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

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Presented at
PSACI PAC Meeting
May 2006

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Outline

- Organization
- Activities
- Invited talks and publications
- Code development
- Physics investigations
- Convergence studies and code comparisons
- Scientific Application Partnership Program activities
- The noise issue
- Summary

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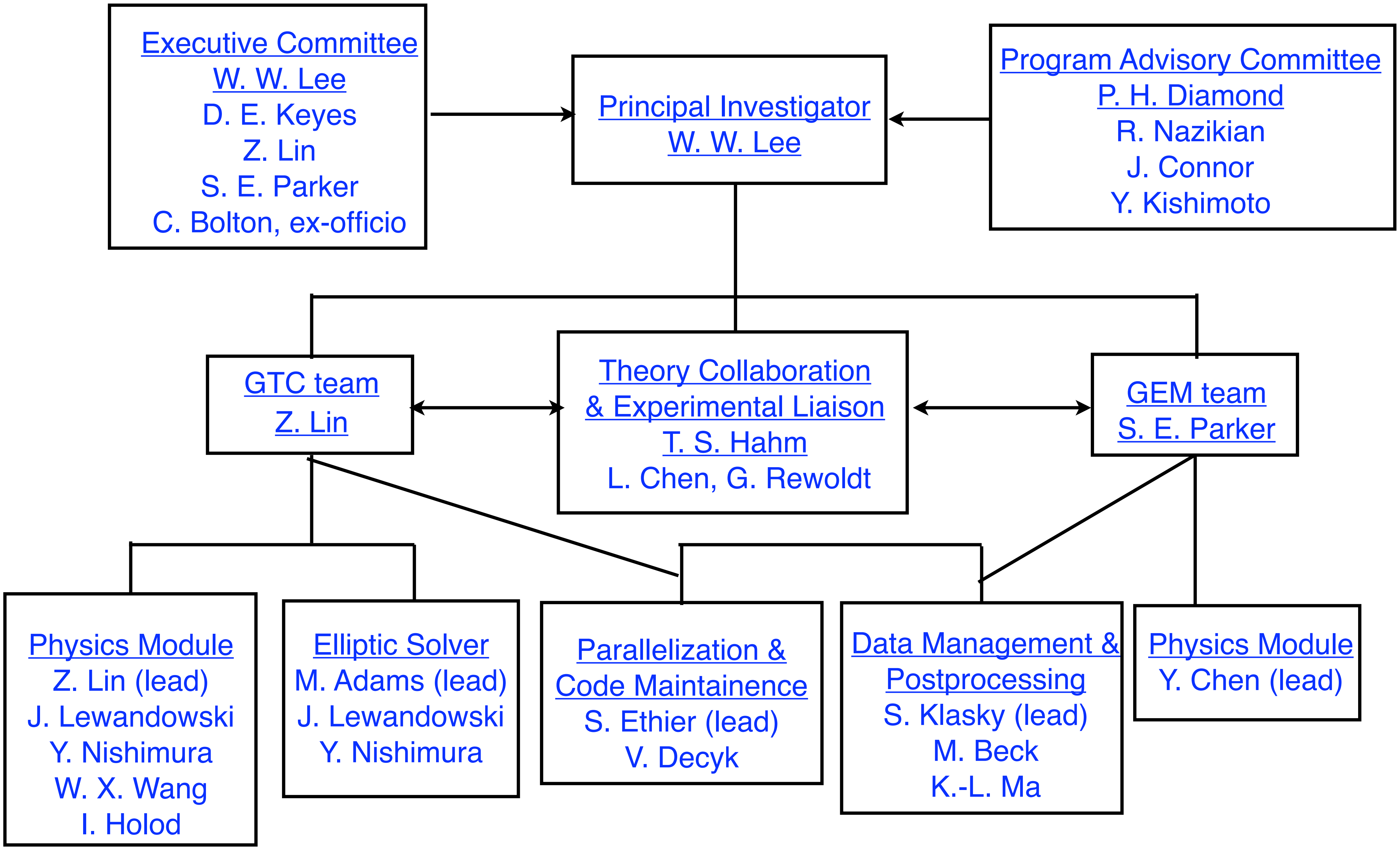

FALL MEETING

SciDAC Center for Gyrokinetic Particle Simulation
of Turbulent Transport in Burning Plasmas
(GPSC)

Governor's Square 9, Adam's Mark Hotel, Denver CO.

October 23, 2005

8:30A Lee - Opening remarks and noise issue in steady state simulations

8:40A Wang - Shaped plasma simulations

8:50A Lewandowski - Kinetic electron simulations

9:00A Ethier - GTC performance and convergence issues

9:15A Lin - GTC code status and ETG simulations

9:30A Nishimura - Progress in the development of electromagnetic GTC

9:45A Holod - Global gyrokinetic particle simulation of energetic particle driven instabilities

10:00A coffee break

10:15A Decyk -- GTC modularization issues

10:30A Adams - GTC parallel strategies, parallel FE solver and FE solver verification

10:45A Y. Chen - Simulation of energetic particle driven toroidal Alfven eigenmodes with the GEM code

11:00A Parker - ETG Particle Number Convergence Studies, GEM Team status and future plan

11:20A Hahm - Turbulence Spreading, Theory Team status and future plan

11:40A Lin - GTC Team status and future plan

12:00A Klasky - Data Management and Visualization accomplishments and future directions for the GPS SciDAC

12:15P Lee -- Concluding remarks and open discussions

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Workshop on Long Time Simulations of Kinetic Plasmas
April 21, 2006
Pryor AB (Atrium Level)
Hyatt Regency, Dallas, TX

Session 1: Manickam
08:30 Lee: Issues to be addressed in this workshop
08:40 Krommes: Physics in Steady State Turbulence
09:00 Lin: Global TEM and ETG Simulations using GTC
09:20 Parker: ITG and ETG Simulations using GEM
09:40 Ethier: Convergence Studies of ITG and ETG using GTC
10:00 Nevins: Discrete Particle Noise in ITG Turbulence (did not present)

10:20 Coffee Break

Session 2: Parker
10:35 Park: Latest Fluctuation Measurements on NSTX
10:55 Ghizzo: Study of Nonlinear kinetic effects in stimulated Raman Back-scattering scenario using semi-Lagrangian Vlasov code
11:15 Qin: Delta-f particle simulations of long time behavior of collective effects in high intensity charged particle beams
11:35 Holod: Transport driven by random fluctuations: theory and simulation
11:45 Jenkins: Fluctuations in nonlinearly saturated drift wave simulations
11:55 Diamond: Fluctuations in Turbulent Plasmas (did not present)

12:15 Lunch

Session 3: Rewoldt
01:30 Chen: EM simulations using GEM
01:50 Wang: Turbulence and Neoclassical Simulations in General Geometry
02:10 Nishimura: Global electromagnetic simulation using GTC
02:30 Xu: Formulation of 5D Edge Gyrokinetic Simulations
02:50 Chang/Ku: Formulation of Edge PIC Gyrokinetic Simulation

03:10 Coffee Break

Session 4: Lee
03:25 Noguchi: Implicit Schemes for Particle Codes
03:45 Dewar: Simulation of Hasegawa-Wakatani Equation
04:05 Klasky: Data Management and Visualization
04:25 Discussions

06:30 Adjourn

PARTICIPANTS

Mark Adams, Allen Boozer, C.S. Chang, Yang Chen, Bruce Cohen. Bob Dewar, Andris Dimits, Stephane Ethier, Alain Ghizzo, Greg Hammett, Fred Hinton, Igor Holod, Tom Jenkins, Scott Klasky, Roman Kolesnikov, Doug Kothe, John Krommes, Seung-hoe Ku, Jae-Min Kwon, Wei-li Lee, Zhihong Lin, John Mandrekas, J. Manickam, Yas Nishimura, Koichi Noguchi, Hyeon Park, Scott Parker, Hong Qin, Greg Rewoldt, Weixing Wang, Xueqiao Xu, Leonid Zakharov

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Invited Talks

*T. S. Hahm, "Overview of outstanding issues in burning plasmas," invited talk, 21st IAEA Fusion Energy Conference, Chengdu, China (2006).

*W. W. Lee, "Gyrokinetic particle simulation of fusion plasmas: path to petascale computing," invited talk, Second Annual DoE SciDAC Conference, Denver, CO (2006).

*W. W. Lee, "Long time simulations of microturbulence," invited talk, Annual Sherwood Theory Conference, Dallas, TX; Bull. Am. Phys. Soc. **51-2**, 111, (2006).

*W. X. Wang, "Neoclassical and Turbulent Transport in Shaped Toroidal Plasmas," invited talk, 47th Annual APS/DPP Meeting, Denver, CO; Bull. Am. Phys. Soc. **50-8**, 180 (2005).

*J. L. V. Lewandowski, "Global particle-in-cell simulations of microturbulence with kinetic electrons," invited talk, 47th Annual APS/DPP meeting, Denver, CO; Bull. Am. Phys. Soc. **50-8**, 181,(2005).

Publications

Review of Modern Physics: 1 submitted
Physics of Plasmas: 7 published, 1 submitted
Journal of Computational Physics: 1 published, 1 submitted
Plasma Physics and Controlled Fusion: 2 published
Contributions to Plasma Physics: 1 published

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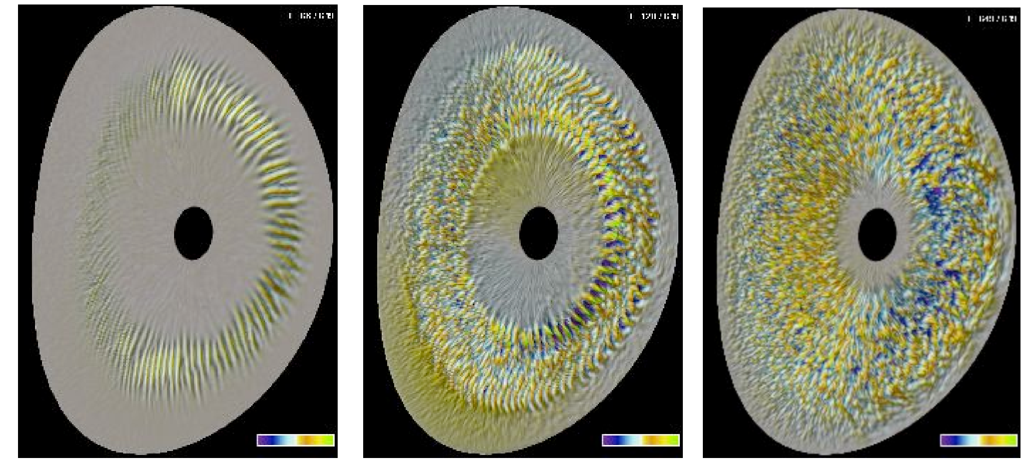
Code Development

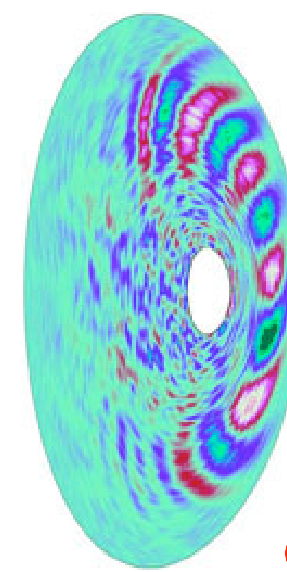


GTC

- GTC (PPPL)
  - -- A global code for turbulence transport simulations
  - -- Shaped plasma in general geometry
  - -- Electrostatic electron dynamics based on the delta-h scheme: non-adiabatic part of delta-f

- GTC (UCI)
  - -- Electromagnetic electron dynamics based on the hybrid scheme: $|\omega/k_{\parallel}v_{\parallel}| \ll 1$
  - -- A global code for both turbulence and gyrokinetic MHD simulations

- GTC-neo (PPPL) -- For neoclassical transport simulations in
  - -- General toroidal geometry
  - -- fully operational collision operators



GEM

- GEM (Colorado)
  - -- A wedge code for turbulence and gyrokinetic MHD simulations
  - -- Shaped plasma in general geometry -- Electromagnetic electron dynamics based on delta-h scheme: non-adiabatic part of delta-f

- Object Oriented GTC (UCLA/UCI/PPPL)
  - -- Based on Fortran-90 to facilitate team coding

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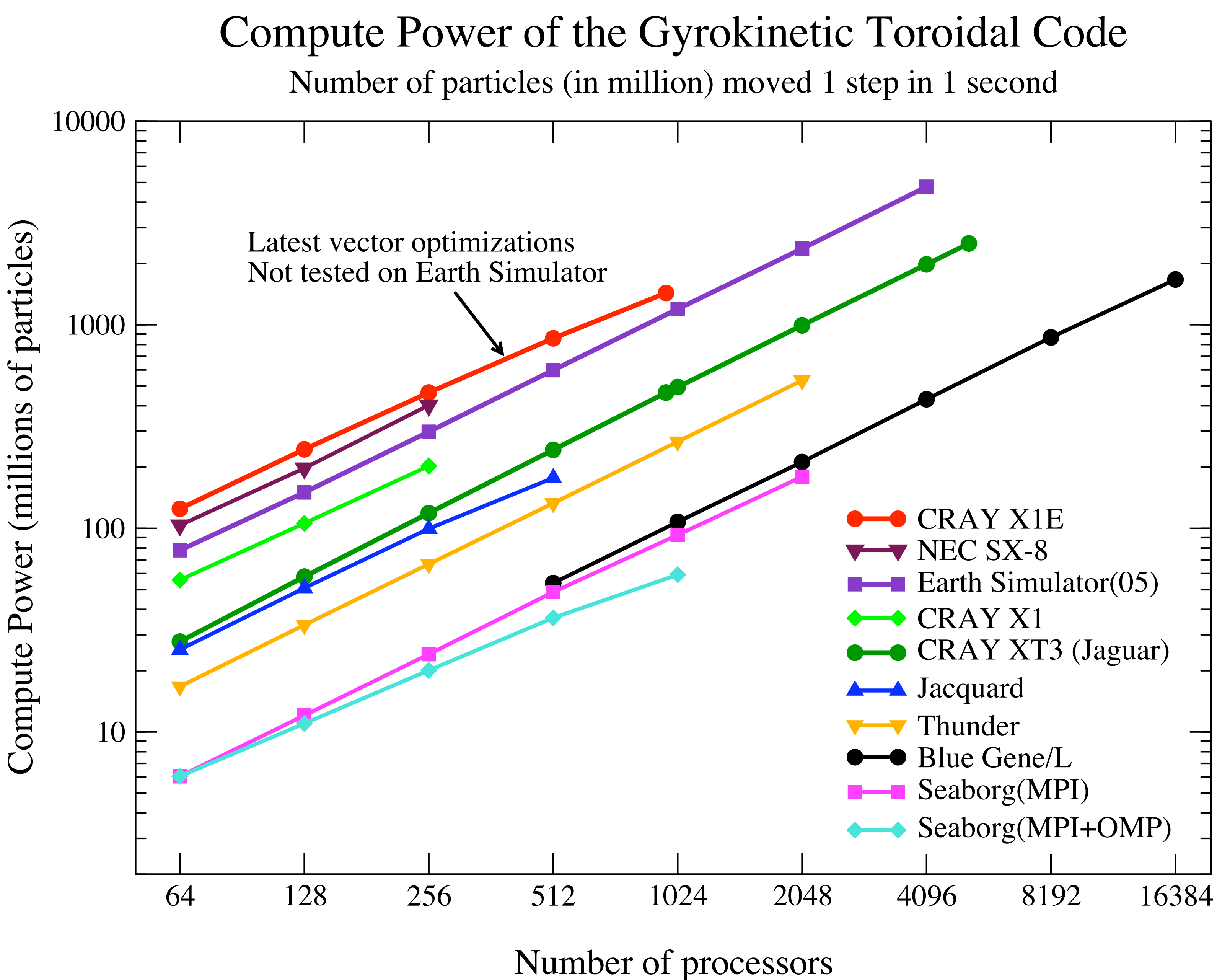
GTC performance on MPP platforms aiming for ITER-size Plasmas

- Gyrokinetic particle codes are very portable, scalable and efficient on both cache-based and vector-parallel MPP platforms
- 7.2 teraflops achieved on the Earth Simulator with 4096 processors using 13.2 billion particles



GPSC computing resources ('05-'06):
Seaborg (2.0 M processor-hrs)
Phoenix (0.2 M processor-hrs)
Jaguar (2.0 M processor-hrs)

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Governing Equations for Gyrokinetic Particle Simulation

- Gyrokinetic Vlasov Equation

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

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

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

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

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

- Gyrokinetic Poisson's Equation

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

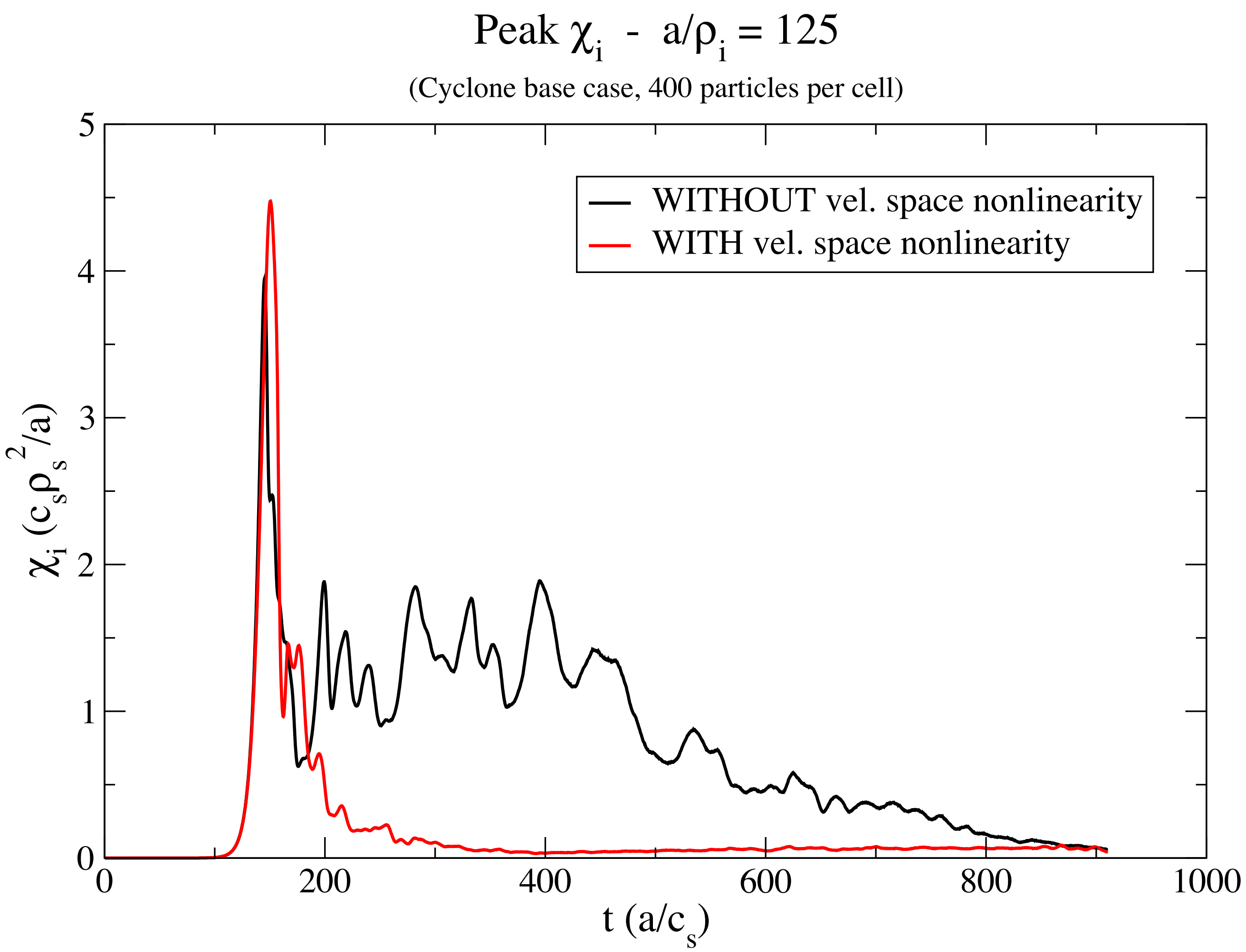
- Gyrokinetic Ampere's Law

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

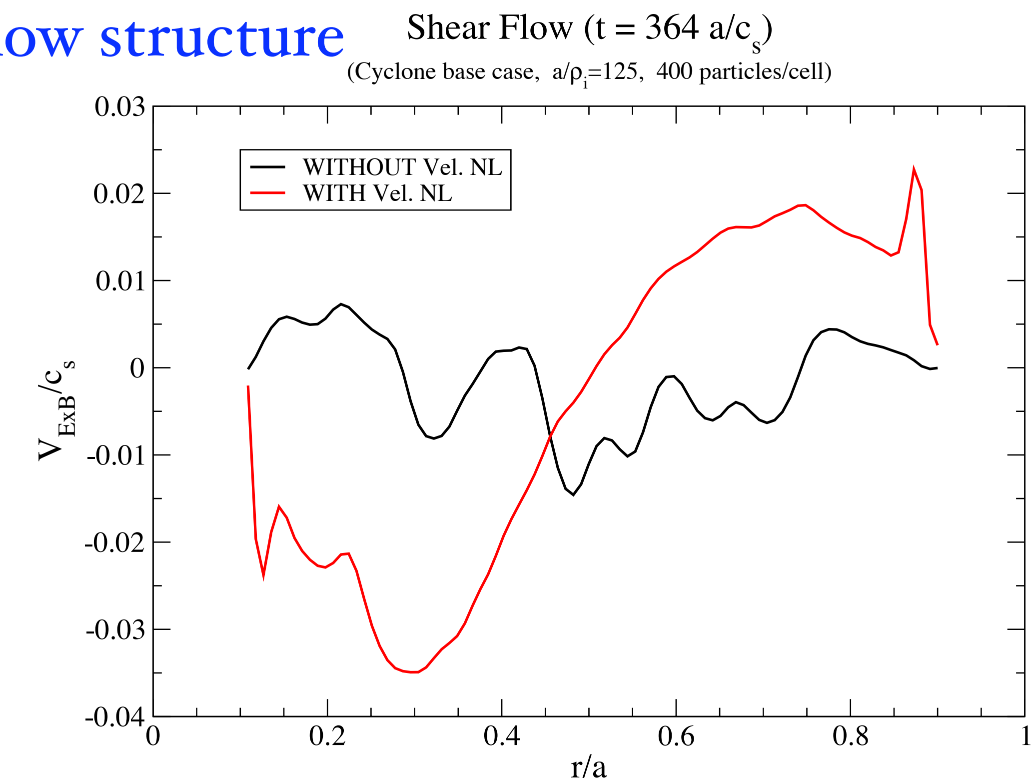
Steady State Simulations of ITG Turbulence with Adiabatic Electrons

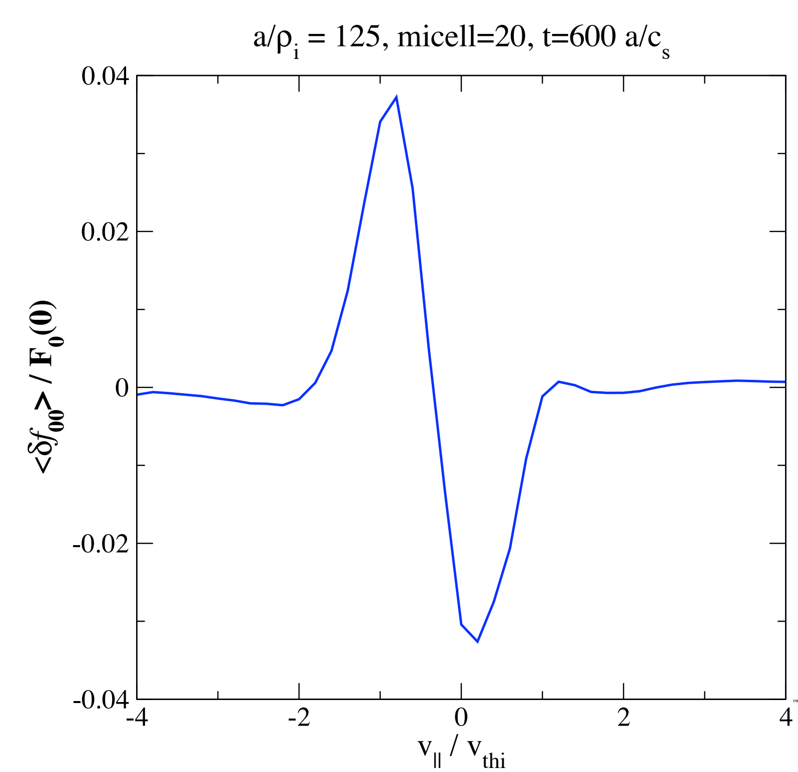
- Cyclone based case with a /rho_i = 125 and 400 particles per cell
- Velocity-space nonlinearity play an important role in achieving state state

- Ion thermal diffusivity vs. time



- Zonal flow structure





- Velocity space nonlinearity produces an ion current: $V_{\parallel} / V_{ti} \approx 2.5\%$ (simulation with 20 particles per cell)

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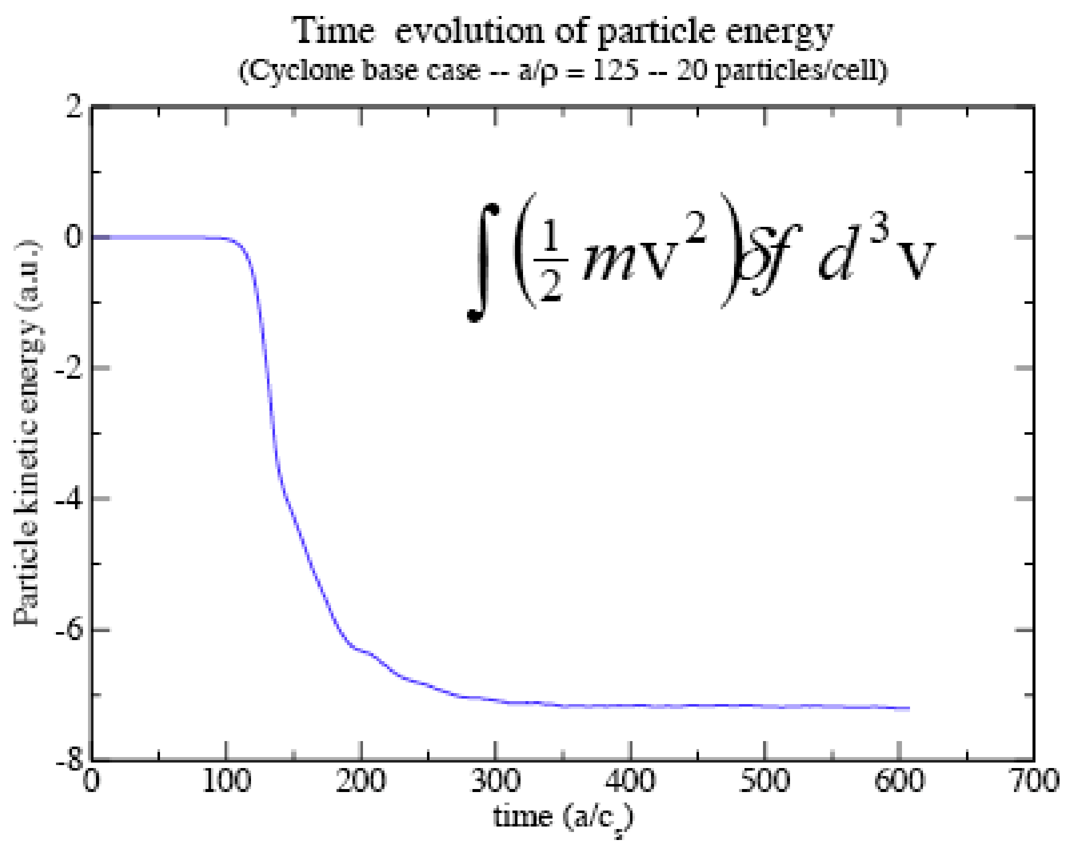
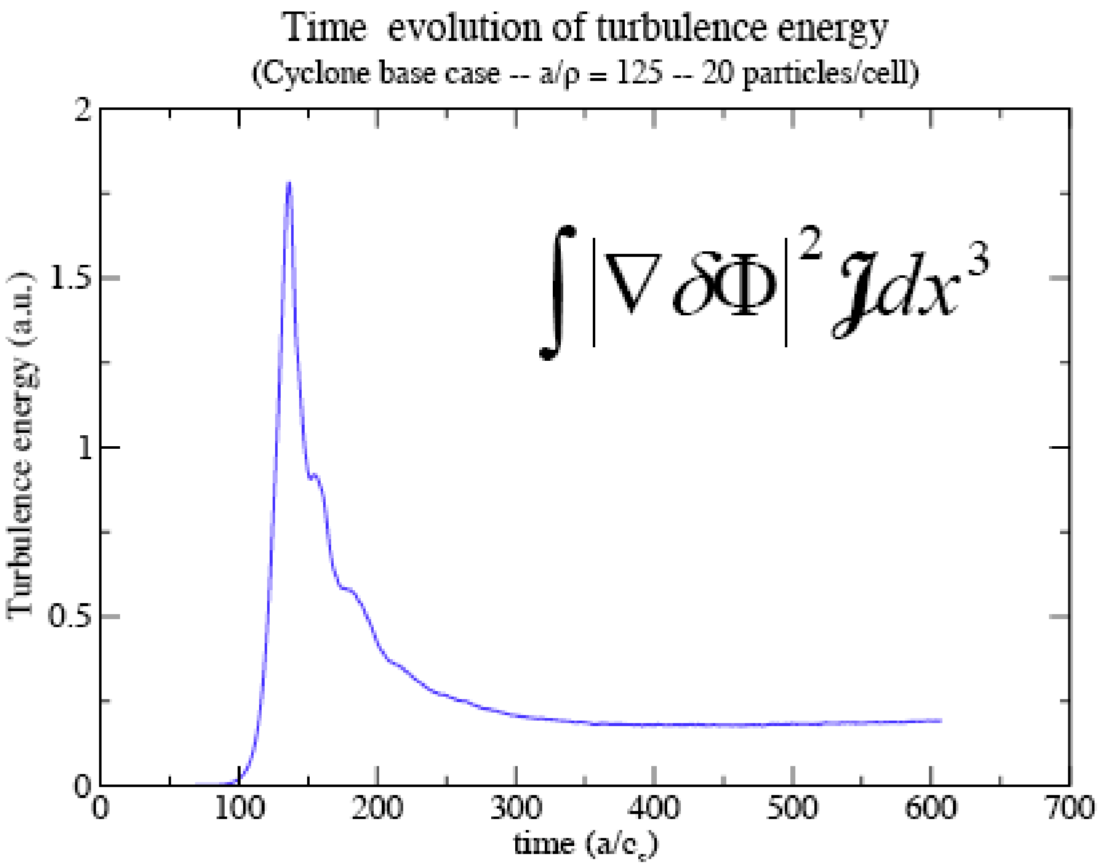
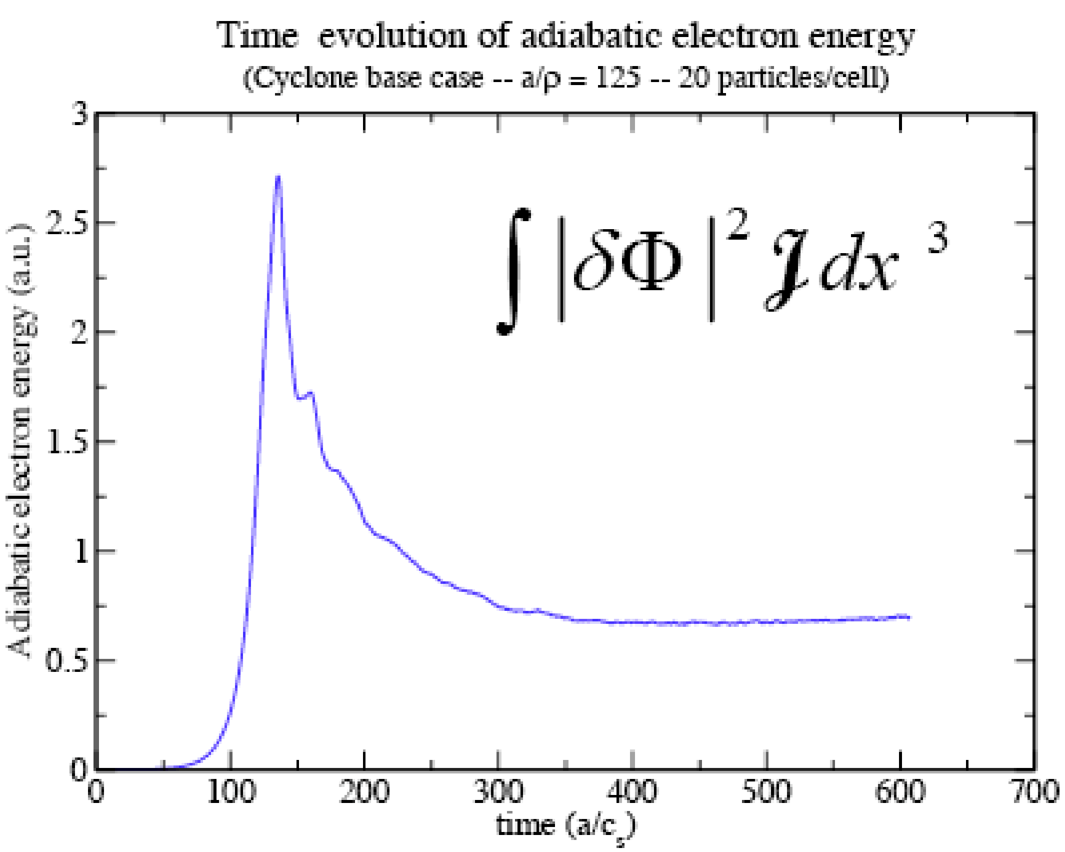
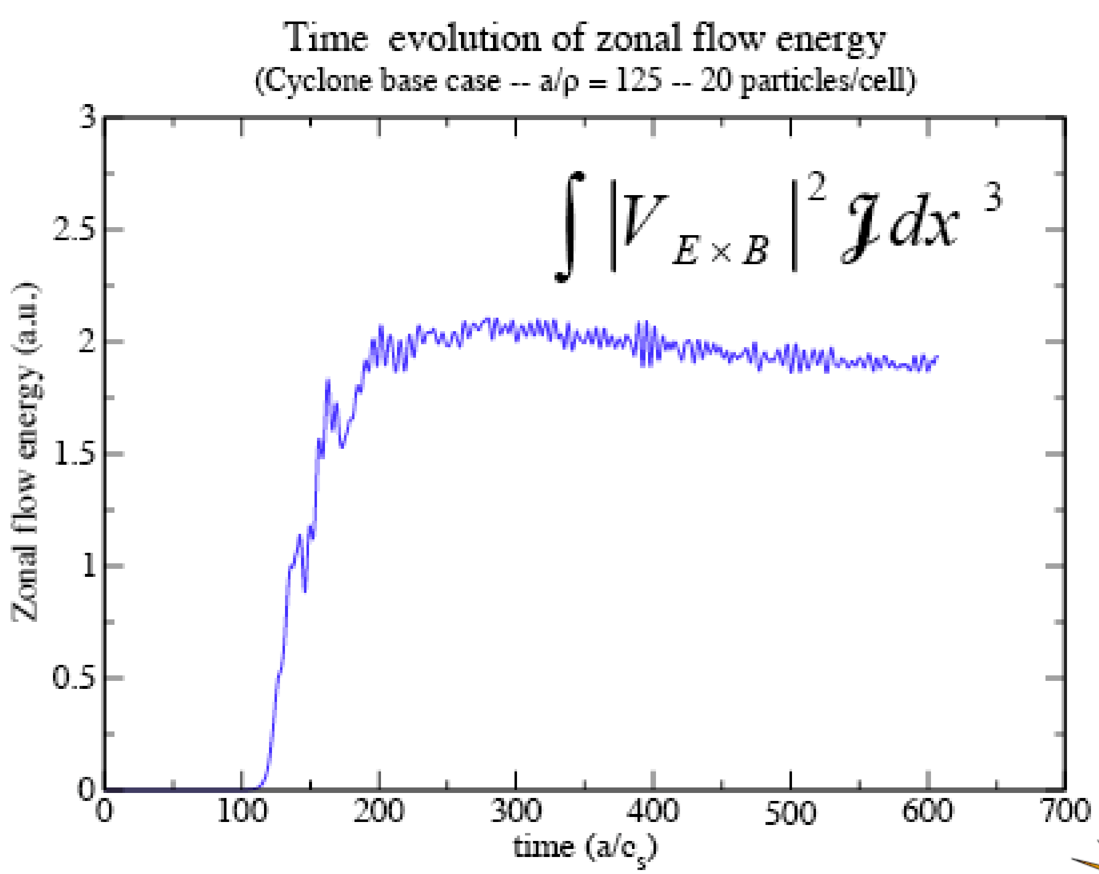
Conservation properties of ITG simulation (20 particles/cell)









20 particles per cell

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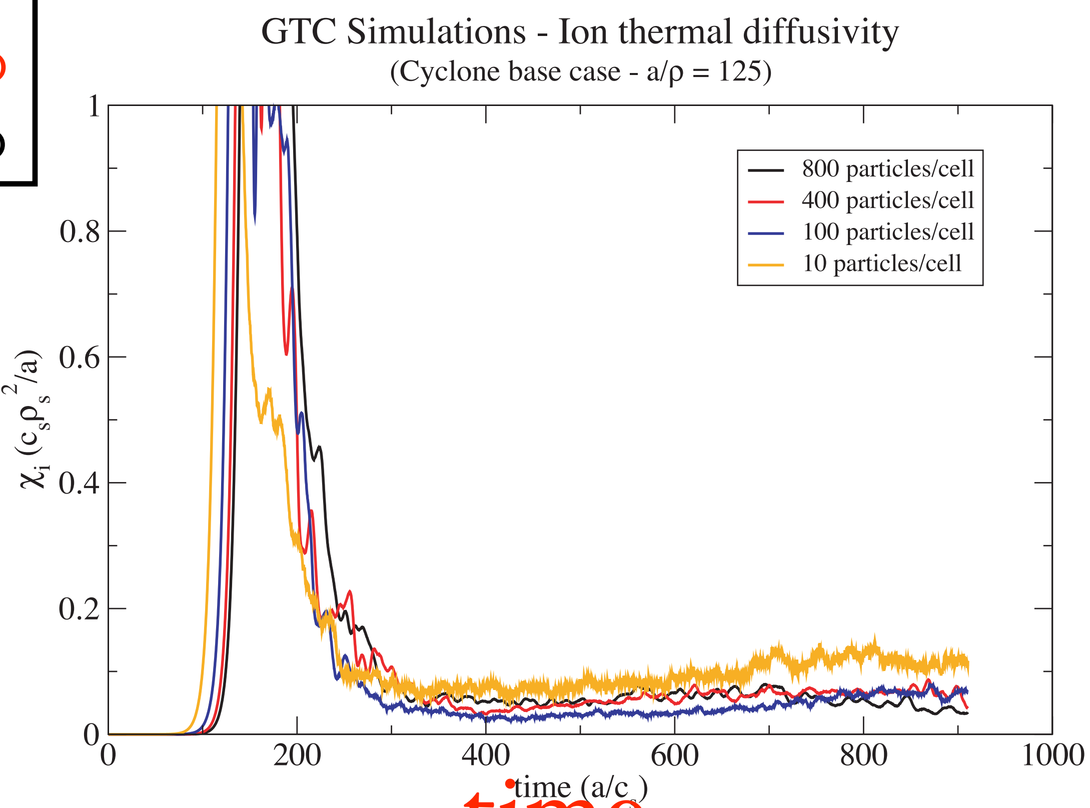
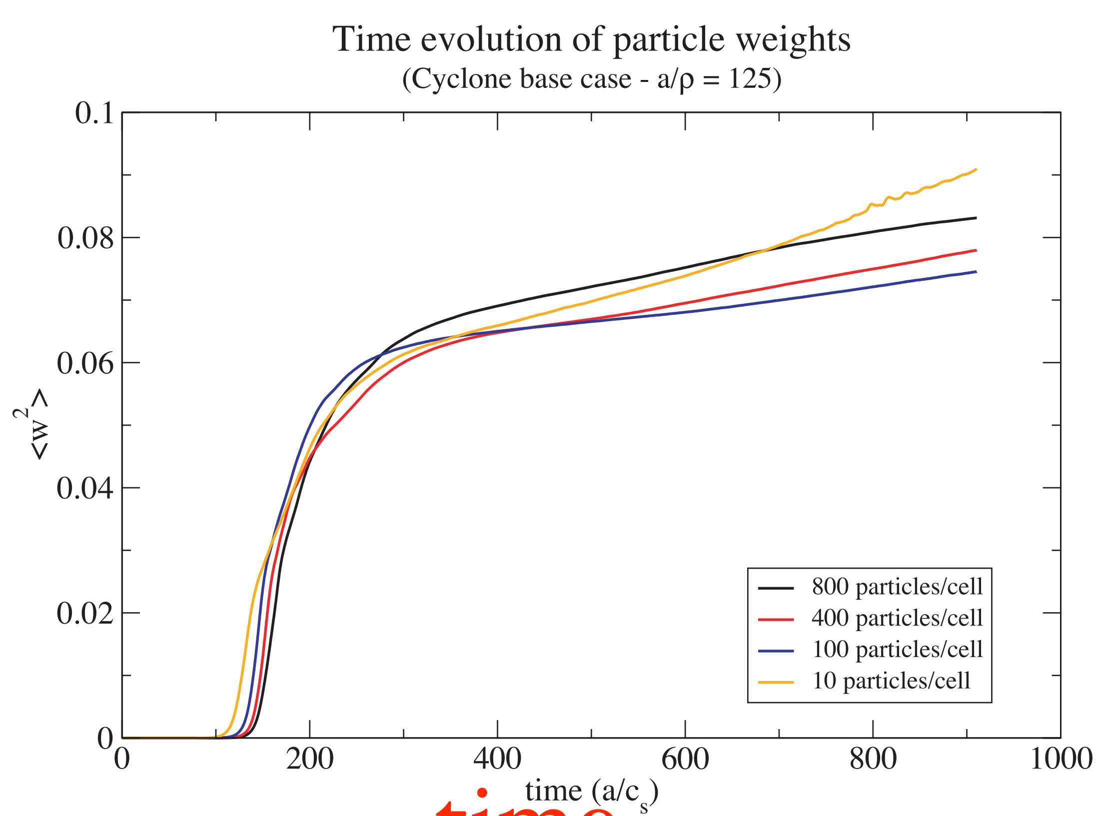
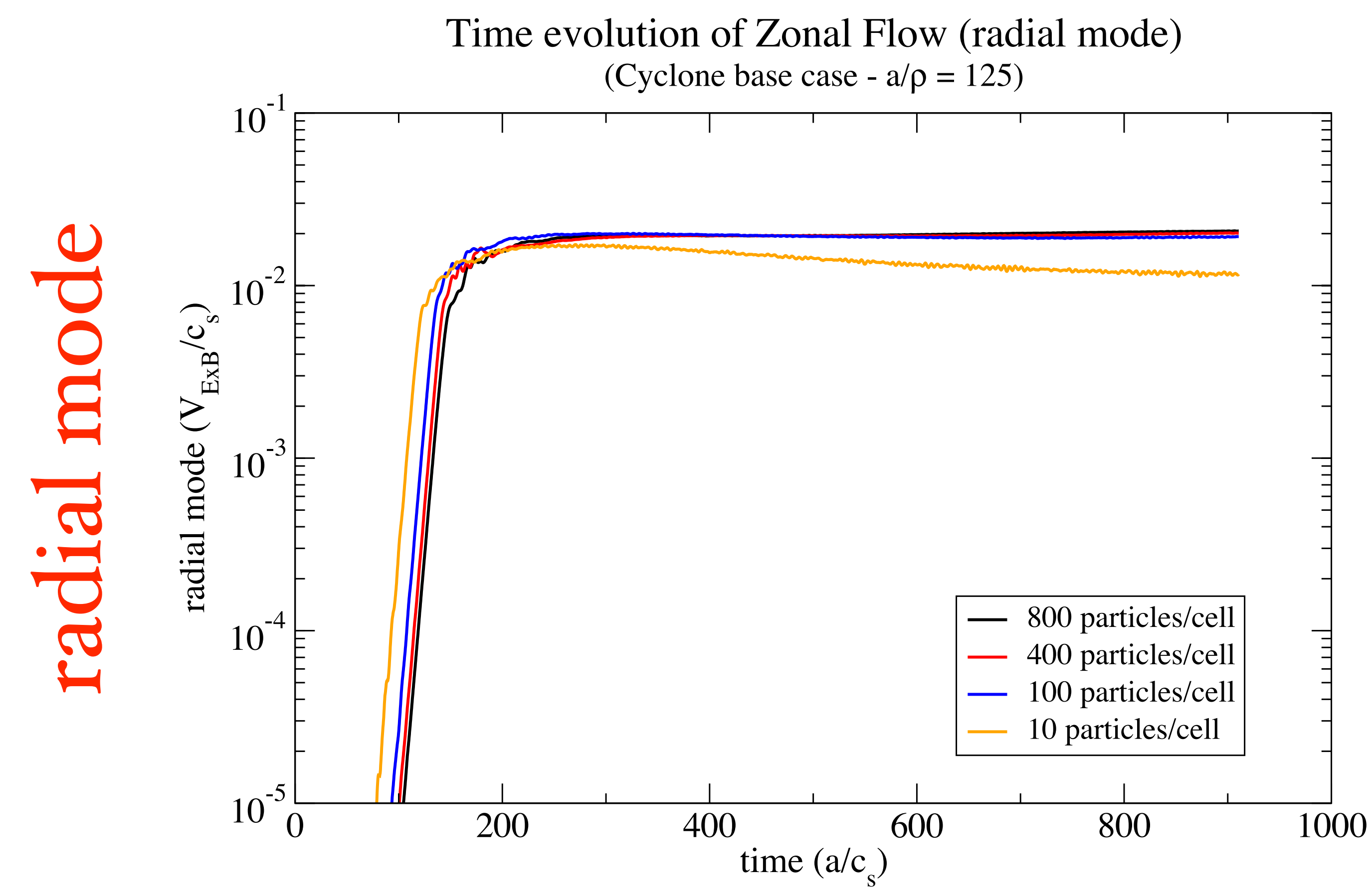
Convergence tests of ITG simulations (LCF- ORNL)

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

10
100
400
800







$$\frac{d}{dt}\sum_{j=1}^{N}\langle w_j^2\rangle = Q$$

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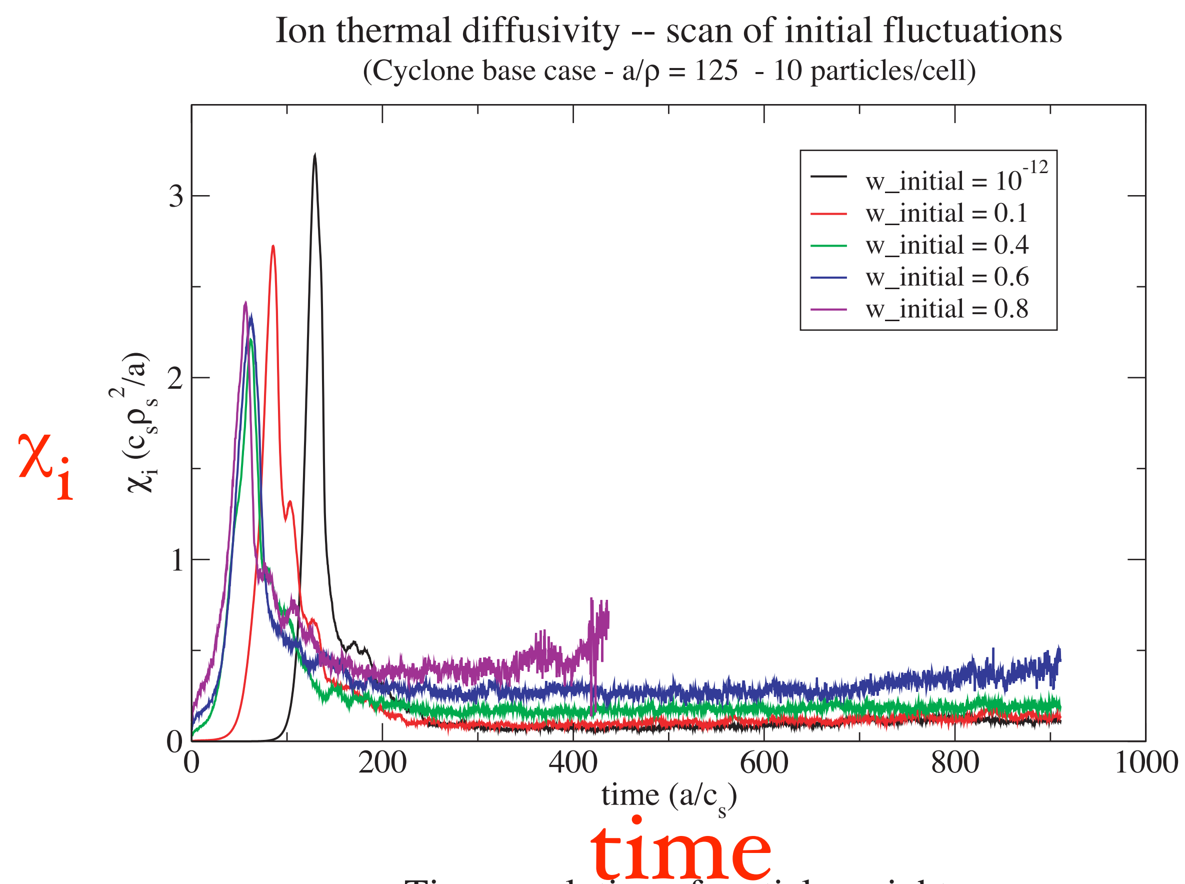
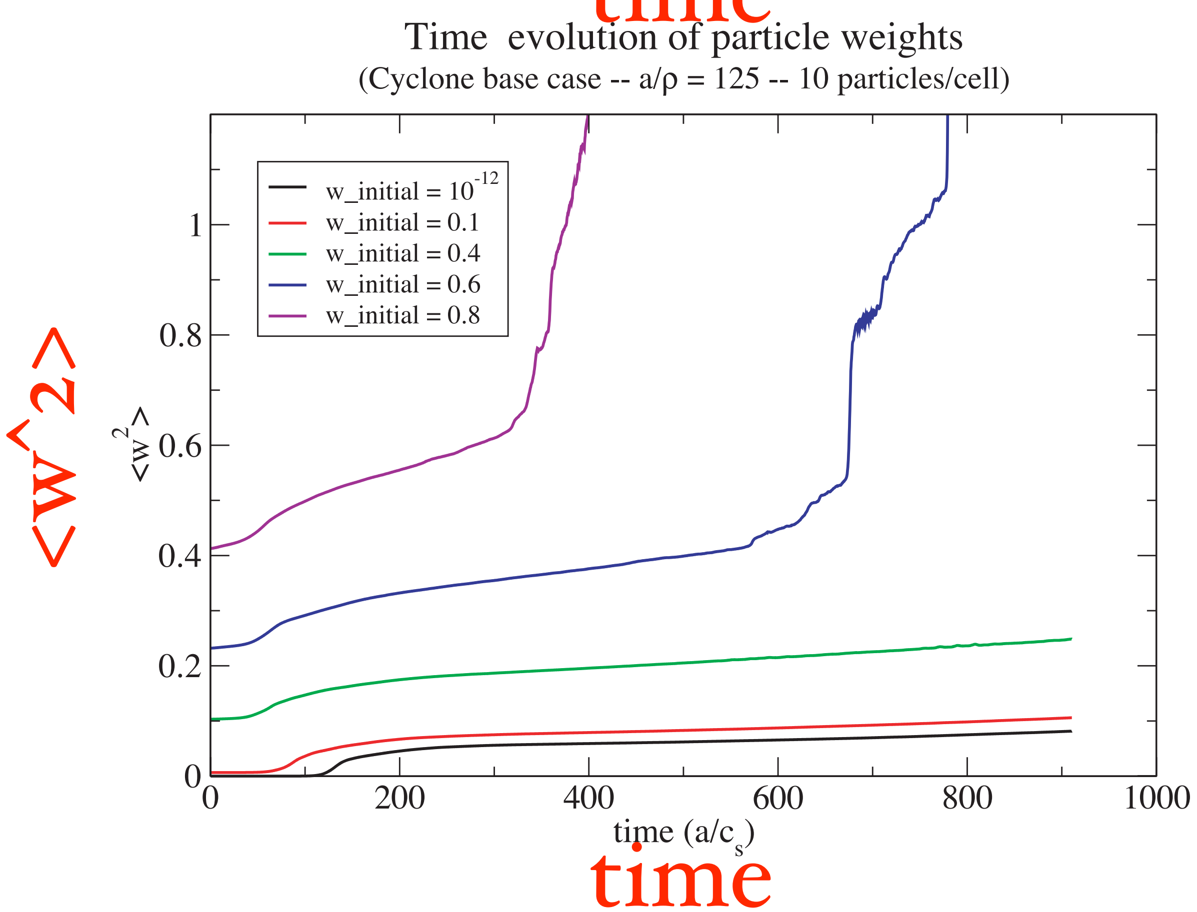
Convergence tests of ITG simulations (LCF- ORNL)

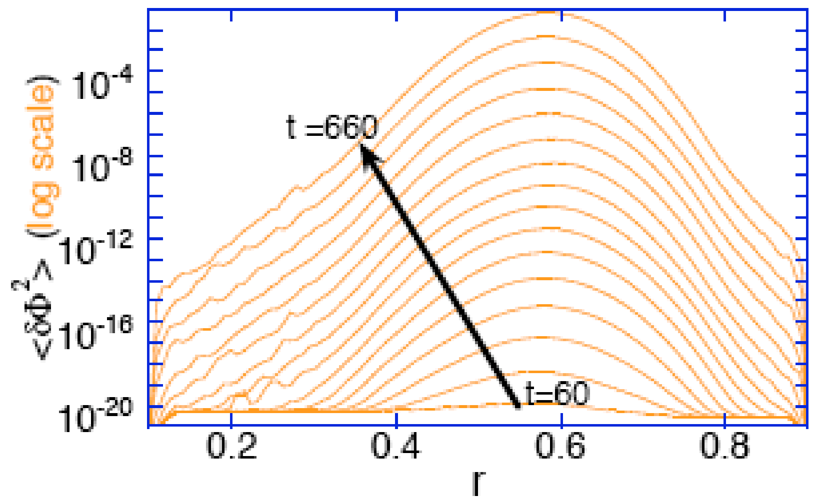


10^-12
0.1
0.4
0.6
0.8

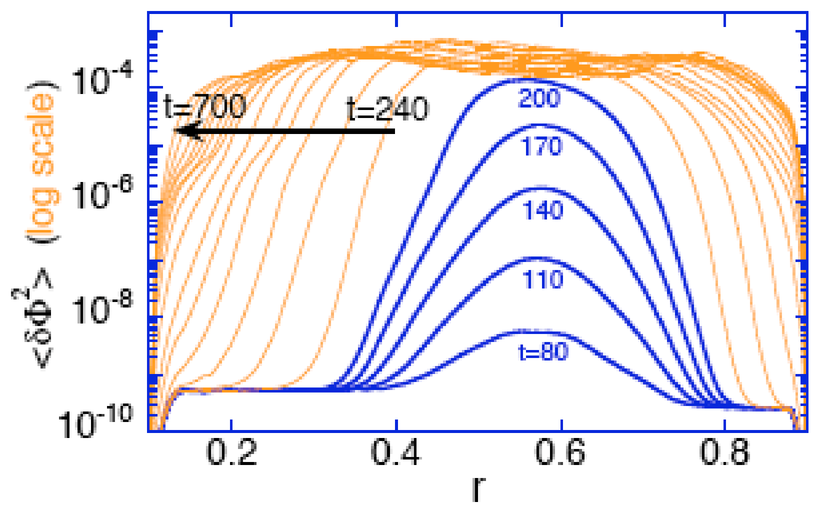


Initial particle weight scan:
growing weights
cause higher fluxes

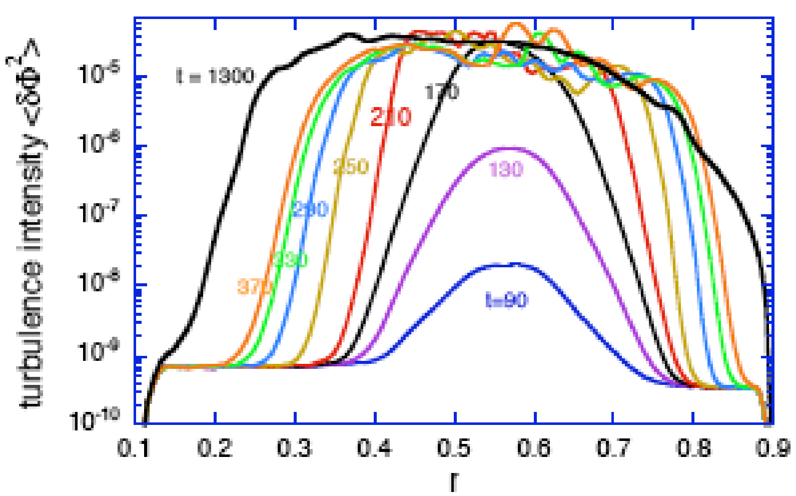
ITG simulations of turbulence spreading using GTC for shaped plasmas



- LINEAR simulation with all modes: toroidal mode coupling induces convective propagation (Garbet et.al); uniform $v_s \sim 1.2(\rho_i/R_0)c_s$, independent of $< \delta\phi^2 >$



- NO ZONAL FLOWS: diffusive nature induced by nonlinear coupling (no longer convective); making spreading faster



- WITH ZONAL FLOWS:
  $\rightarrow$ lowers $< \delta\phi^2 >$ by a factor of 10
  $\rightarrow$ reduces turbulence spreading

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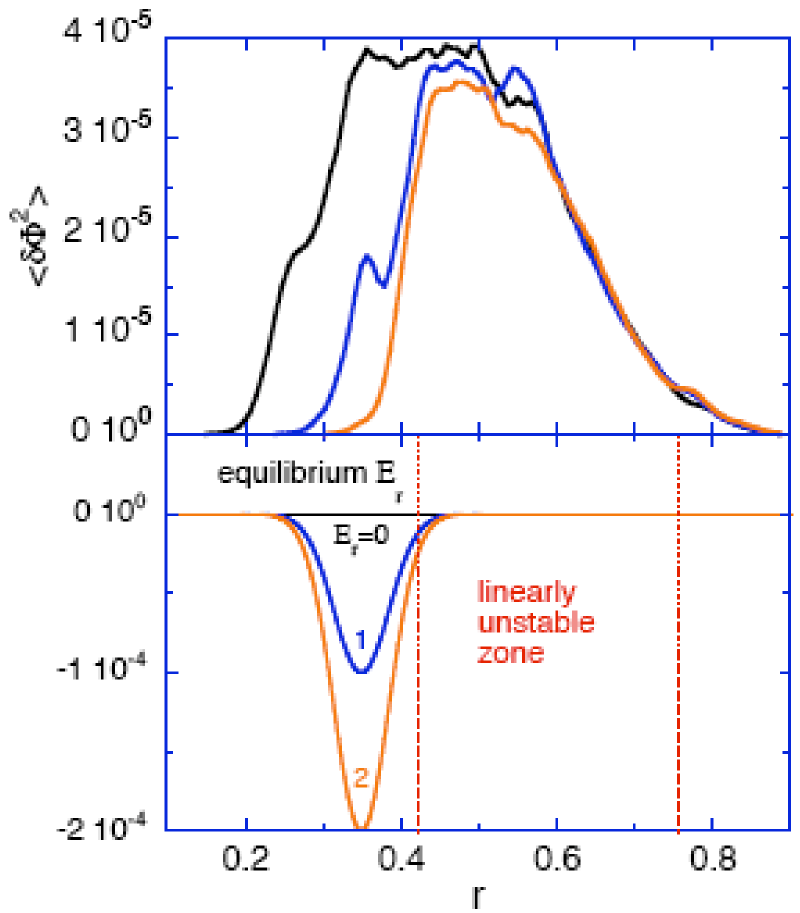
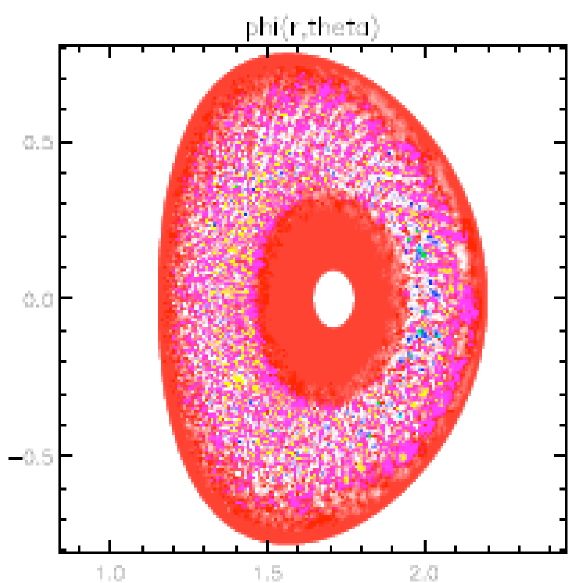
$E \times B$ Shear Layer Blocks Turbulence Spreading





- $\omega_{E\times B}^{max} = 0$: turbulence widely spreads to fill up big area in both directions
- $\omega_{E\times B}^{max} = 0.13\frac{c_s}{a}$: inward spreading partially blocked
- $\omega_{E\times B}^{max} = 0.26\ c_s/a$: almost completely blocked
- Shear layer not only reduces turbulence spreading extension but also slows down the spreading
- Turbulence level not increased in source region as spreading blocked
- Outward spreading is not affected

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Turbulence Spreading Theory

[Hahm, Diamond, Lin, Rewoldt, Gurcan,and Ethier, PoP, 12, 090903 ‘05]

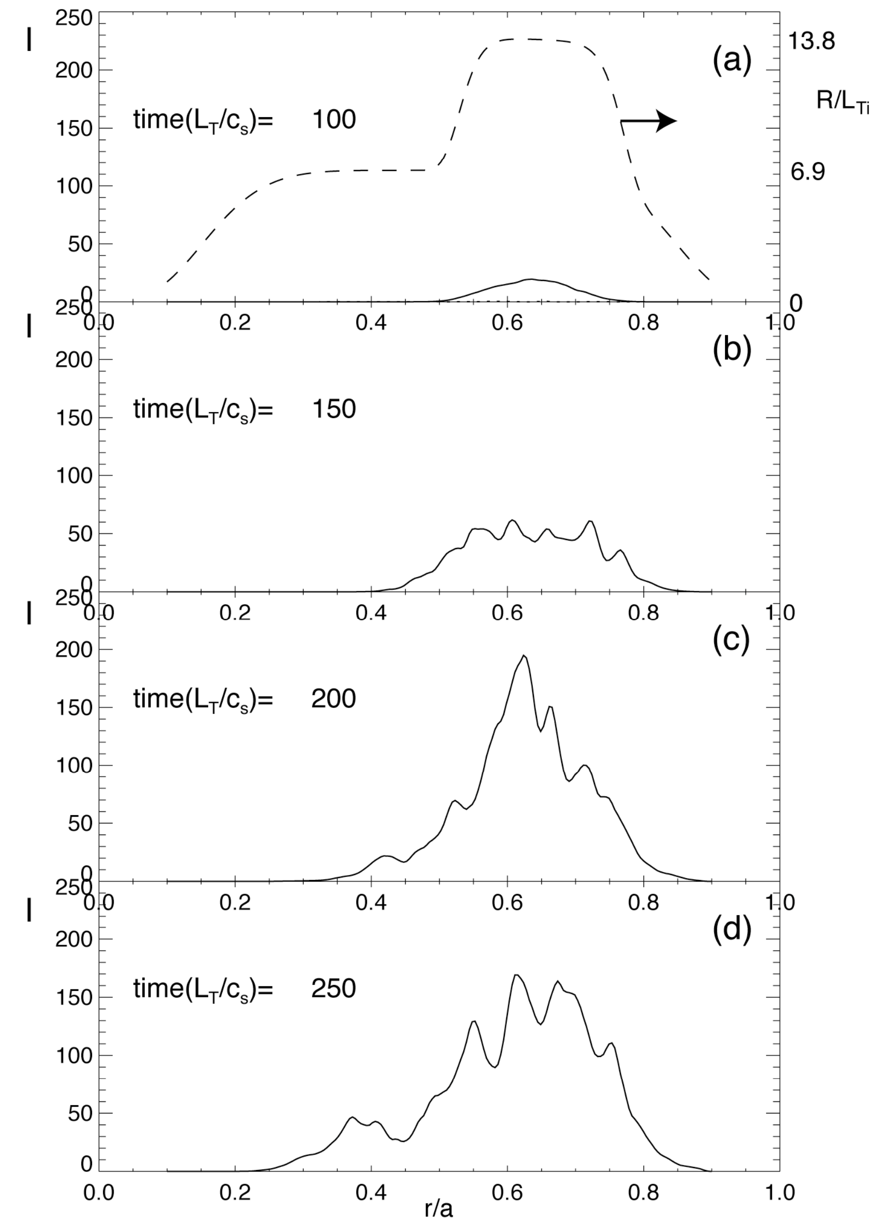
- A model nonlinear diffusion equation

$$\frac{\partial}{\partial t} I = \gamma(x) I - \alpha I^2 + \chi_0 \frac{\partial}{\partial x}\left(I \frac{\partial}{\partial x} I \right)$$

- predicts **Ballistic Front Propagation** with

$$U_x = \gamma^{1/2} \times \left(\frac{\chi_0 I}{2} \right)^{1/2}$$

- From simulation, initial turbulence growth at the edge is followed by ballistic front propagation into core
- Front speed increases with R/L_T
- Related to Sudden Core confinement improvement after H-mode transition in JET, JT-60U, … [Cordey, Neudatchin, et al., NF ‘94]



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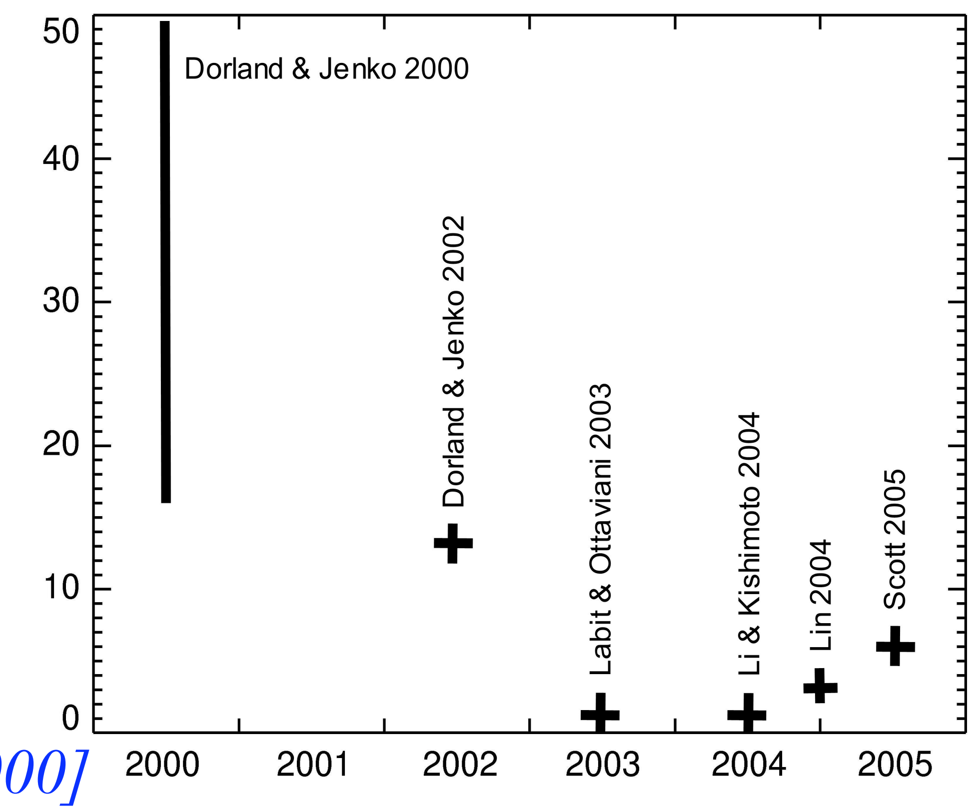
Controversy on ETG simulations



• Difference in electron thermal diffusivities with Cyclone based case using different codes in the worldwide fusion community

• Difference in saturation mechanism

-- Kelvin-Helmholtz secondary instability was conjectured as the ETG saturation mechanism *[Jenko & Dorland, PoP2000, PRL2000]*

- Radial streamers drive large transport

-- Nonlinear toroidal coupling was found to be responsible for ETG saturation *[Lin, Chen, & Zonca, PoP2005, PPCF2005]*

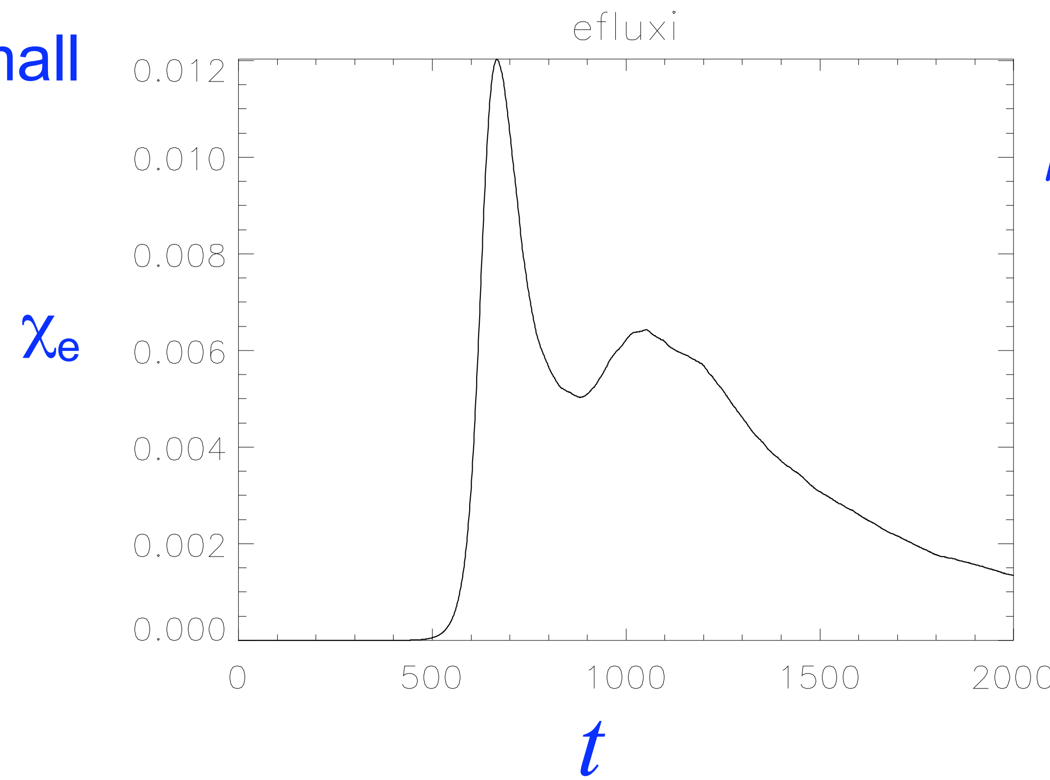
- Transport level independent of streamer length: electrons do not rotate with streamers
- Important role of long wavelength quasimodes

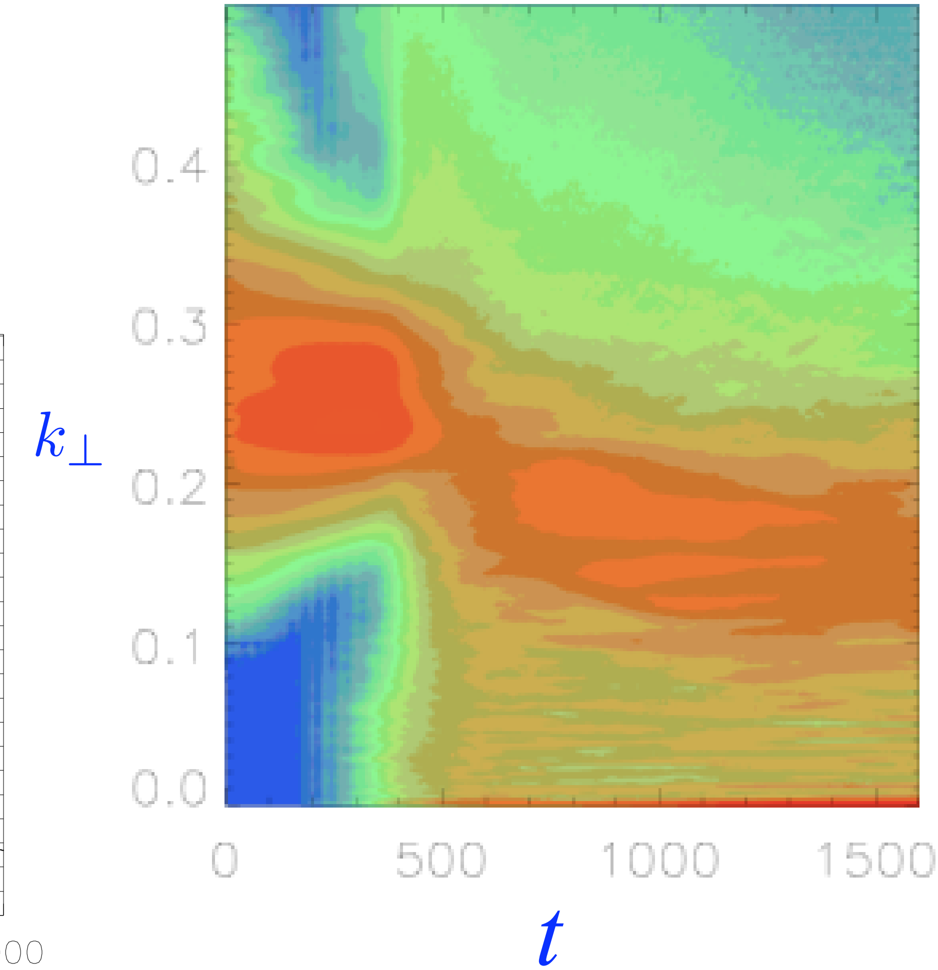
-- Recent GS2 simulation of ETG turbulence in MAST *[Joiner, Applegate, Cowley, Dorland, Roach, PPCF 48, 685 (2006)]*

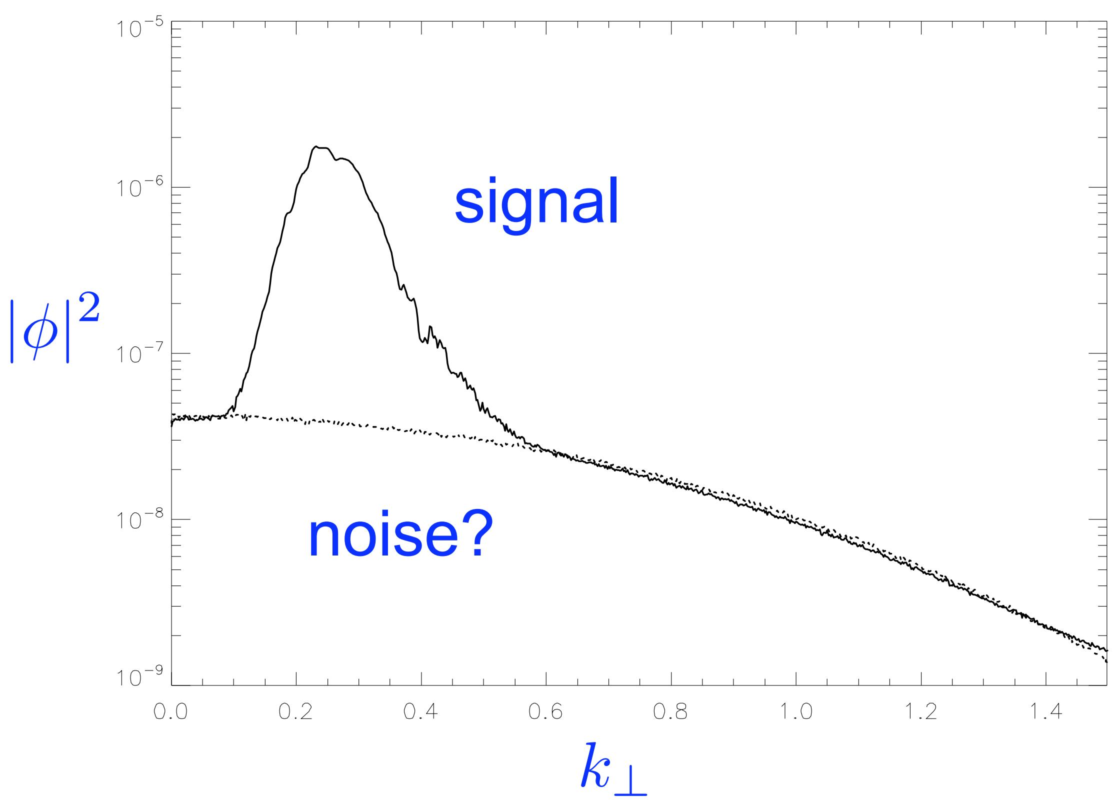
- Confirms role of long wavelength mode and nonlinear couplings
- Confirms that electron do not rotate with streamers, $\Delta r \sim 20\rho_e$
- $\chi_e \sim 3\chi_{GB}$ for s=0.3 and 2.4

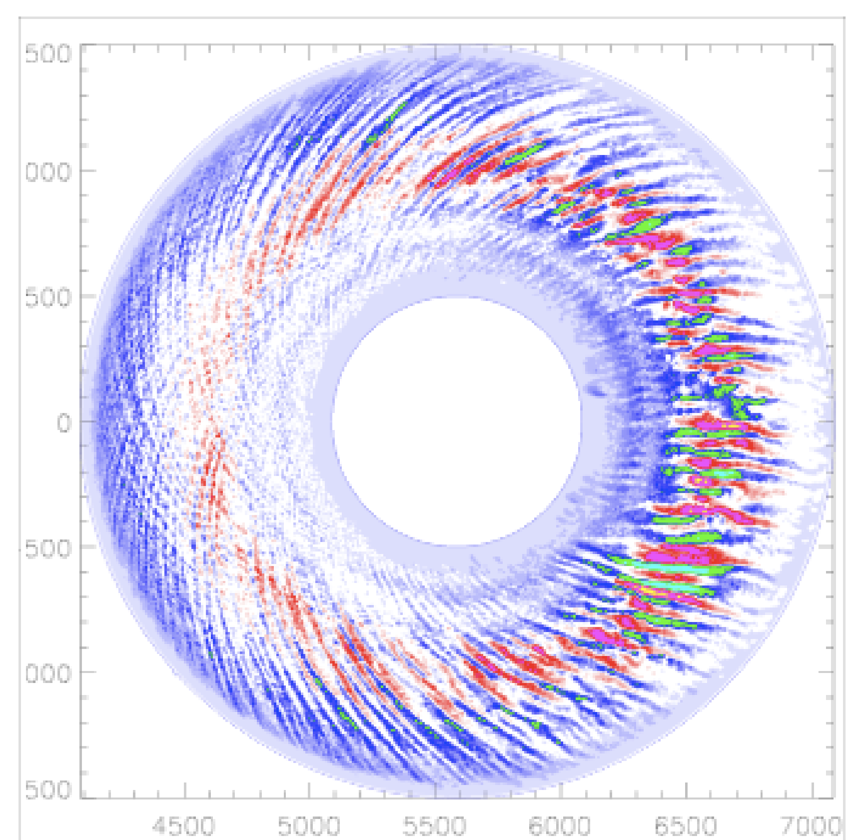
Global ETG simulations using GTC on XT3 (ORNL)

- $R/L_T=5.3$, $q=1.4$, $s=0.78$, 40-400 particle/cell
- Energy cascade to longer wavelength modes
- χ_e due to noise is small
- Streamers persist
- Why flux drops?









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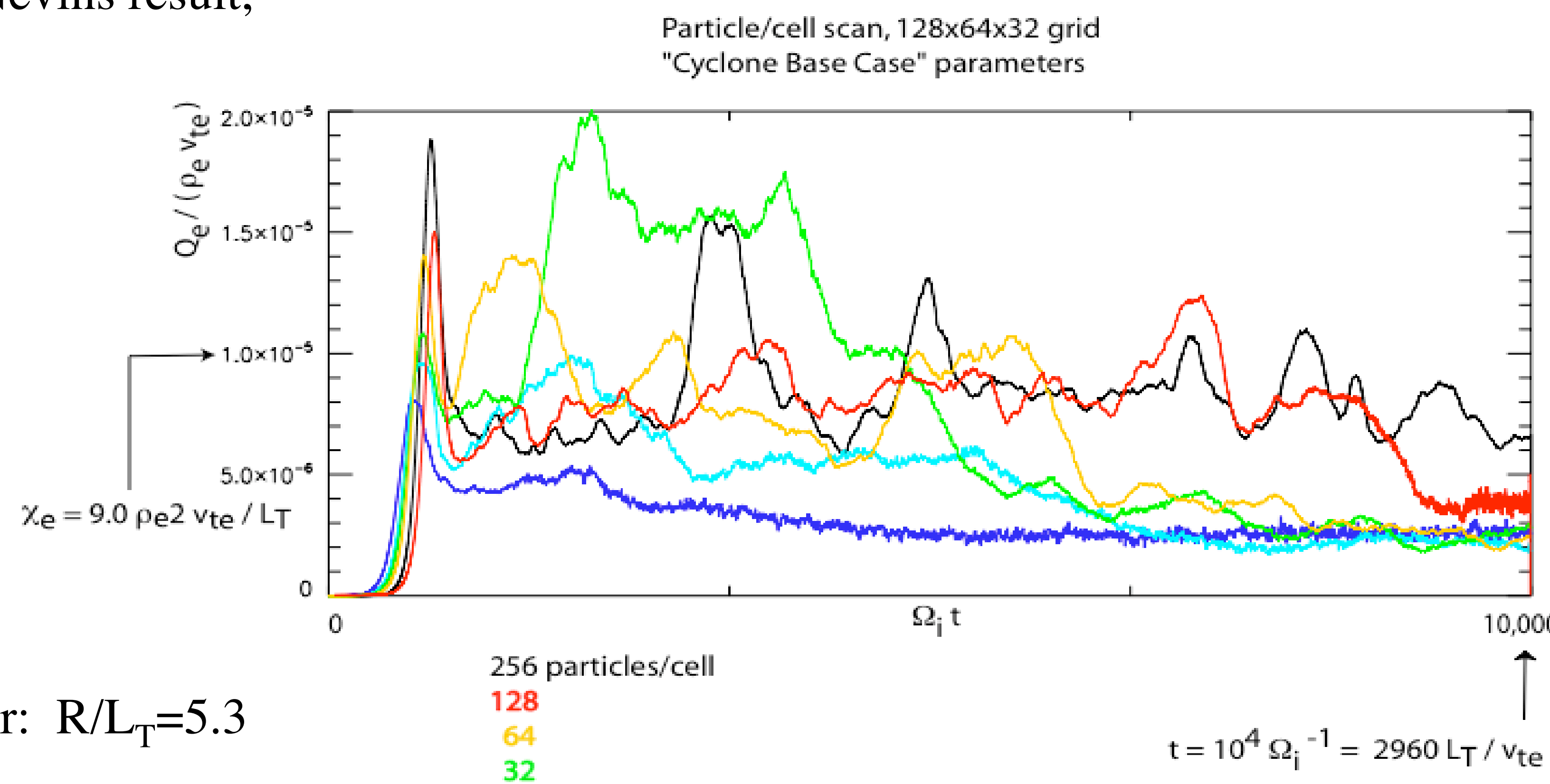
Flux-tube ETG simulations using GEM

GEM shows convergence wrt particle number: R/L_T=6.9

Qualitatively similar to Dorlan/Jenko and Nevins result, disagrees with GTC

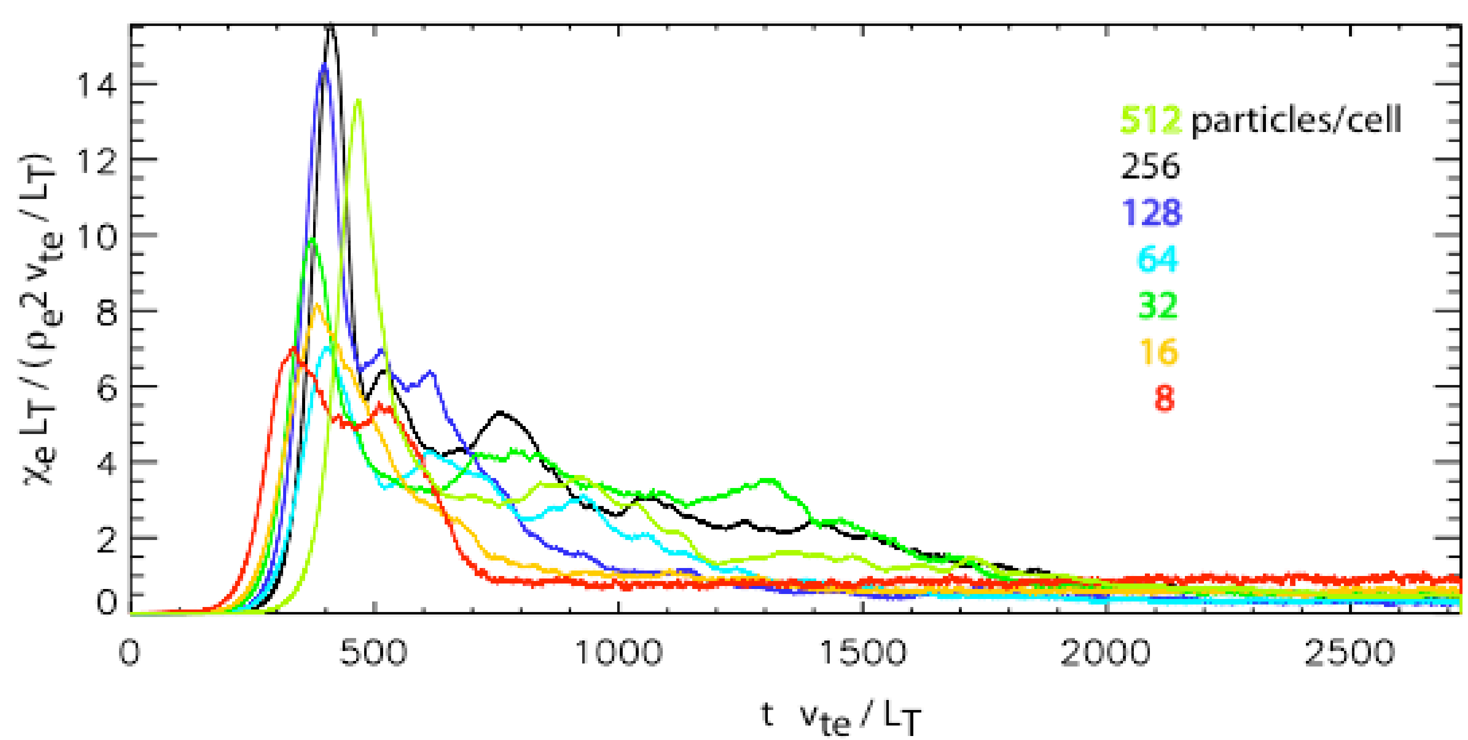


GEM shows convergence wrt particle number: R/L_T=5.3

Now agrees with GTC! What is causing the drop? It's not noise…

<u>Explanation of ETG flux drop:</u>

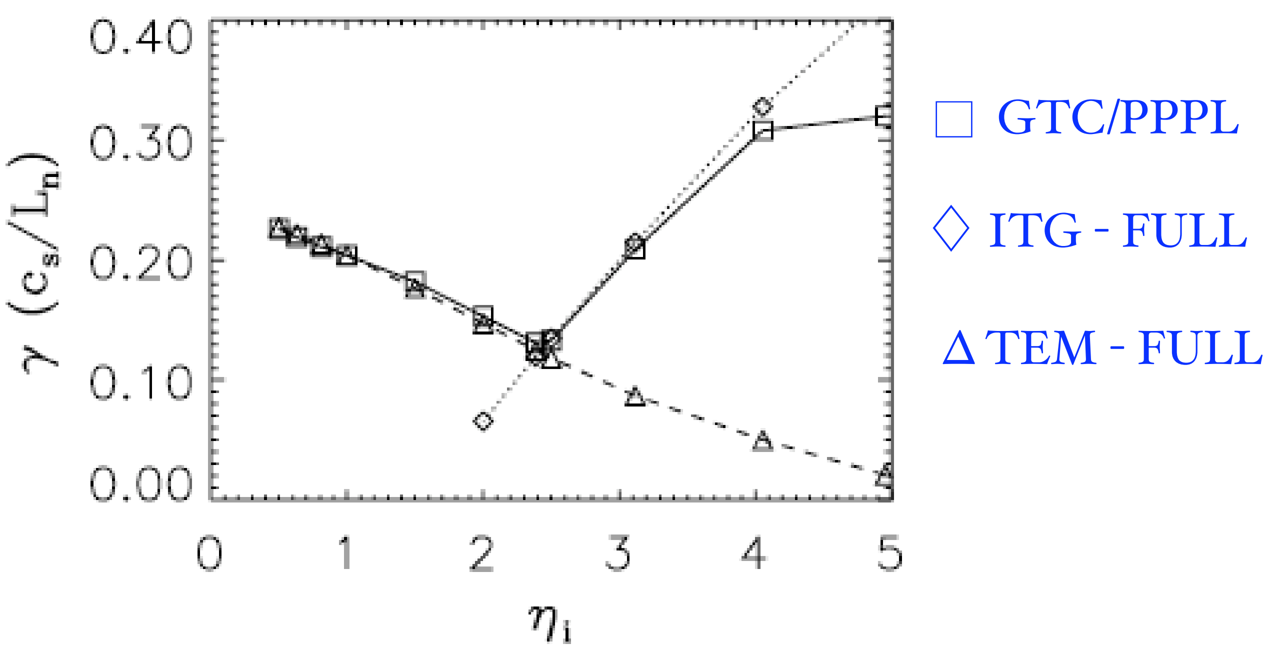
<u>Zonal flow suppression</u>

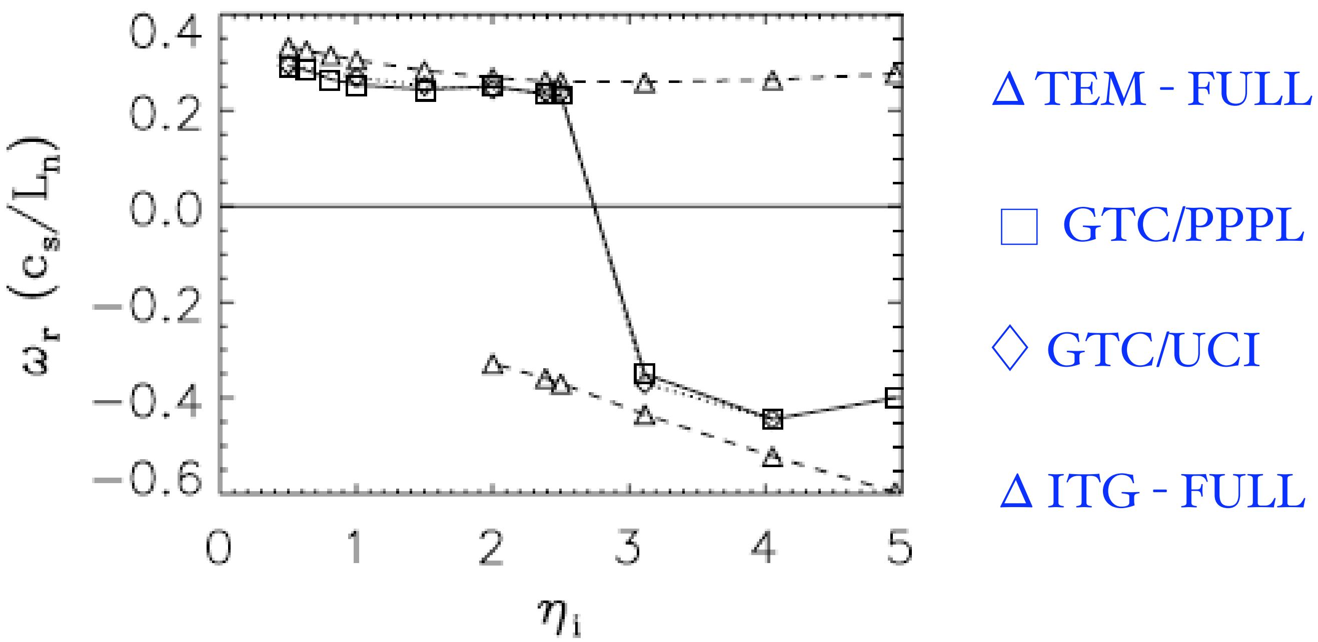


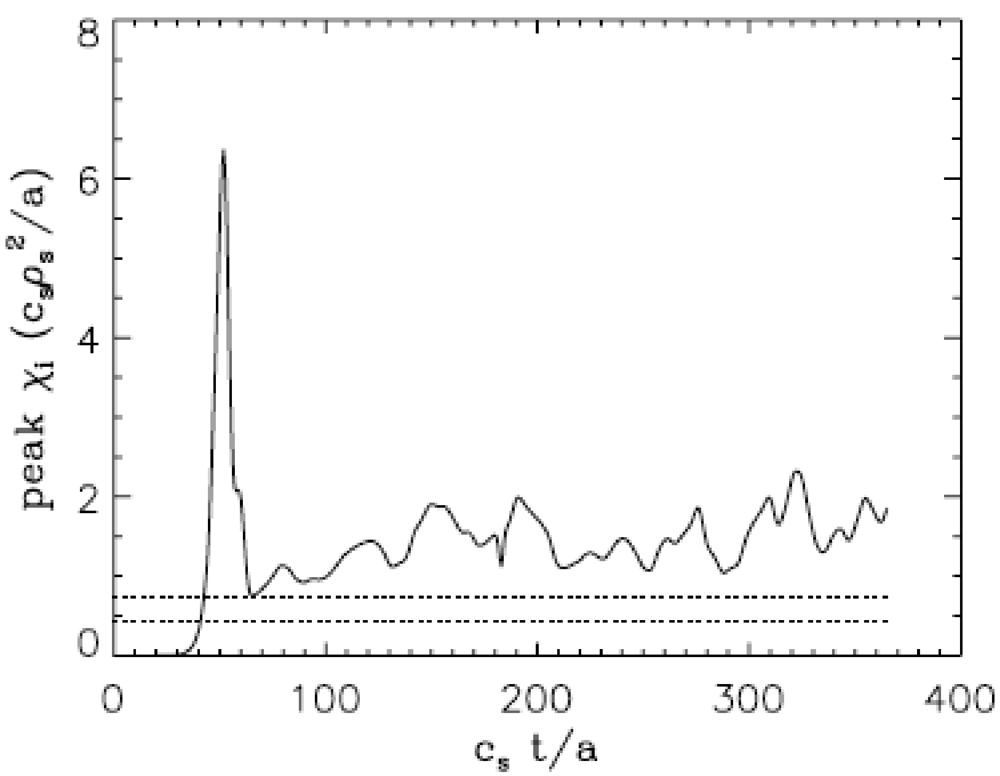
Colorado

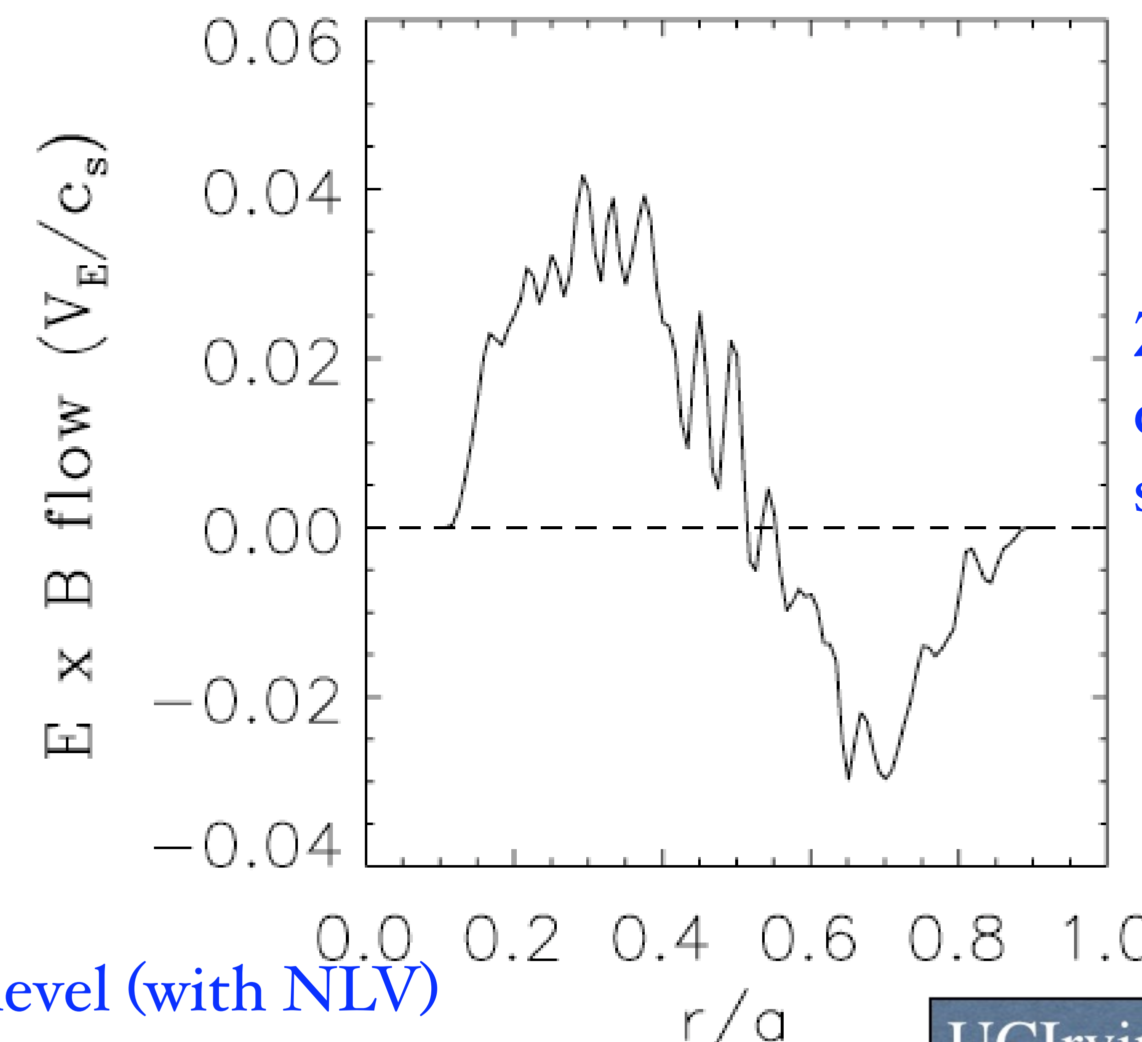
ITG & TEM modes with non-adiabatic electrons using GTC and FULL

$k_\theta \rho_i = 0.336$









Zonal flows develop finer structures

χ_i is enhanced above the adiabatic electron level (with NLV)

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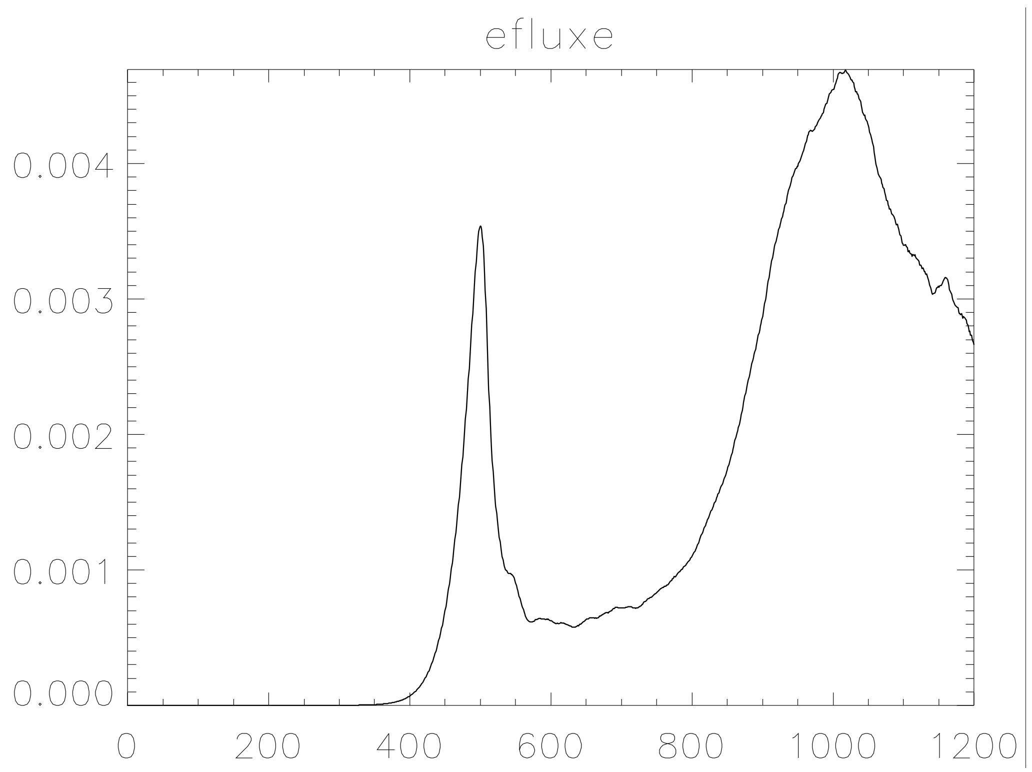
Trapped electron modes using GTC/UCI

- Short wavelength modes drive mostly electron heat flux
- Long wave modes drive significant ion heat flux and particle flux

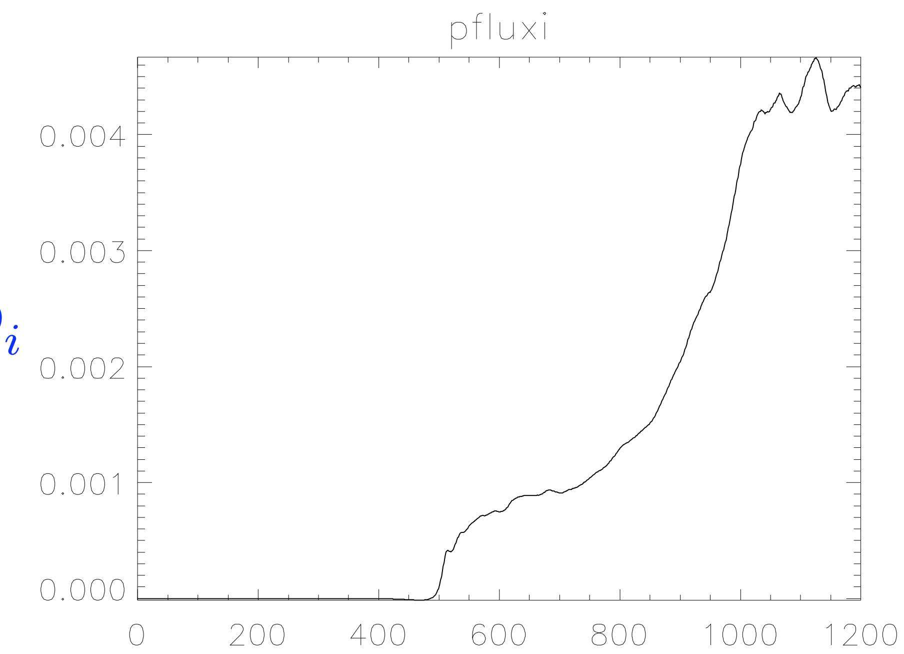
Equilibrium ω_{ExB} could suppress long wavelength modes, while short wavelength modes survive?

- Residue electron transport in ITB?



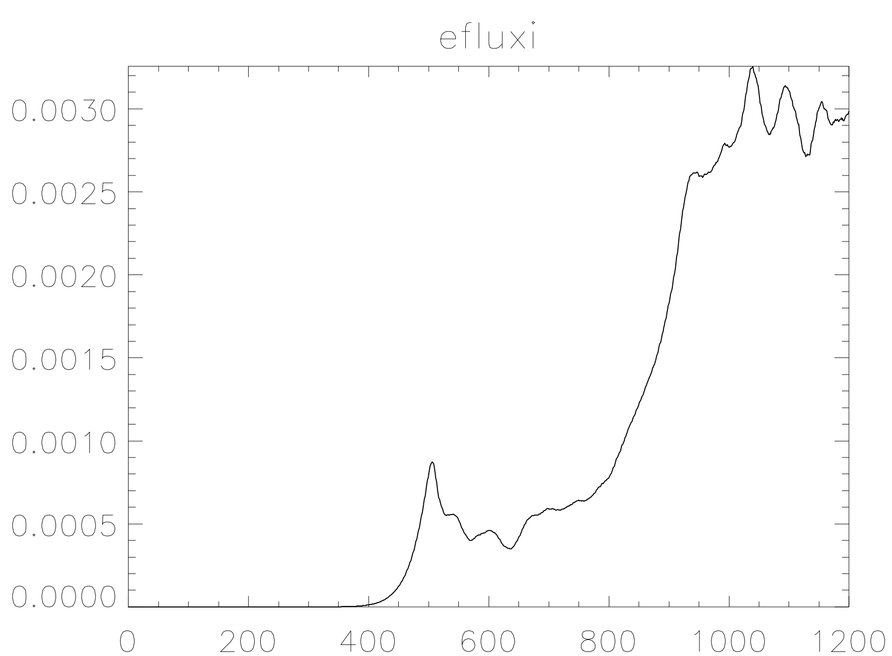
χ_e

t



D_i

t



χ_i

t

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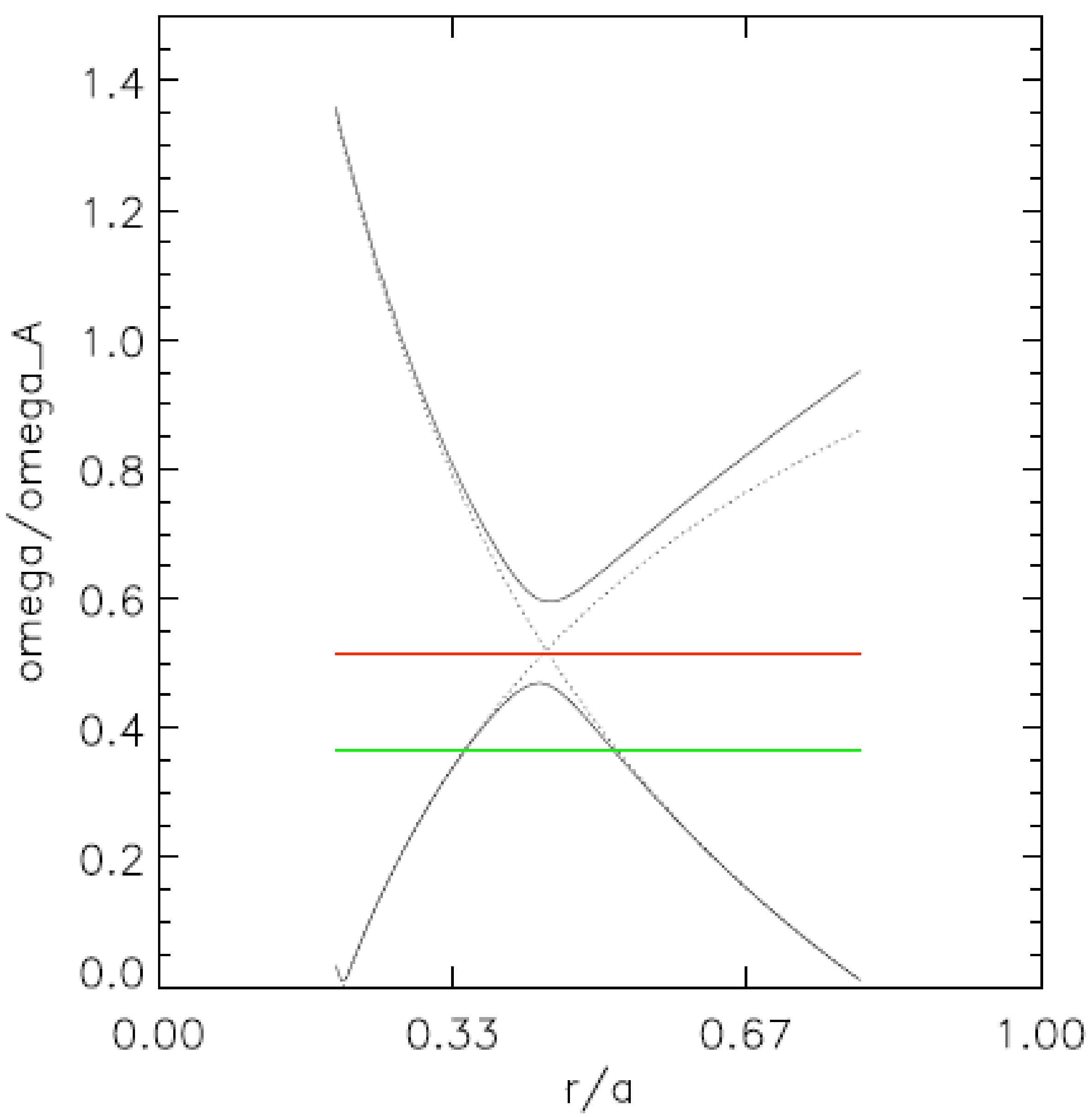
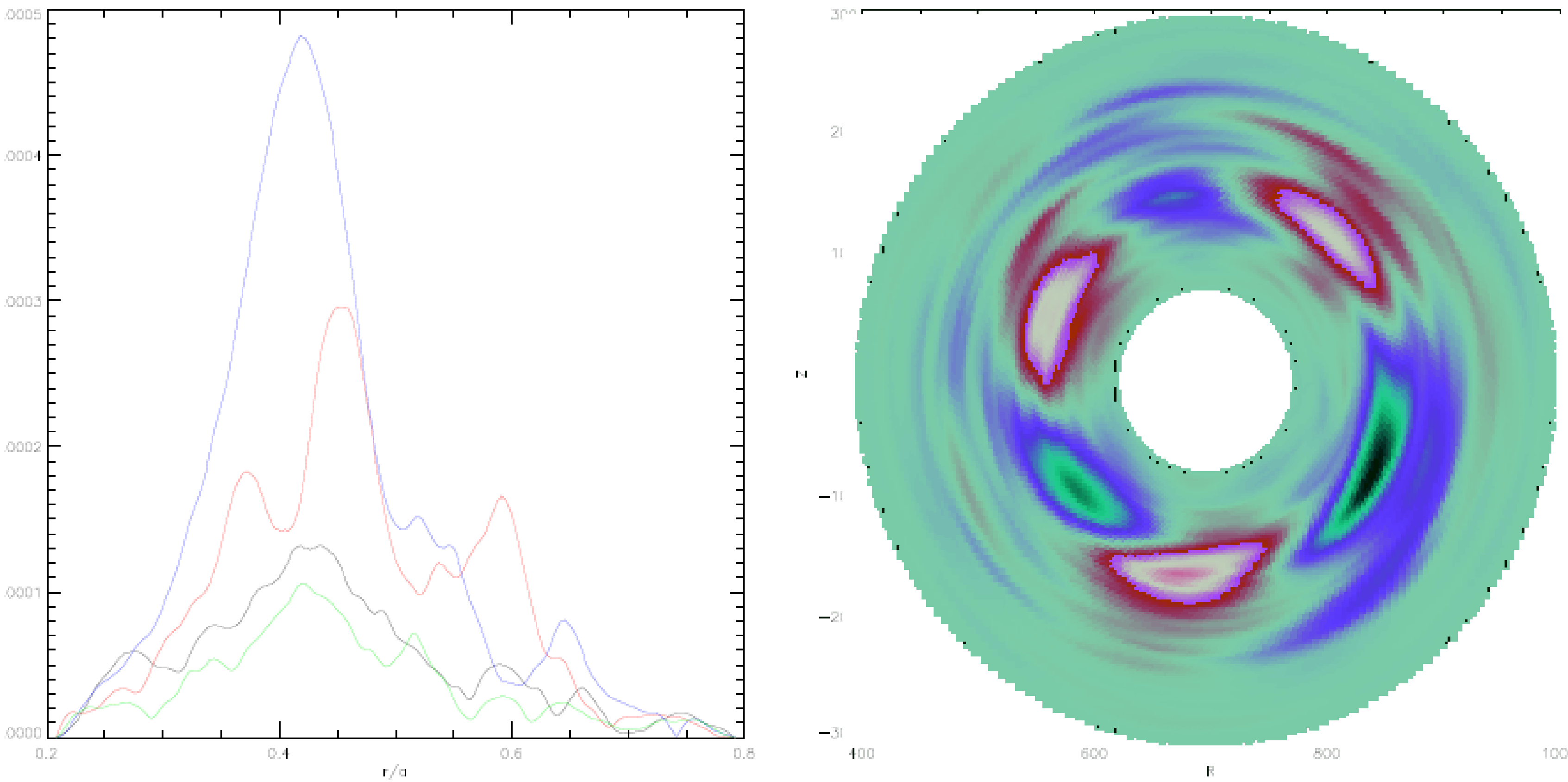
EM simulations using GEM (kinetic and zero-mass electrons)

TAE Frequency Eigenmode Observed at Low β

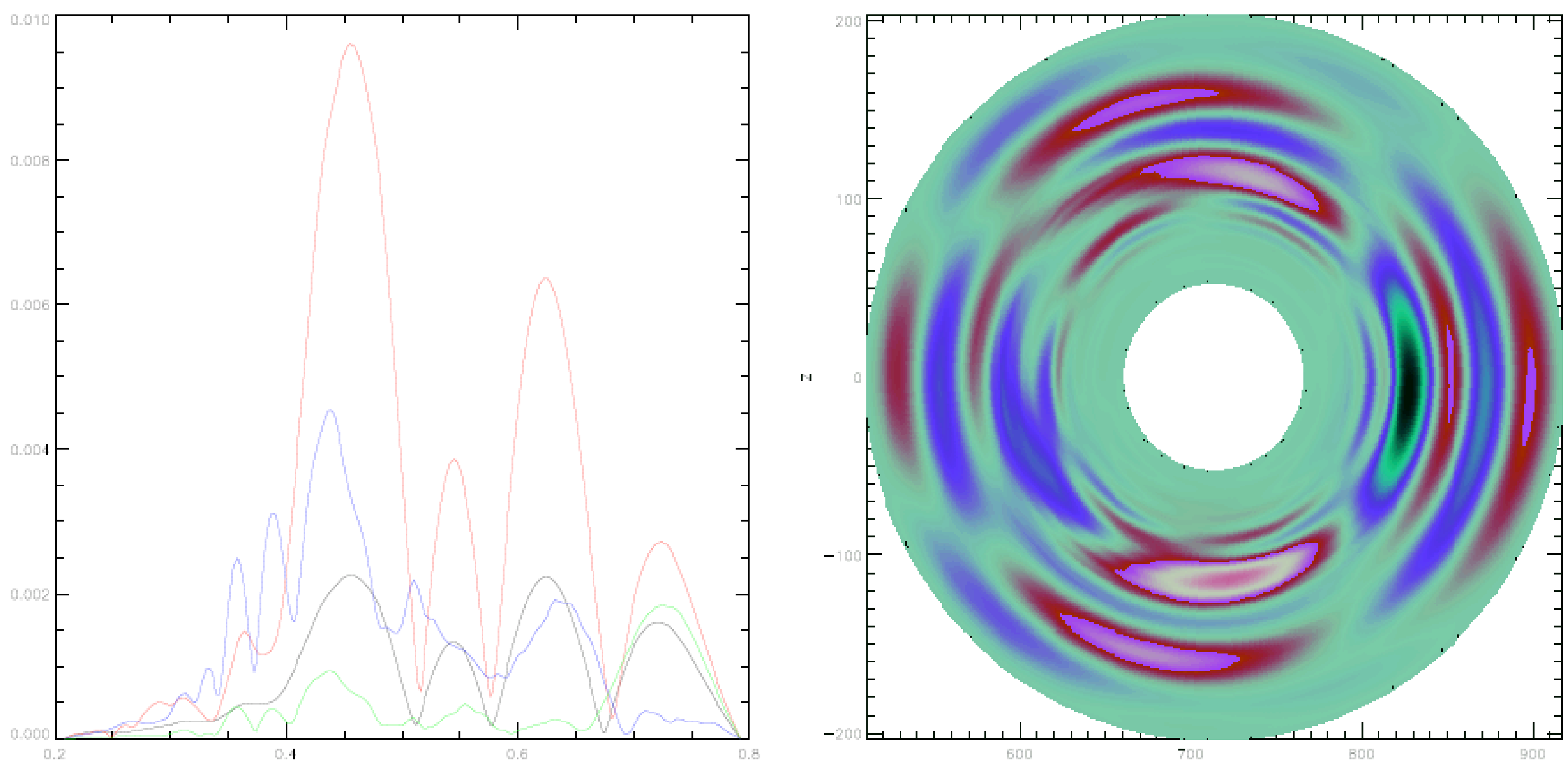
- $B_0 = 1.91T$, $T_i = T_e = 2KeV$, $1/L_T = 1/L_n = 0$, $R_0 = 1.67m$, $a = 0.36R_0$
- $q(r) = 1.3(\frac{r}{r_0})^{0.3}$, $r_0 = a/2$, $rq'/q = 0.3$
- $m_p/m_e = 500$, $m_i/m_p = 2$
- Scan over β is equivalent to changing n_0, with above parameters fixed
- Simulation domain $[0.2a, 0.8a]$.
- Add external $n = 2$ current for 200 steps, then observe the subsequent oscillation and mode structure
- Fluid electron case $E_\parallel = 0$



Mode structure–kinetic electrons



Mode structure–fluid electron

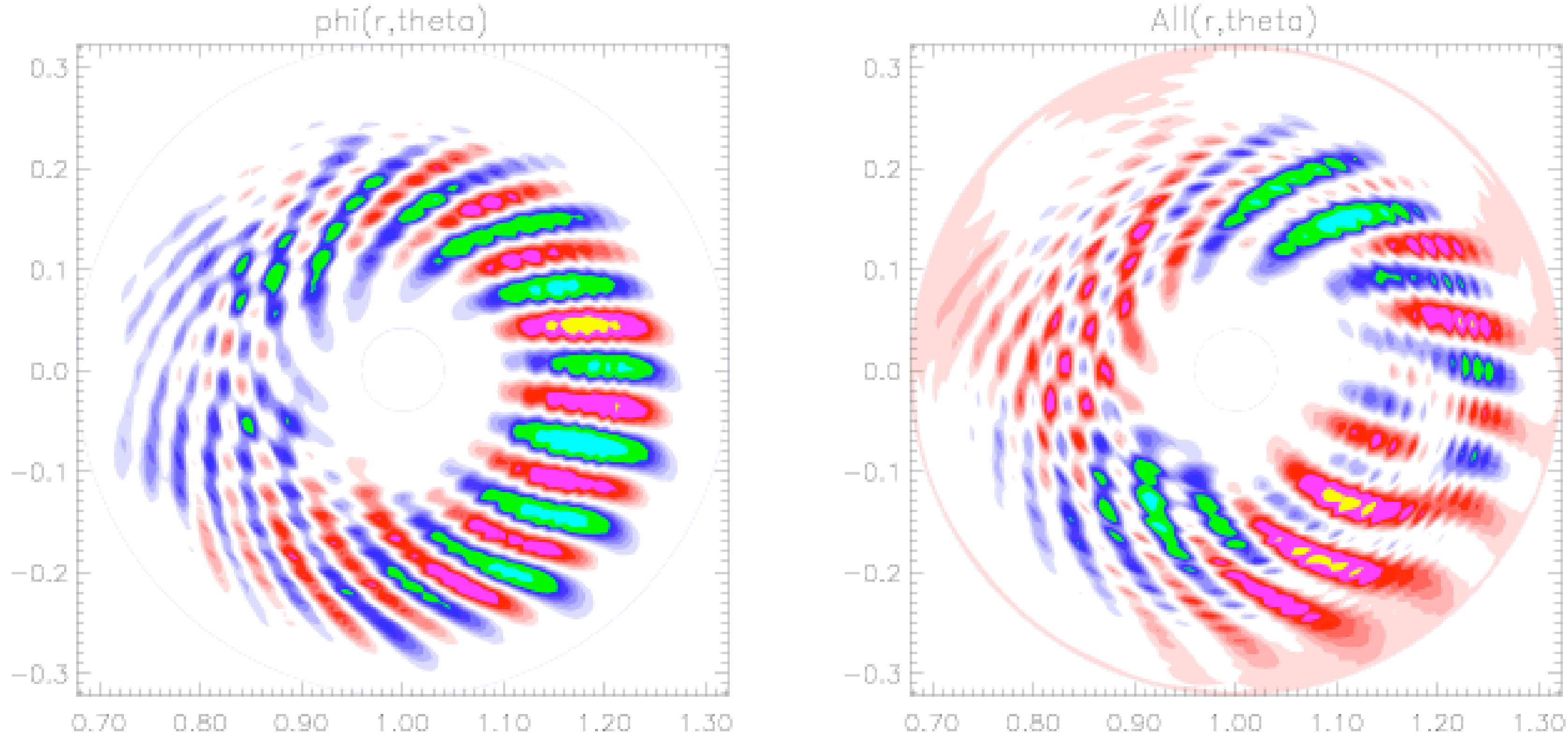


EM simulations using GEM

Colorado

EM simulations using GTC

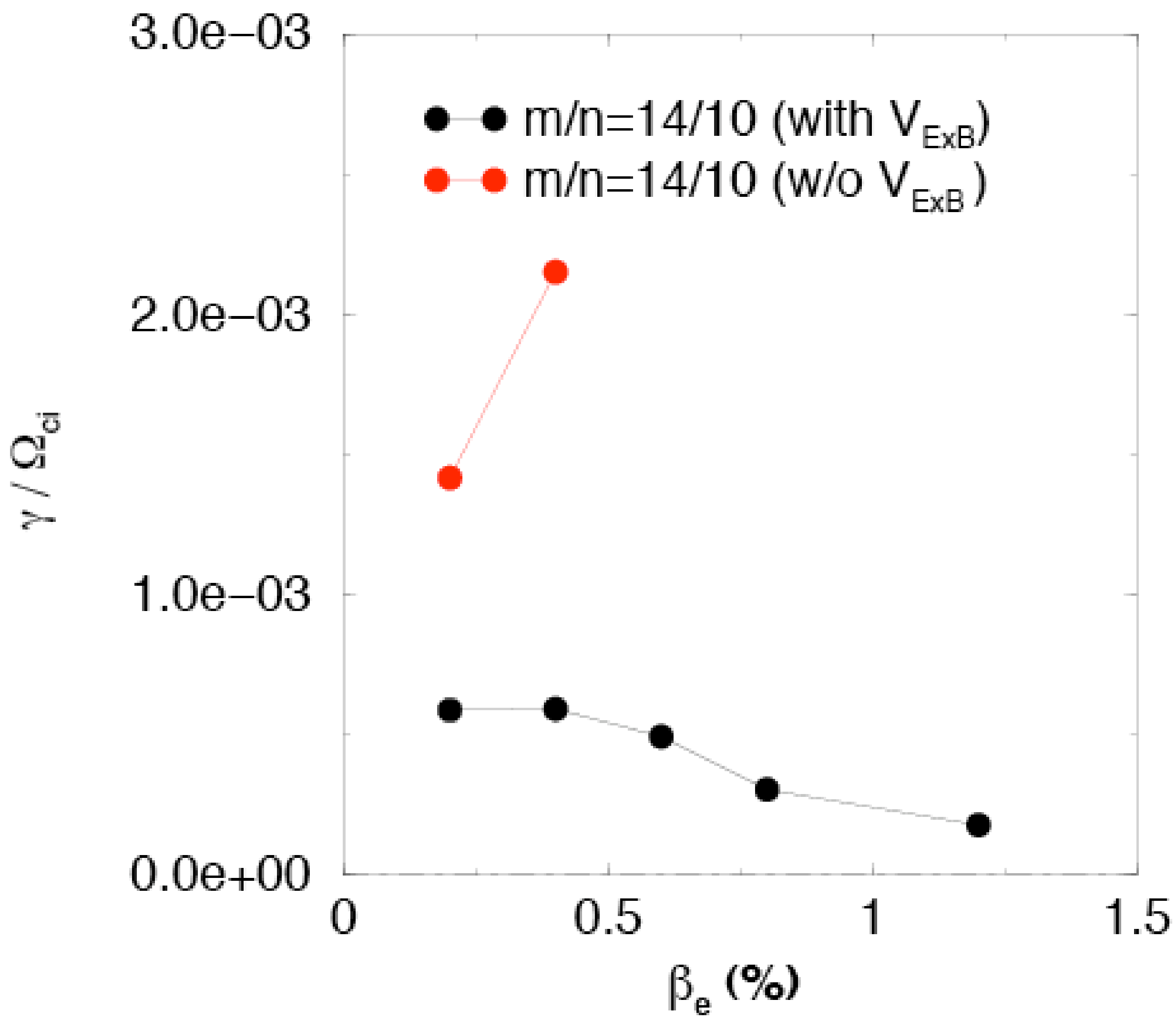
Linear global eigenmode of finite β modified ITG is obtained by using GTC



(**Left**) A Φ contour plot. (**Right**) An $A_{||}$ contour plot. Note the difference in the parity.

EM simulations using GTC

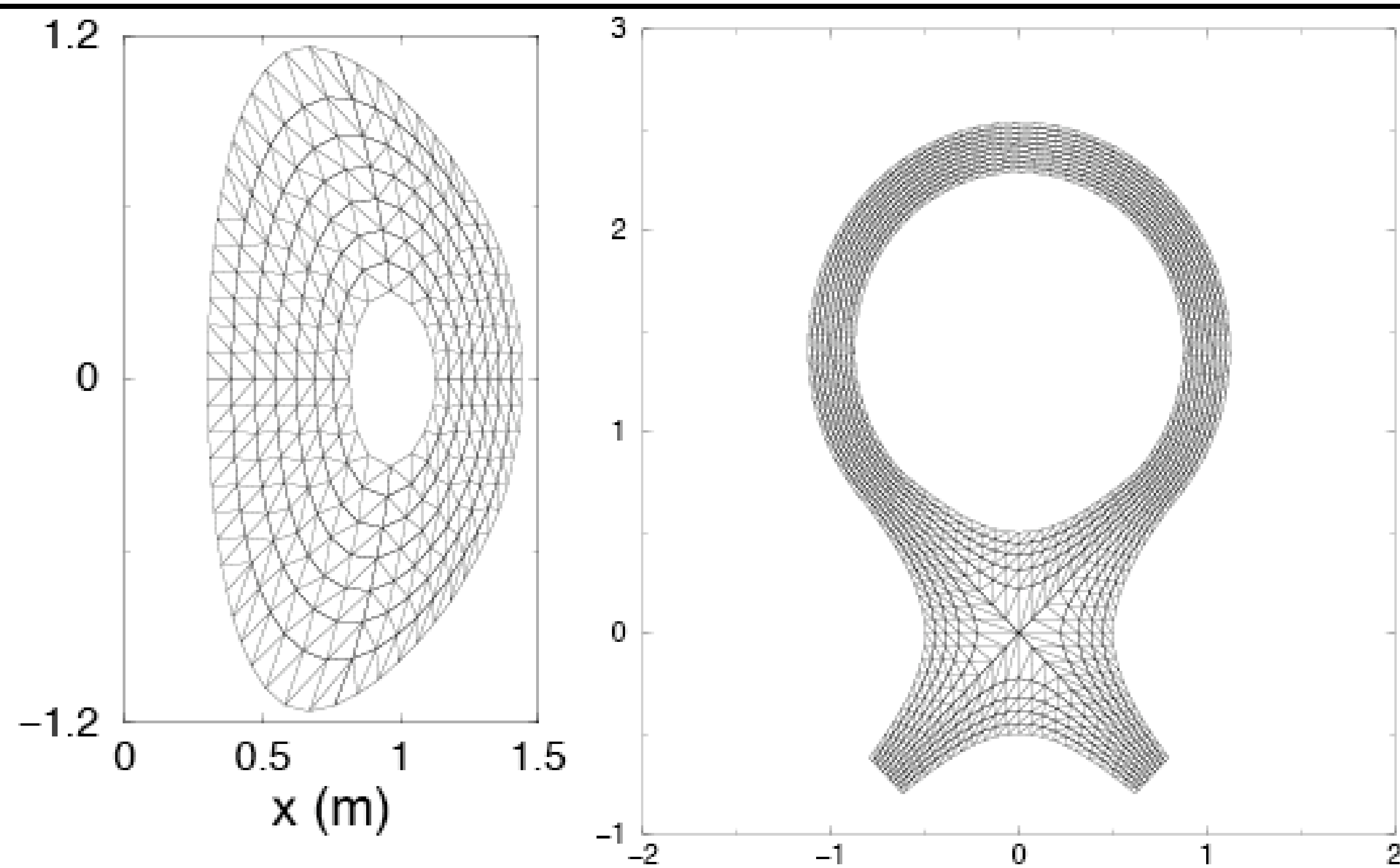
Effect of finite beta on the ITG linear growth rate is demonstrated



We expect excitations new EM branches (AITG/KBM).

UCIrvine

A finite element field solver is applied to global gyrokinetic particle code



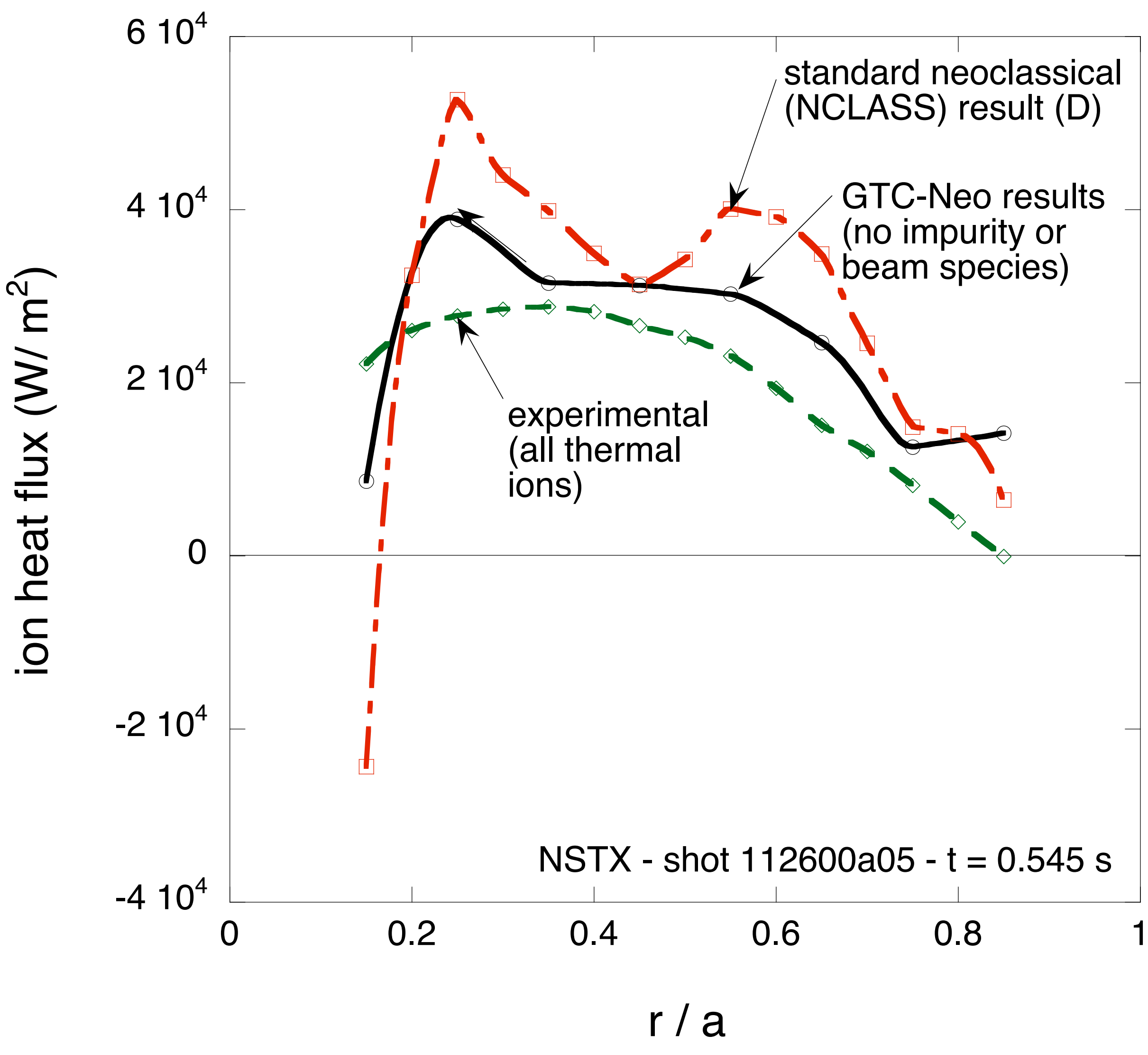
(**Left**) Patched NSTX equilibrium.[a]
(**Right**) An application to the divertor geometry.

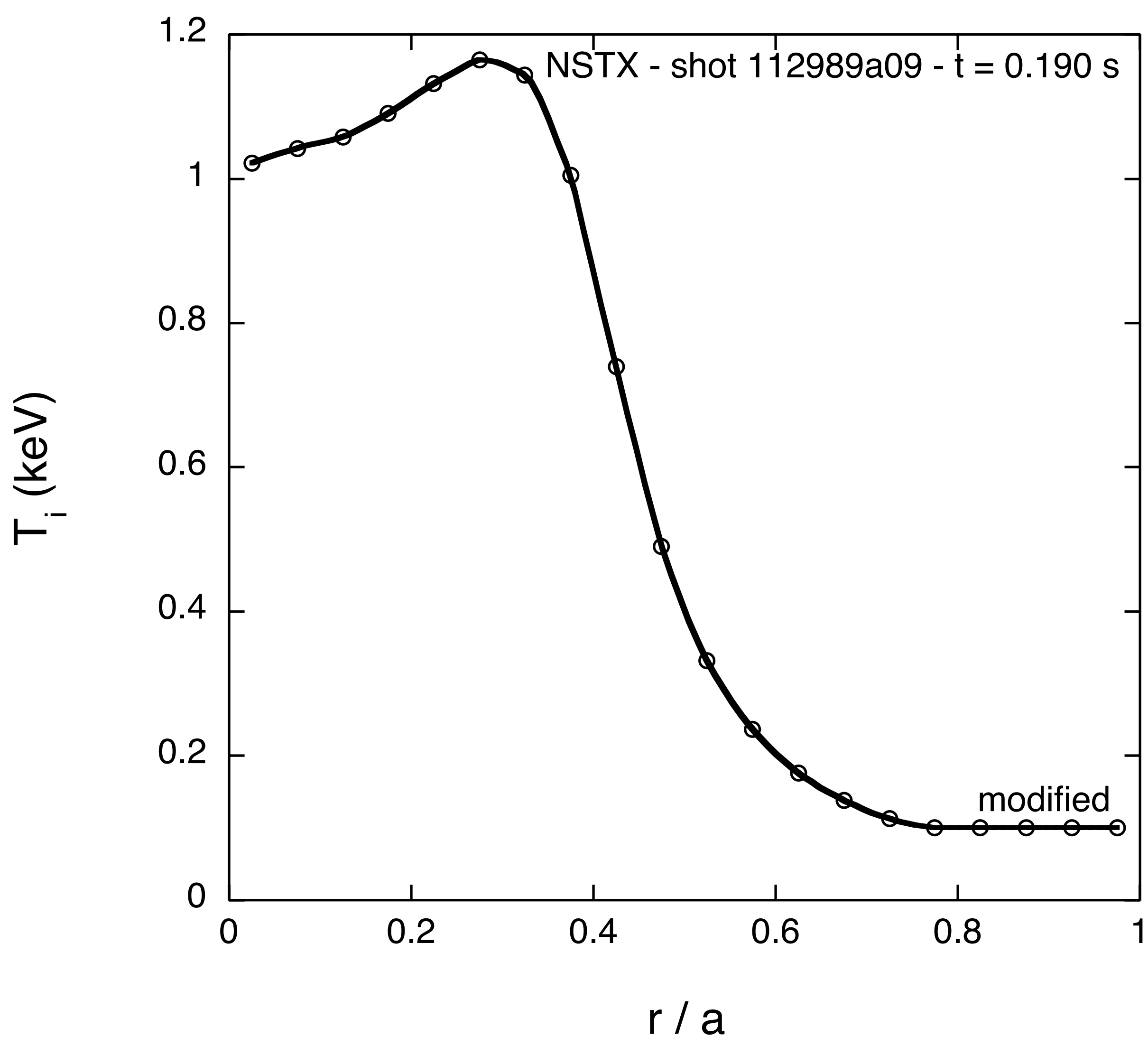
[a] By the courtesy of J.Manickam.

UCIrvine

Nonlocal Neoclassical Transport in NSTX

- GTC-neo has been used to study 12 NSTX cases and 3 D3D cases using realistic MHD equilibria
- Large orbit effects give rise nonlocal transport
- Ion heat flux q_i is outward even for a reversed local ∇T_i near magnetic axis
- Nonlocal smoothing for q_i profile





PPPL
PRINCETON PLASMA PHYSICS LABORATORY

Questions Posed by GPSC Advisory Committee Chairman

1.) What is the metric of good performance against noise, i.e. - How many particles per wavelength are needed to resolve e-phi/T of X% on scale y for time T?

2.) What sets noise and Limits Performance in Gyrokinetic-PIC simulations?

3.) How does resolution limit performance in Gyrokinetic-Continuum Codes?

4.) What aspects of drift wave physics are most likely to be obscured in noisy PIC simulations?

5.) How might we mitigate noise in PIC codes and still extract the relevant physics/

6.) What might constitute a sensible PIC GPSC research program for the coming 1-2 years?

1) For a typical fluctuation level of 1% in the steady state, we need 10,000 $k_\perp \rho_s \approx 0.2$ particles for the wave of interest and, for 0.01%, we need 100,000,000 particles for . If simulation time is too long, we need more particles.

2), 3) & 4) Need interactions between the PIC and continuum groups.

5) Particle number convergence studies.

6) See next page.

Summary

• Substantial progress has been made and more needs to be done for the competition, which is less than one year away.

• GPSC has taken the noise issue seriously and we have spent considerable amount of manpower and computing resources for that purpose for the past year.

• Because of this commitment, collisional effects, as recommended by the PSACI panel, have only been studied in conjunction with neoclassical transport.

• For the coming year
  -- more convergence studies if needed
  -- collisional and finite-beta effects in turbulence transport using GTC
  -- more case studies with GTC-neo for NSTX and D3D plasmas
  -- transport barrier physics using GTC-shaped
  -- gyrokinetic MHD physics, energetic particle physics using GTC and GEM
  -- two-dimensional domain composition for the scalar and vector potential fields
  -- preparations for ITER-type plasmas simulations in terms of physics fidelity and size.
  -- extension of Fluctuation-Dissiaption theorem to the driven cases:
    † marginal stable
    † nonlinearly saturated