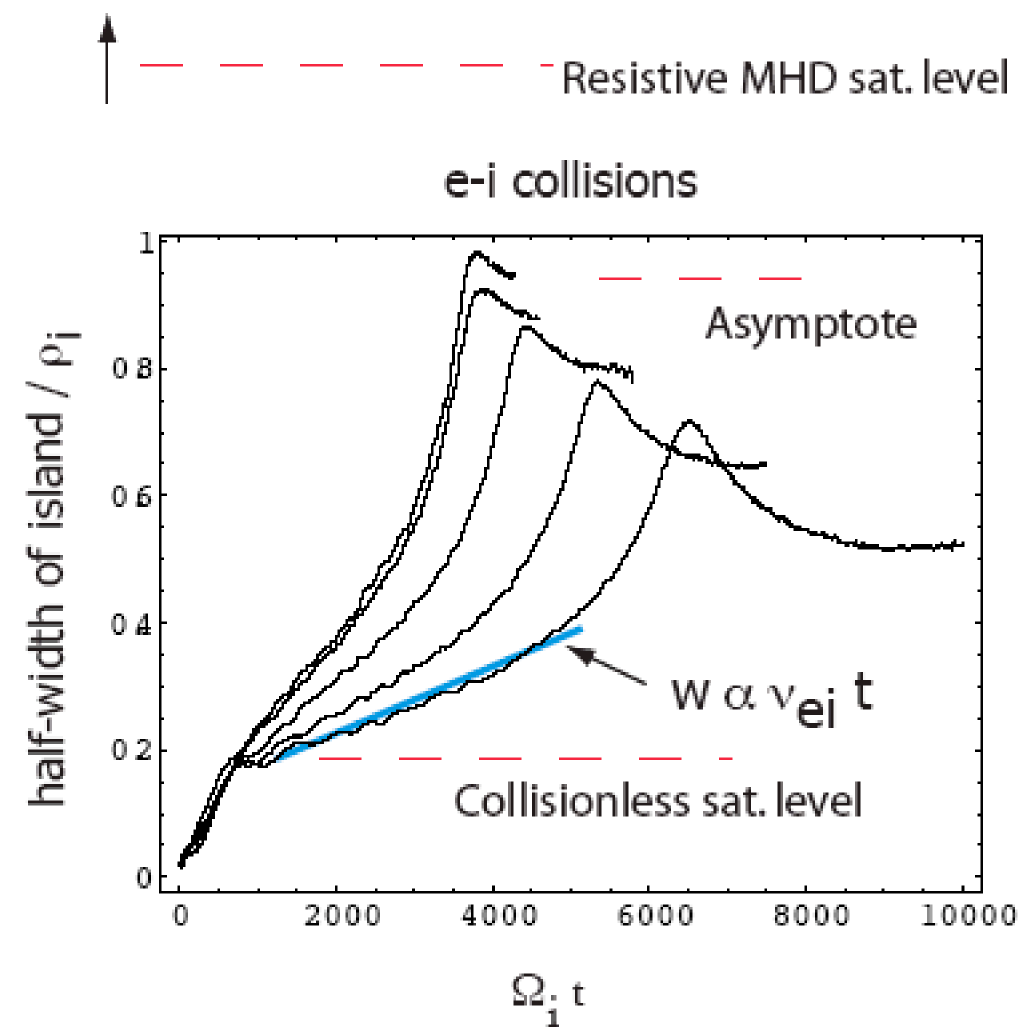
Katanuma '80
Sydora '01

Wan, Chen, Parker, Phys. Plasmas (2005)

GEM - gyrokinetic, electromagnetic,
general geom. Chen and Parker, J. Comput. Phys. (2003)

Nonlinear saturation of collisionless and semi-collisional tearing modes

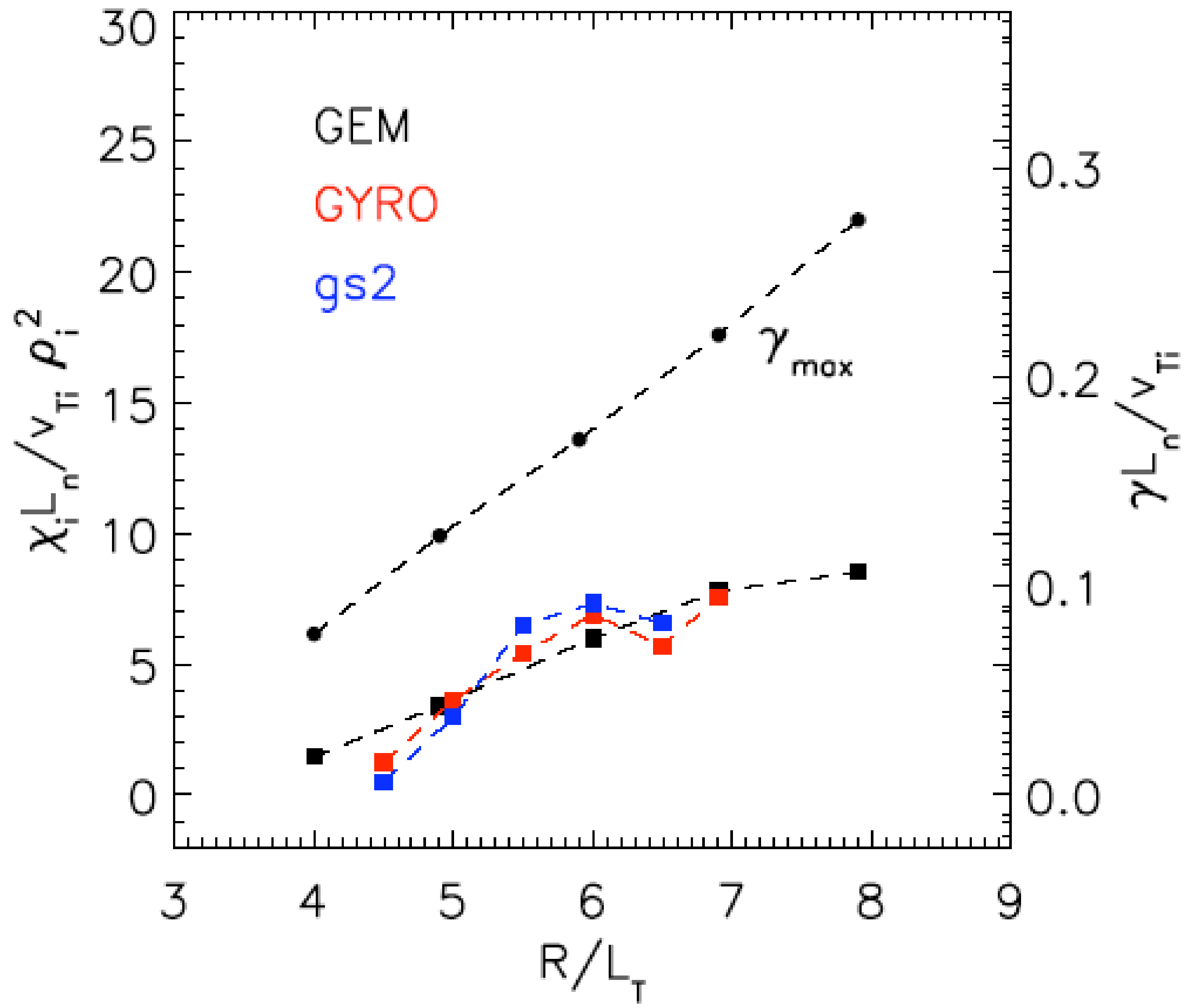




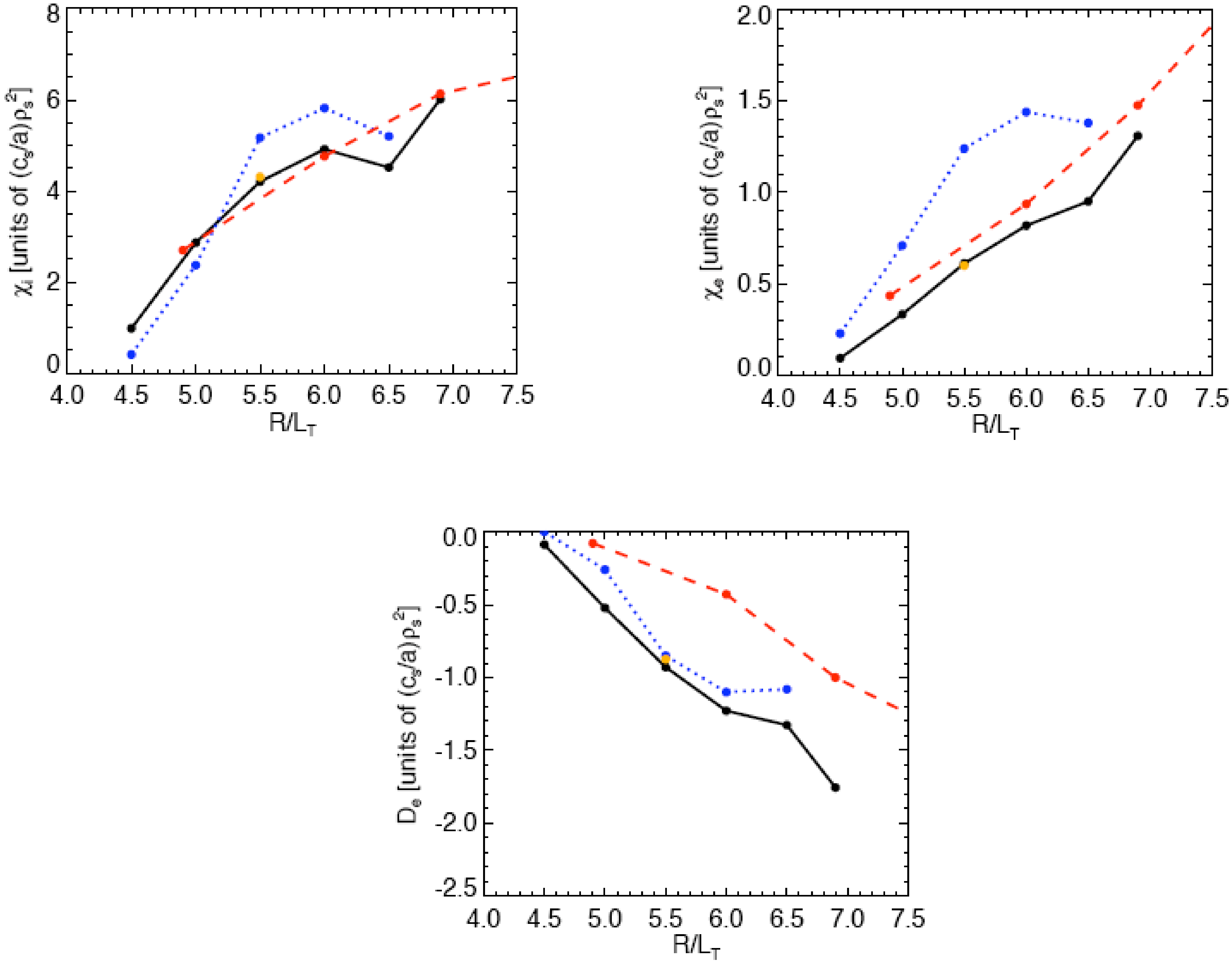
Theory - Drake and Lee '77

Simulation - Wan, Chen and Parker, Phys. Plasmas (2005)

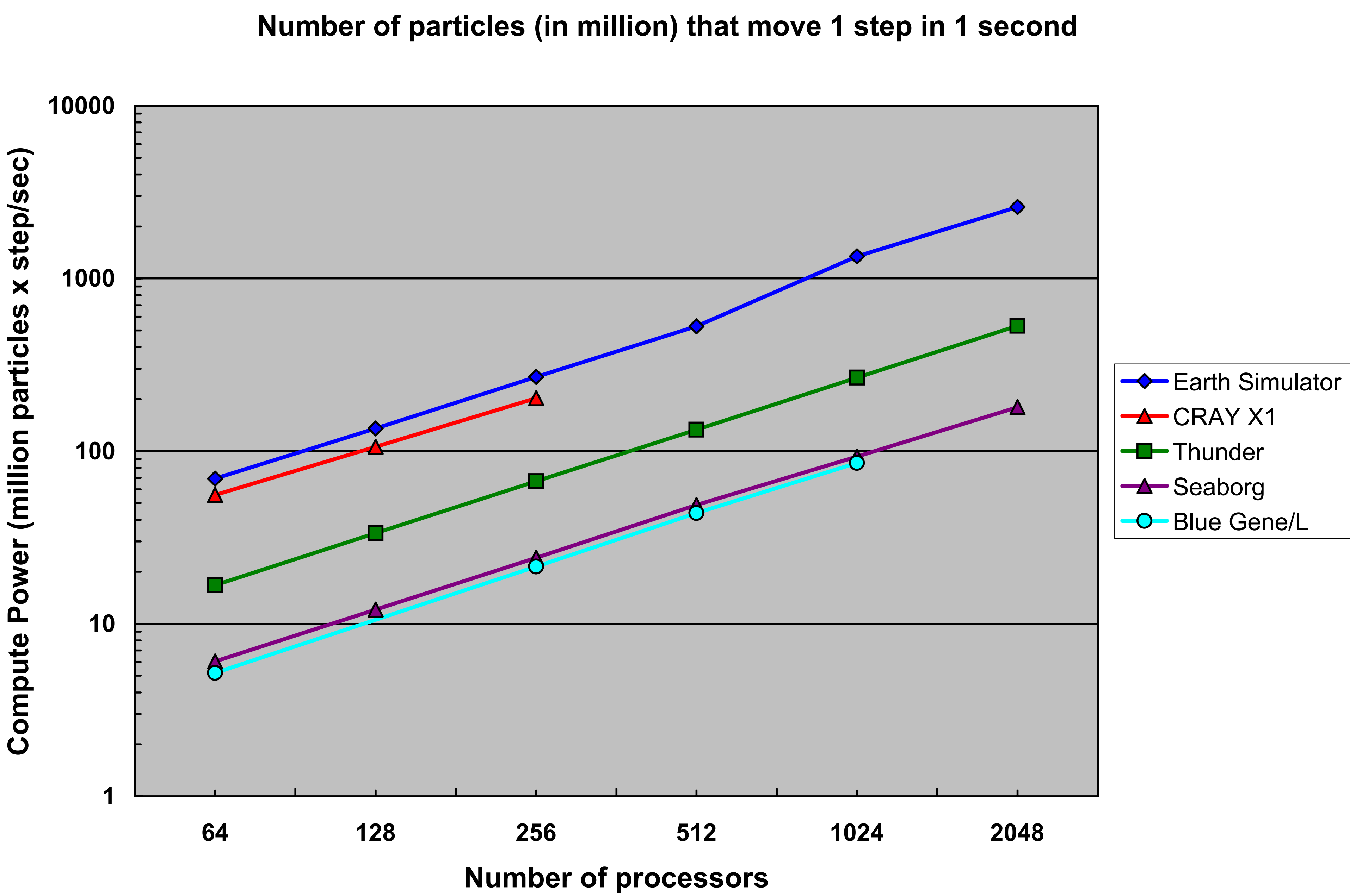
Differences between particle and continuum near critical gradient



GS2, GYRO, GEM Nonlinear Benchmarks



GTC performance on MPP platforms



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

S. Ethier

GTC performance

# of proc.	#part (Bil-lion)	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!!

S. Ethier

Finite Element (FEM) Elliptic Solver Developed for GTC Global Field Aligned Mesh

- FEM adapted for logically non-rectangular grids.
  Need adjustments of elements at different toroidal angles.

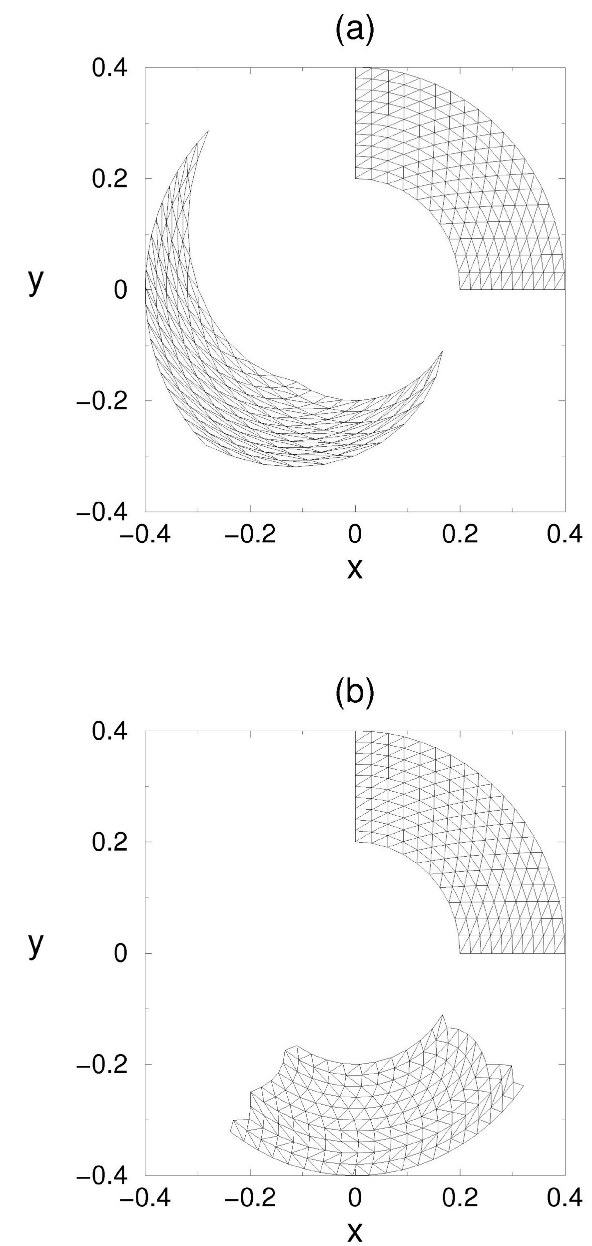
- Linear sparse matrix solver
    - PETSc (ANL)

- Enabled implementing split-weight *(Manuilskiy & Lee, POP2000)* and hybrid electron models *(Lin & Chen, PoP2001)*

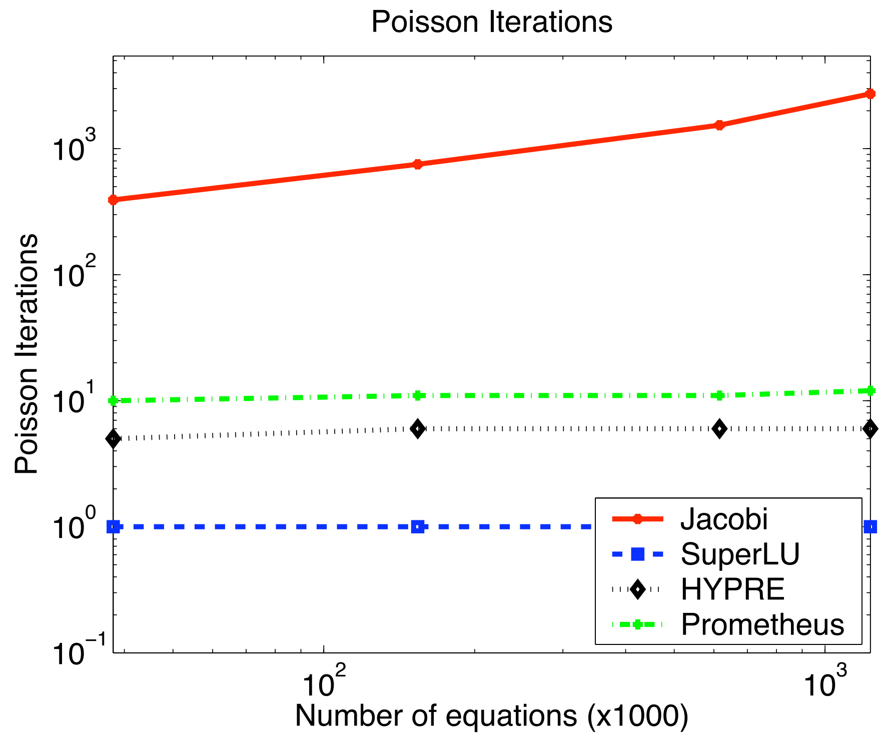
- Ongoing studies of kinetic electron effects on ITG and TEM turbulence

- Ongoing studies of electromagnetic turbulences: AITG/KBM & TAE/EPM

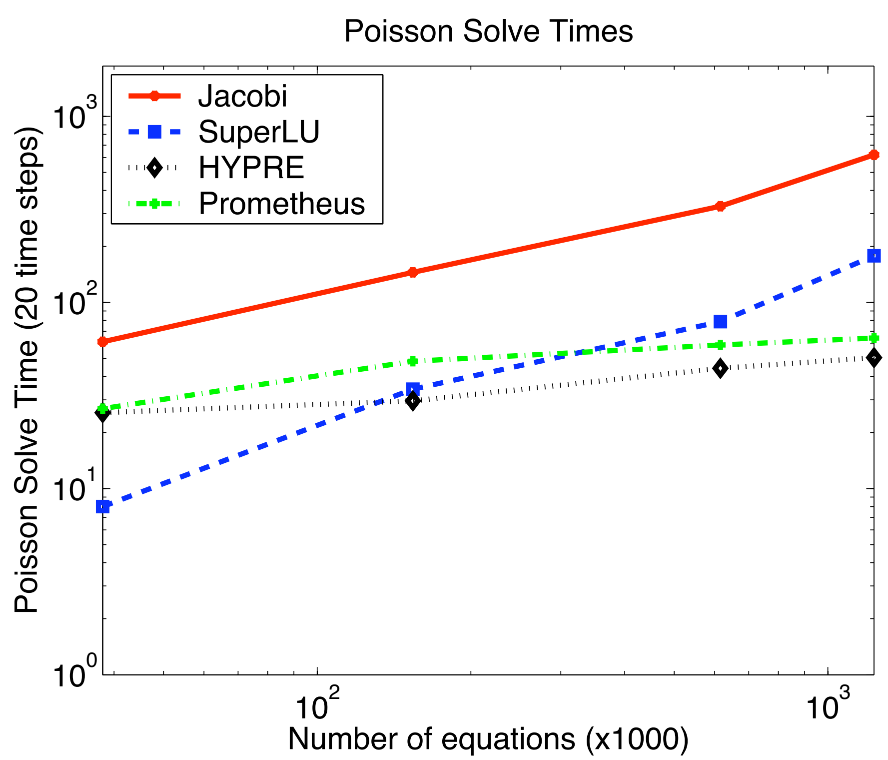
Nishimura, Ethier, Lewandowki & Lin, submitted to JCP, 2004

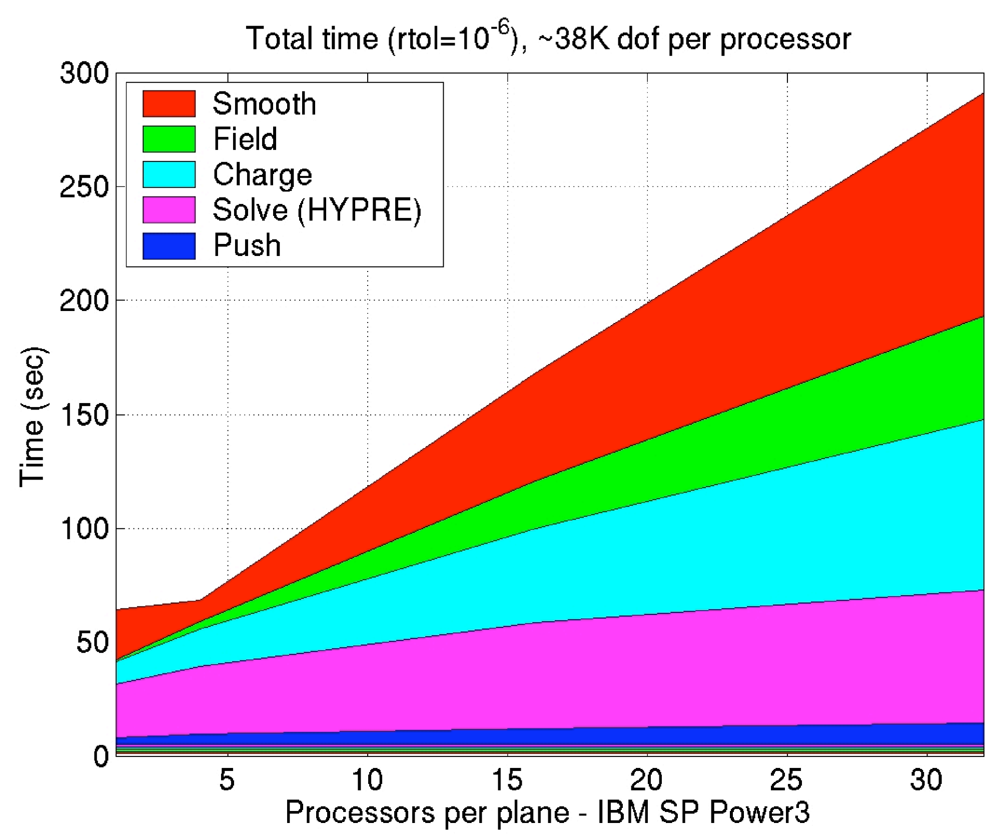


Poisson Solver Performance



- 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 and Y. Nishimura, submitted to CPC

Toward Team Programming -- GTC

- Object Oriented programming based on Fortran 90
- Eight classes and one module have been implemented

  mesh2d_class
  flr_class
  equilibrium_class
  interpolation2d_class
  scalar_field2d_class
  vector_field2d_class
  gk_particles_class
  dk_particles_class
  multi_species

- The first four classes currently have no methods (functions), except for a constructor. They exist primarily to group together data which appear in other classes.

- The remaining four classes contain methods which provide data to the original subroutines in GTC, but with simpler arguments. Currently, this data points to the original data in the code, but eventually it will replace the original data.

- Finally, there is a module which has methods which involve various particle types. This may eventually become a class.

Decyk, Nishimura, Ethier, Adams, Klasky

Data Management challenges

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

- This data needs to be post-processed
  - Essential to parallelize the post-processing routines to handle our larger datasets.
  - We need a cluster to post process this data.
    - > M (supercomputer processors) x N (cluster processors) problem.
    - > QOS becomes more important to sustain this post-processing.
    - > Workflow automation becomes essential to automate this process of moving data, analyzing data, and finally visualizing/publishing data.

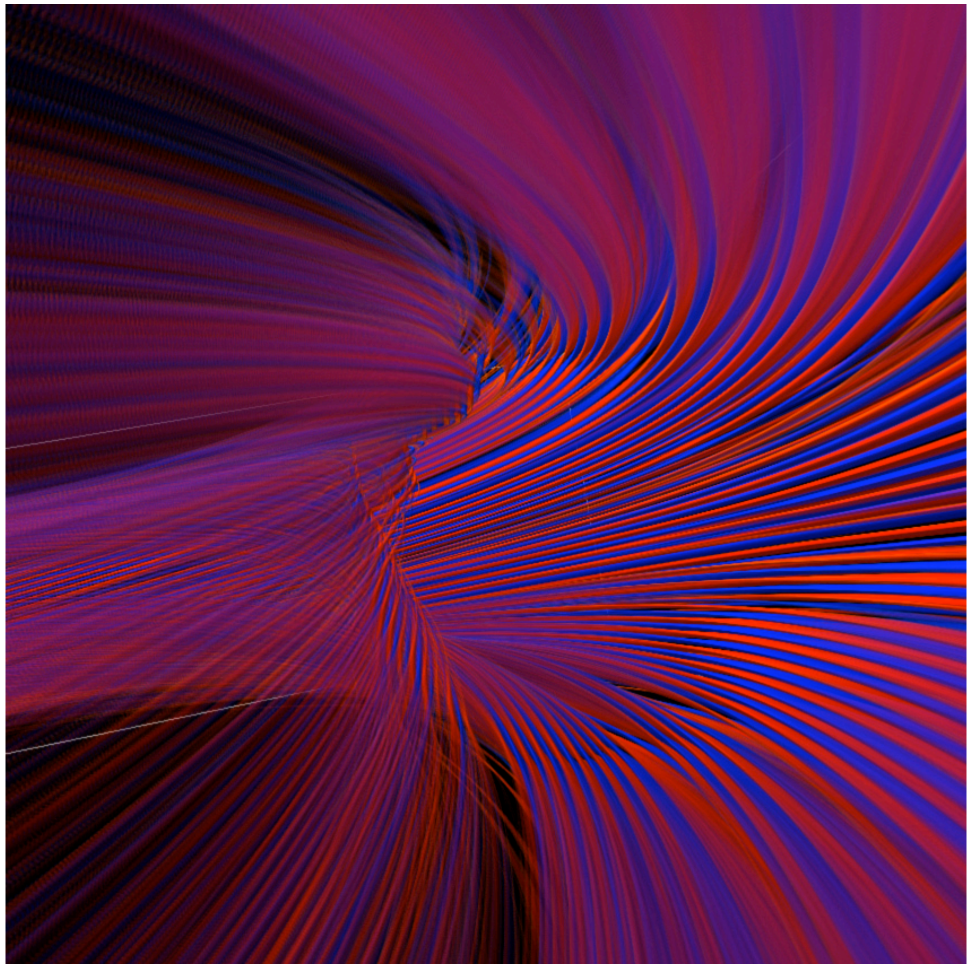
- The post-processed data needs to be shared among collaborators
  - Different sections of the post-processed data may go to different users .
  - Post-processed data, along with other metadata should be archived into a relational database.
  - This technology is critical for data sharing of large datasets.

Beck, Bhat, Klasky, Ma, Parashar

Post processing of GTC Data

- Particle Data
  - No compression possible [already compressed by a factor of 10].
  - Sent to 1 cluster for visualization/analysis.
  - Work being done with K. Ma, U.C. Davis: Visualize a million particles.
  - Gain new insights into the theory.

- Field Data
  - Geometric/Temporal compression of the data is possible [a factor of 10 or more].
  - Data needs to be streamed to a local cluster at PPPL.
  - Reduced subset needs to be sent to PPPL + collaborators.
    - > Use Logistic Network. [Beck, UT-K]
    - > Data transfer needs to be automatic, and integrated into a dataflow/webflow for use with parallel analysis routines.
  - We desire to see post-processed data during the simulation.



Beck, Bhat, Klasky, Ma, Parashar

After the analysis

- Post-processed data needs to be saved into a relational database

  - How do we query this abstract data to compare it with experiments?

  - 3D correlation functions

  - Processing of TBs of data/run now, 100's of TBs of data/run in 5 years.

  - Data mining techniques will be necessary to understand this data.

  - Everything should be parallelized: Data Transfer, Data Analysis, Visualization

Beck, Bhat, Klasky, Ma, Parashar

Thermal Noise in Particle Simulation of Drift Waves in 1D - Parker & Lee, PFB '93

*N*_particle_ = 987
*N*_grid_ = 16

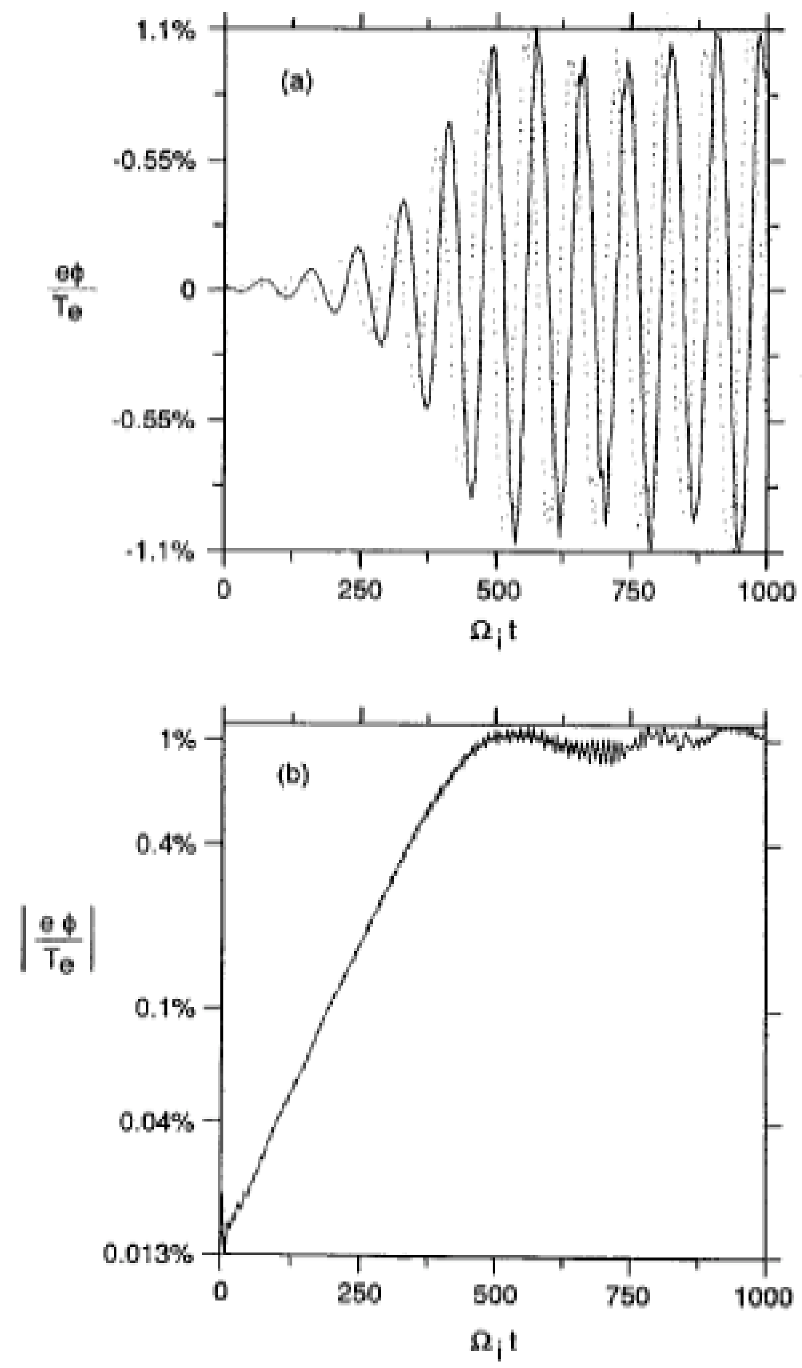


FIG. 1. The $n=1$ drift instability ($k_\perp \rho_i = 0.8$) for the run with 987 particles on a 16-grid system. (a) The time history for the real (solid line) and imaginary (dashed line) parts of the electrostatic potential and (b) the corresponding amplitude evolution.

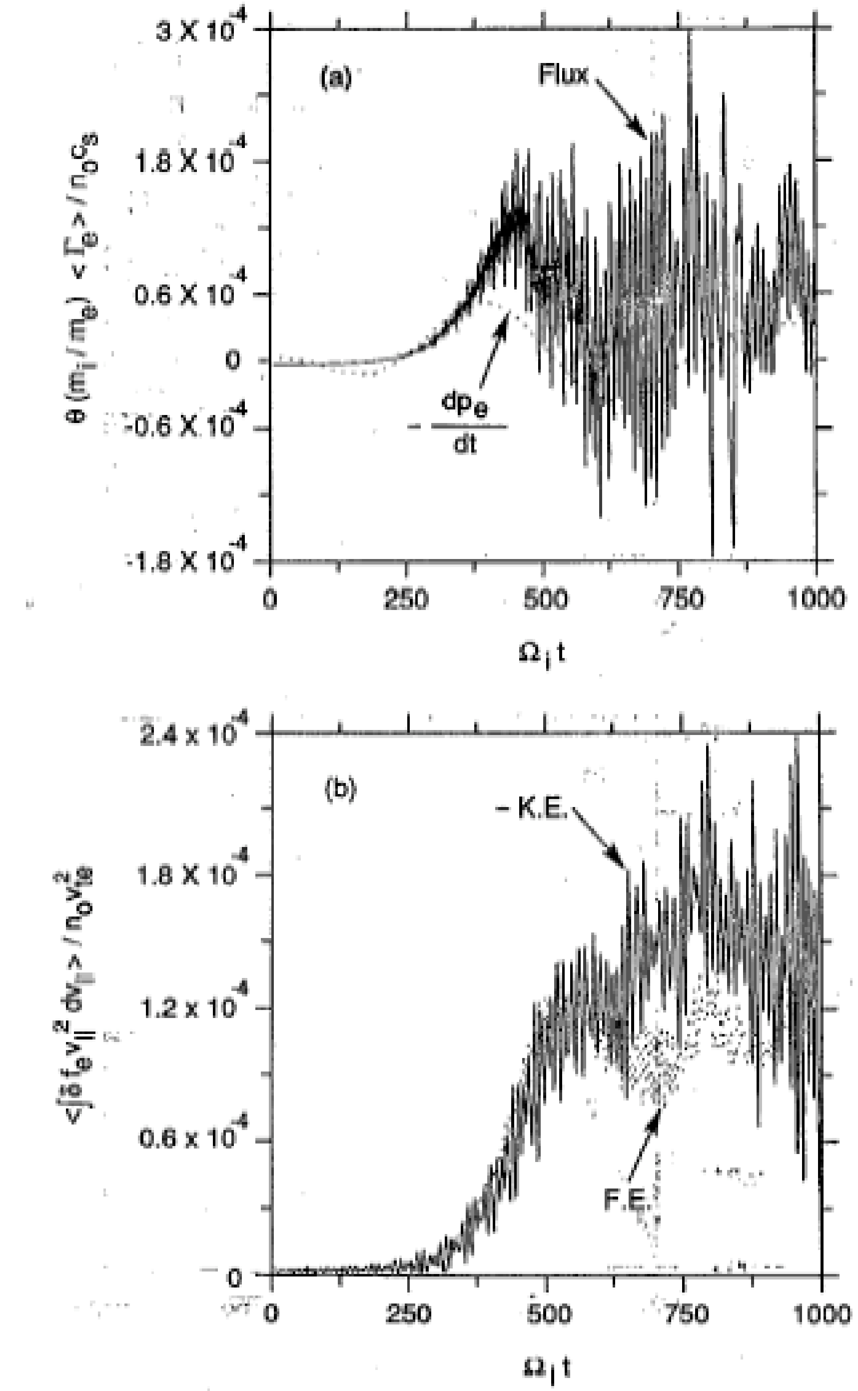


FIG. 3. The 987 particle run. (a) Time history for the electron particle flux (solid line) and the time rate of change for the electron parallel momentum (dashed line) and (b) the time evolution for the perturbed electron kinetic energy (solid line) and the field energy (dashed line).

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

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

Thermal Noise in Particle Simulation of Drift Waves in 1D (cont.) - Parker & Lee, PFB '93

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

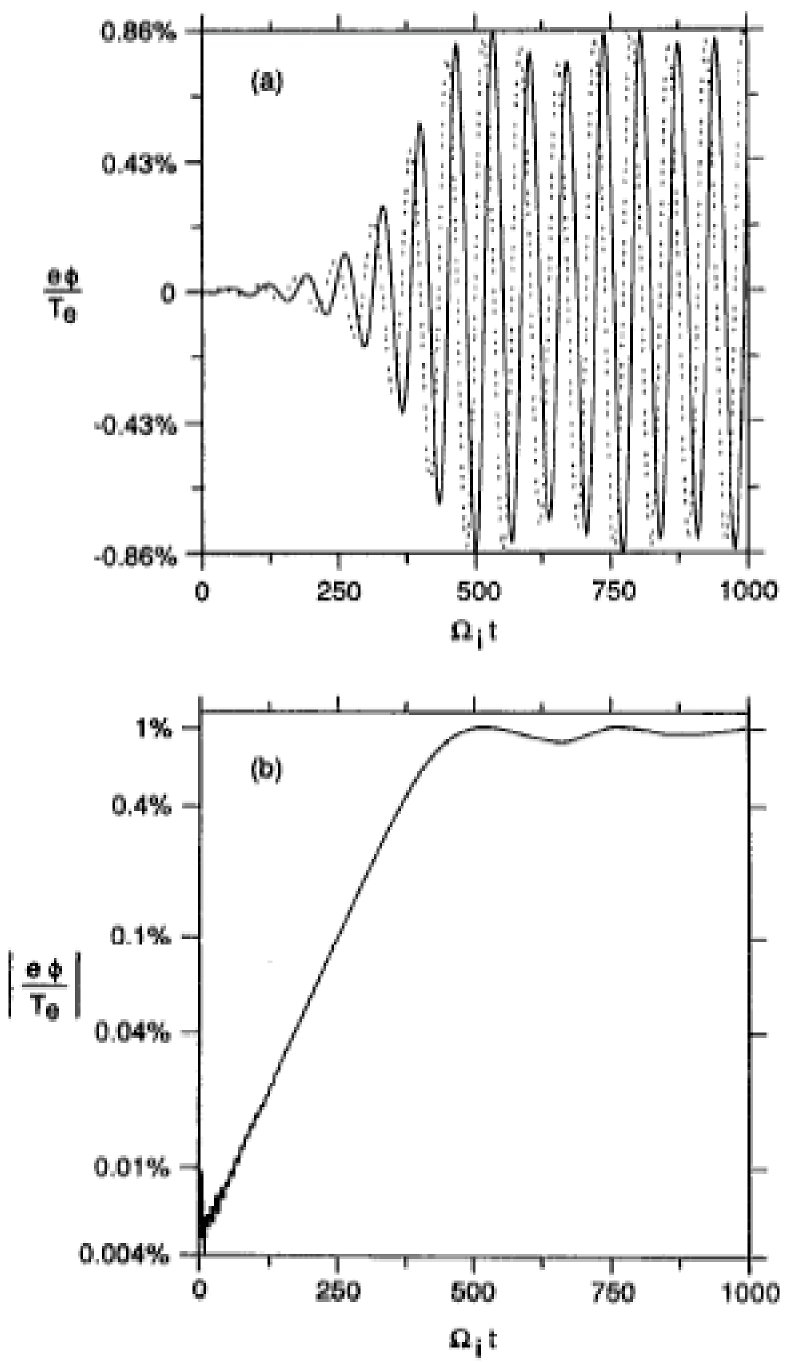


FIG. 4. The $n=1$ drift instability ($k_\perp \rho_i = 0.8$) for the run with 46 368 particles on a 64-grid system. (a) The time history for the real (solid line) and imaginary (dashed line) parts of the electrostatic potential and (b) the corresponding amplitude evolution.

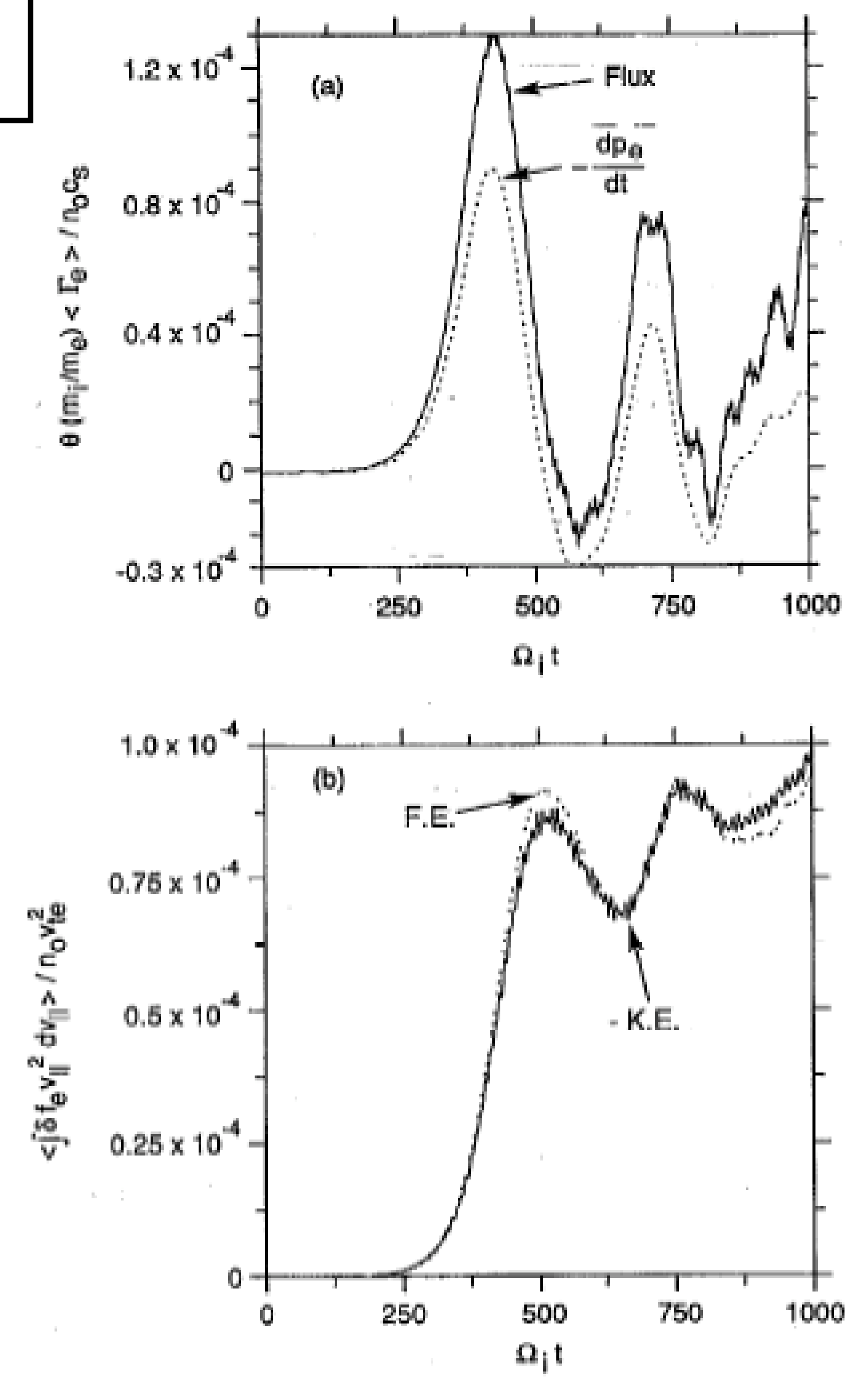


FIG. 6. The 46 368 particle run. (a) Time history for the electron particle flux (solid line) and the time rate of change for the electron parallel momentum (dashed line) and (b) the time evolution for the perturbed electron kinetic energy (solid line) and the field energy (dashed line).

Kadomtsev, Plasma Turbulence, Academic Press, 1965, pp.46.

Thermal Fluctuations

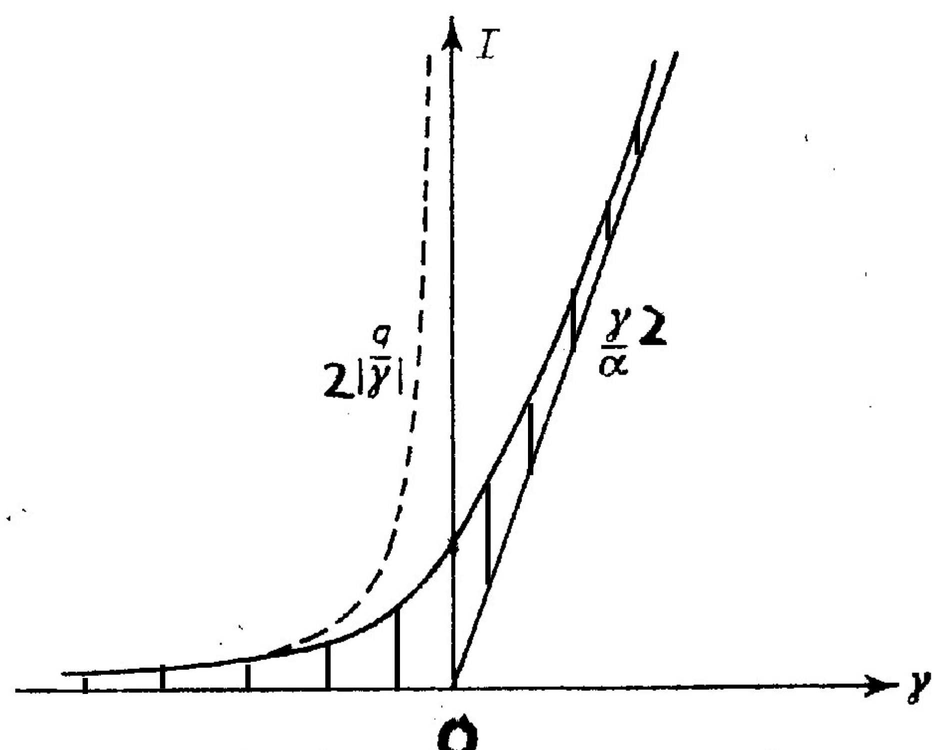
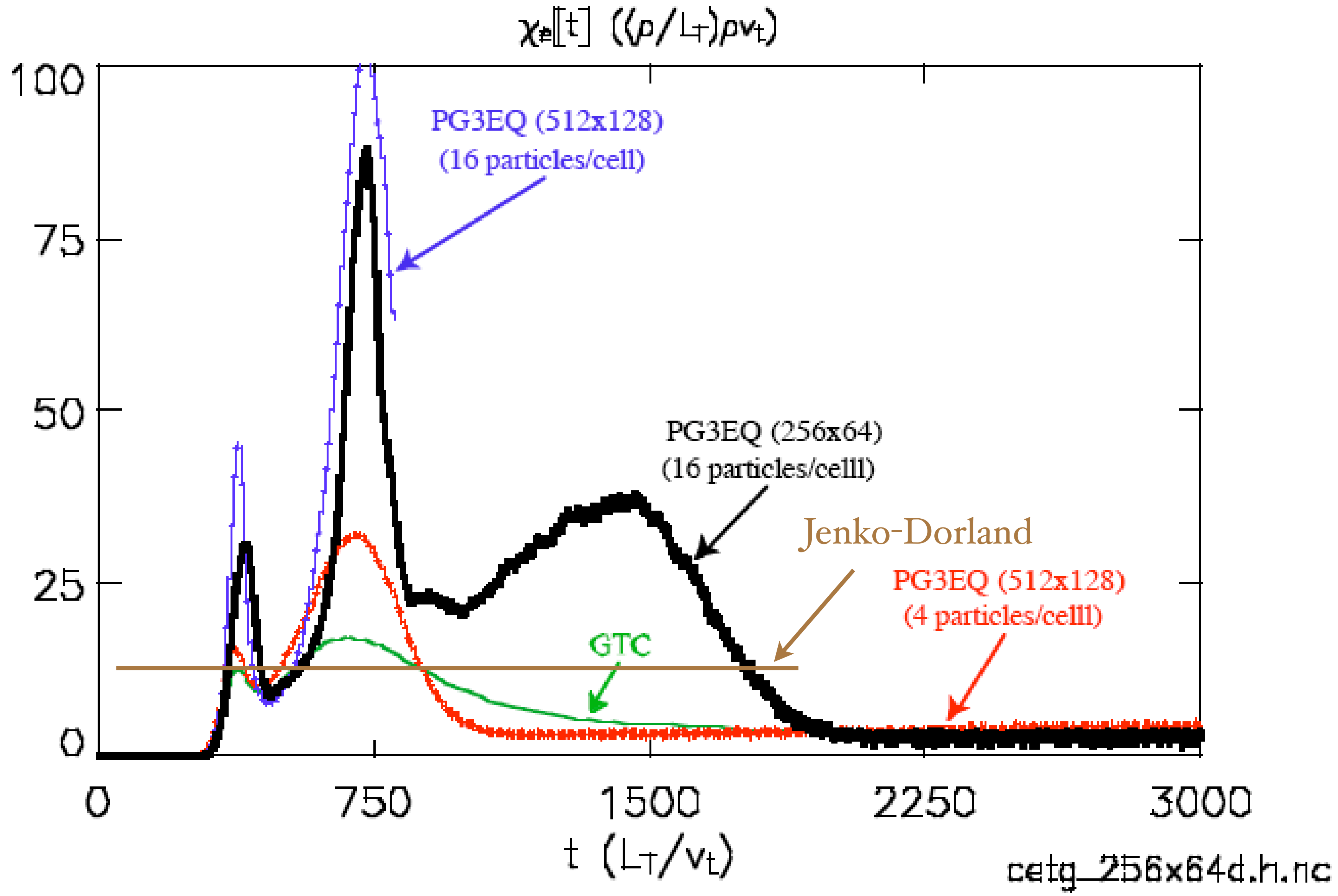


FIG. 11. Dependence of noise intensity on growth rate of small oscillations

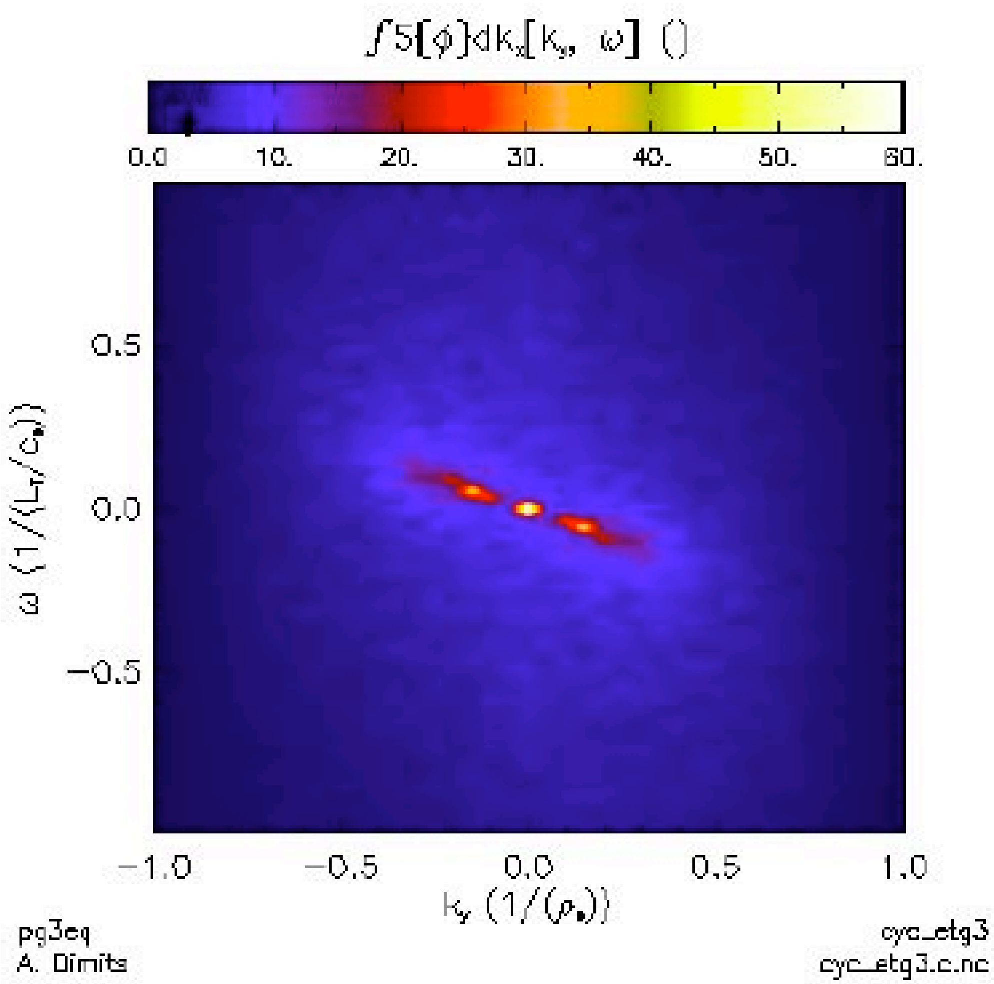
Cyclone base-case-like ETG Turbulence



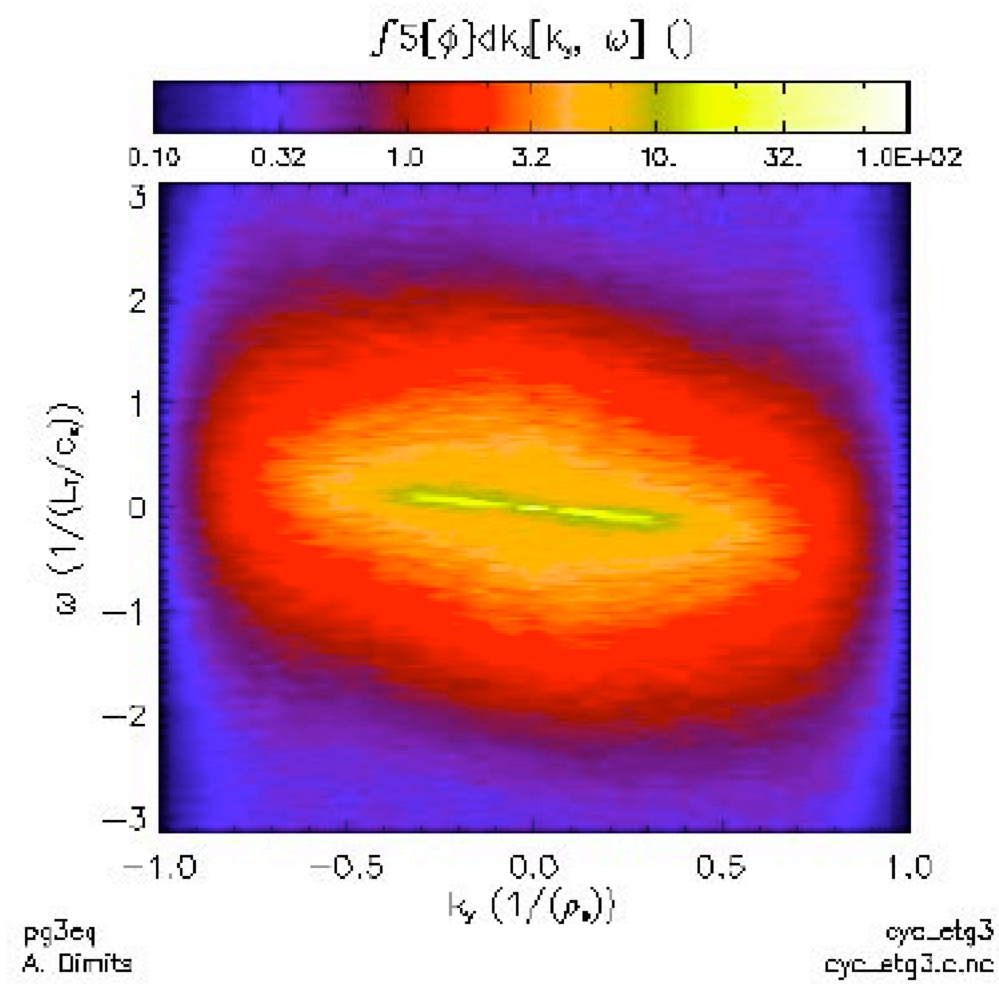
Nevins, Dimits, and Hammett, private communication

Frequency Spectrum

Drift waves at low-$k_\perp$



Broad-band noise at high-$k_\perp$



Nevins, Dimits, and Hammett, private communication

Summary and Conclusions

- GPSC is a true multi-discipline SciDAC project: integration of algorithms design, applied mathematics, parallelization, optimization, data management, visualization, team coding $\longrightarrow$ simulation vs. theory-experiment

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

- Interesting physics insights associated ITG and ETG turbulence and tearing modes have been obtained

- Velocity space nonlinearity is important in achieving steady state turbulence and is also important for conservation properties in the simulation

- The concept of steady state turbulence is essential for time-integrated transport-time-scale simulation

- We are looking forward to the spatially-integrated core-edge simulation

- Our ultimate goal is the development of multiscale gyrokinetic particle codes including wave-heating, turbulence and gyrokinetic-MHD.

- Numerical noise in particle codes has been studied extensively, but we still need to pay attention in the future. However, same type of scrutiny is needed for the artificial dissipation in continuum codes.