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

W. W. Lee
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Princeton, NJ 08543

Presented at
PSACI PAC Meeting
June 2007

UCDAVIS UCIrvine UCLA Colorado ornl OAK RIDGE NATIONAL LABORATORY PPPL PRINCETON PLASMA PHYSICS LABORATORY

Outline

- Center Activities
  -- Fall Meeting
  -- Invited talks and Publications

- Code Development

- Code Validation

- Physics Investigations

- The noise and growing weight issues

- Conclusions

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Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas

Executive Committee
W. W. Lee
D. E. Keyes
Z. Lin
S. E. Parker
C. Bolton, ex-officio

Principal Investigator
W. W. Lee

Program Advisory Committee
P. H. Diamond
R. Nazikian
J. Connor
Y. Kishimoto

GTC team
Z. Lin

Theory Collaboration & Experimental Liaison
T. S. Hahm
L. Chen, G. Rewoldt

GEM team
S. E. Parker

Physics Module
Z. Lin (lead)
J. Lewandowski
Y. Nishimura
W. X. Wang
I. Holod

Elliptic Solver
M. Adams (lead)
J. Lewandowski
Y. Nishimura

Parallelization & Code Maintainence
S. Ethier (lead)
V. Decyk

Data Management & Postprocessing
S. Klasky (lead)
M. Beck
K.-L. Ma

Physics Module
Y. Chen (lead)

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FALL MEETING

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

Room 407-408
Philadelphia Marriot Hotel, Philadelphia, PA

November 2, 2006

7:00P Lee - Opening remarks

7:10P Wang - Shaped plasma simulations and future plans

7:25P Ethier - GTC performance and optimization issues

7:40P Lin - Status and plan in global GTC turbulence simulation

7:55P Nishimura - Shear Alfven wave studies in electromagnetic global gyrokinetic simulation of tokamak plasmas

8:10P Parker - ETG Convergence Studies, GEM Team status

8:25P Y. Chen - The growing weight problem

8:40P Rewoldt -- Application of GEM code for experimentally-realistic tokamak cases

8:55P Hahm - Theory team status and plan

9:10P Coffee break

9:25P Holod - Particle noise-driven flux in GTC simulations

9:35P Xiao - Theory of zonal flow residual level with arbitrary wavelength and collisionality

9:45P Jenkins – Particle noise issues

9:55P Diamond – Concluding remarks

10:05P Klasky - Data Management, Visualization and MPP issues

10:15P Plans for re-competition

11:15P Recess

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Invited Talks and Review Papers

• Wang, W.X., T.S. Hahm, G. Rewoldt, J. Manickam and W.M. Tang, "Gyrokinetic studies of Nonlocal Properties of Turbulence-driven and Neoclassical Transport", 21th IAEA Conference on Plasma Physics and Controlled Nuclear Fusion Research, (Chengdu, China, 2006)

• Lee, W.W., S. Ethier, T. G. Jenkins, W. X. Wang, J. L. V. Lewandowski, G. Rewoldt, W. M. Tang, S. E. Parker, Y. Chen, and Z.Lin, 21th IAEA Conference on Plasma Physics and Controlled Nuclear Fusion Research, (Chengdu, China, 2006)

• Lee, W.W., S. Ethier, W. X. Wang, W. M. Tang and S. Klasky, "Gyrokinetic particle simulation of fusion plasmas: path to petascale computing", Presented at SciDAC 2006, Denver CO., J. of Phys.: Conference Series **46**, 73 (2006).

• Brizard, A.J., and T.S. Hahm, "Foundations of Nonlinear Gyrokinetic Theory", Rev. Mod. Phys. **79**, 421 (2007).

Publications

Review of Modern Physics: 1
Physics of Plasmas: 11 published, 2 submitted
Journal of Computational Physics: 2 published
IAEA: 4 published
Other Journals: 3 published
Conference Proceedings: 11 published

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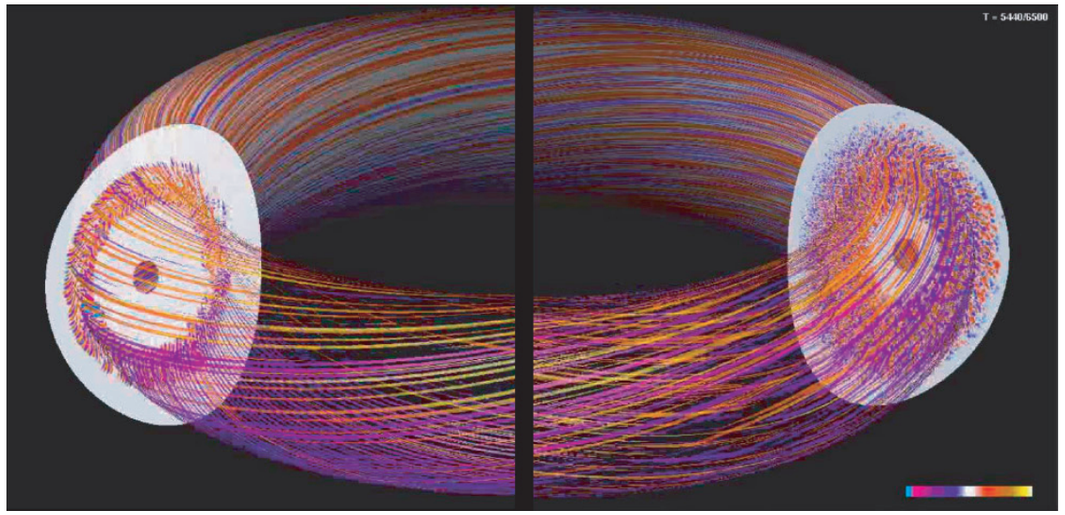
Code Development

- GTS
  - -- A global code for turbulence transport simulations
  - -- Shaped plasma in general geometry interface with TRANSP, JSOLVER and ESC
  - -- Electron dynamics based on the split-weight scheme: delta δh, non-adiabatic part of δf
  - -- GK Poisson's equation is solved simultaneously for zonal flows and perturbed potentials

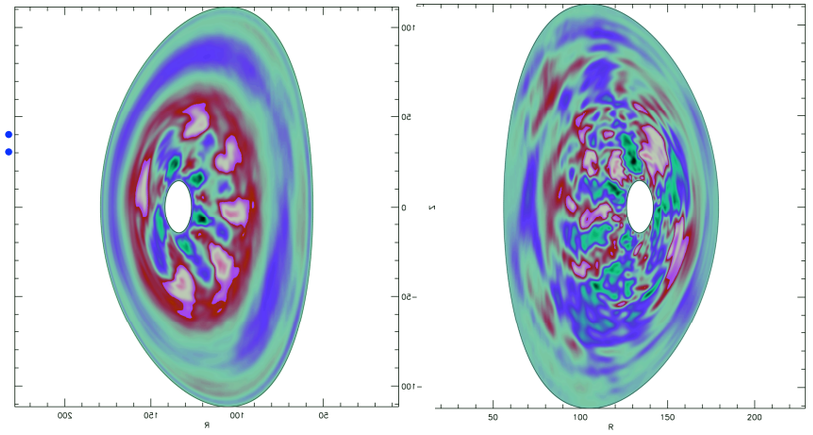


GTS

- GTC
  - -- Adiabatic electron version for high performance computing
  - -- Electrostatic electron dynamics based on the hybrid scheme
  - -- Electromagnetic electron dynamics based on the hybrid scheme:

$$|\omega/k_{||}v_{||}| \ll 1$$

- GTC-neo -- For neoclassical transport simulations in
  - -- General toroidal geometry
  - -- Fully operational collision operators



GEM

- GEM
  - -- A wedge code with multi-ion species for turbulence and gyrokinetic MHD simulations
  - -- Shaped plasma in general geometry with interface with TRANSP and JSOLVER
- Object Oriented GTC framework -- Based on Fortran-90 to facilitate team coding

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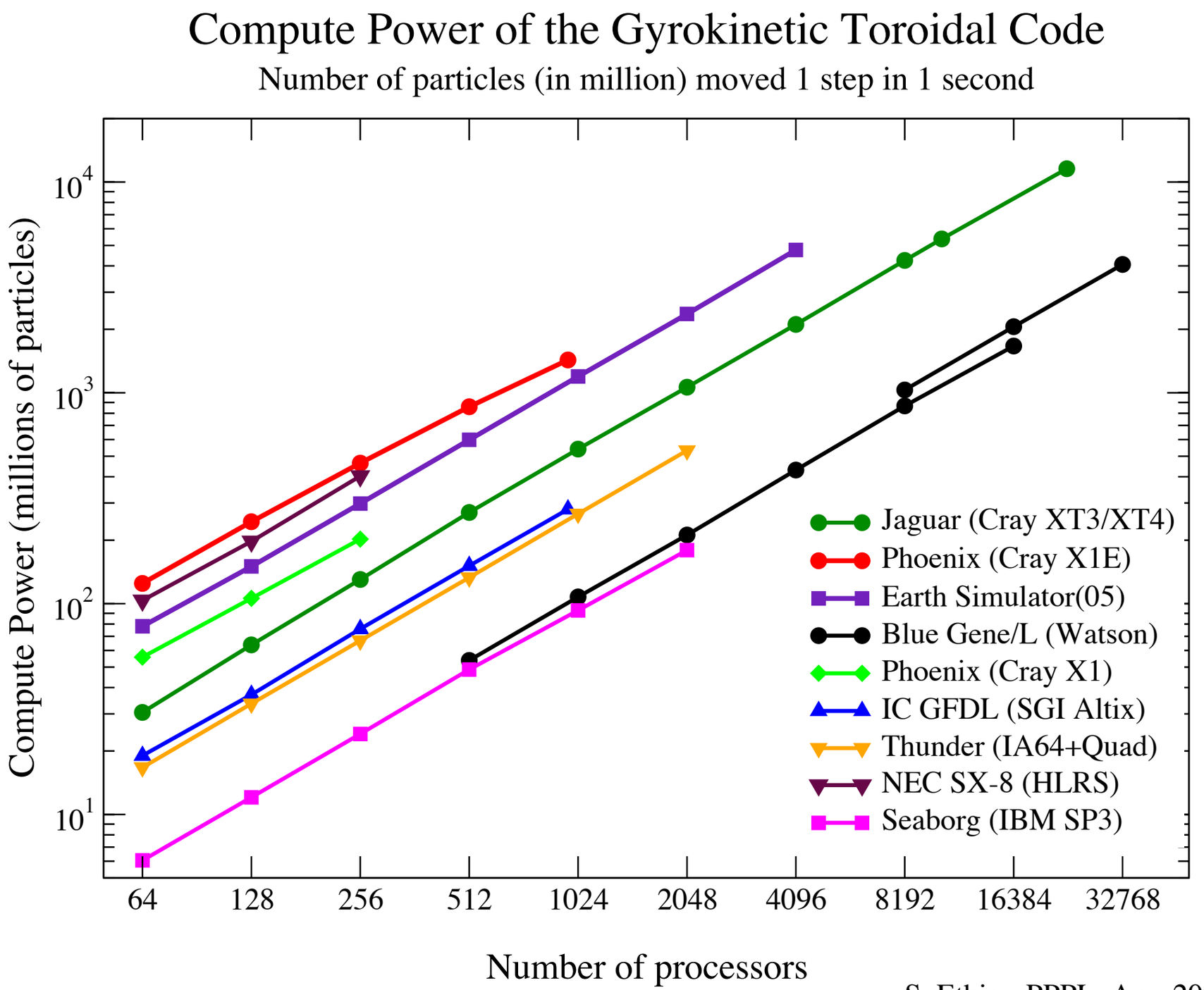
GTC performance on MPP platforms aiming for ITER-size Plasmas

- GTC is very portable, scalable and efficient on both cache-based and vector-parallel MPPs.
- 20 TeraFlops/sec performance has been achieved with 74 billion particles on Jaguar (ORNL) with 22,976 cores and 2.8 times faster than with 32,786 BG/L cores



Joule Applications & 250 TF campaign at ORNL

S. Ethier, PPPL Apr. 2007

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Numerical Considerations for Gyrokinetic Simulation Codes

- Flux Tube codes are valid for large (m, n) modes
- Wedge codes include radial variations and some are valid only for large (m,n) modes
- Global codes are valid for any (m, n) modes and are truly five dimensional
- Physics of turbulence transport alone dictates the the usefulness of these codes, i.e.,

  -- are radial modes local or global?

  -- does energy cascade to lower or higher (m, n) modes ?

-- how about enstrophy, to higher (m,n) modes?

-- perpendicular spatial resolution: ion gyroradius, electron skin depth or electron gyroradius?

-- parallel spatial resolution: field line following coordinates?

-- velocity space resolution?
- √ trapped particle dynamics
- √ wave-particle interactions
- √ artificial dissipation
- √ discrete particle noise

-- collisions: can neoclaasical transport be simulated?

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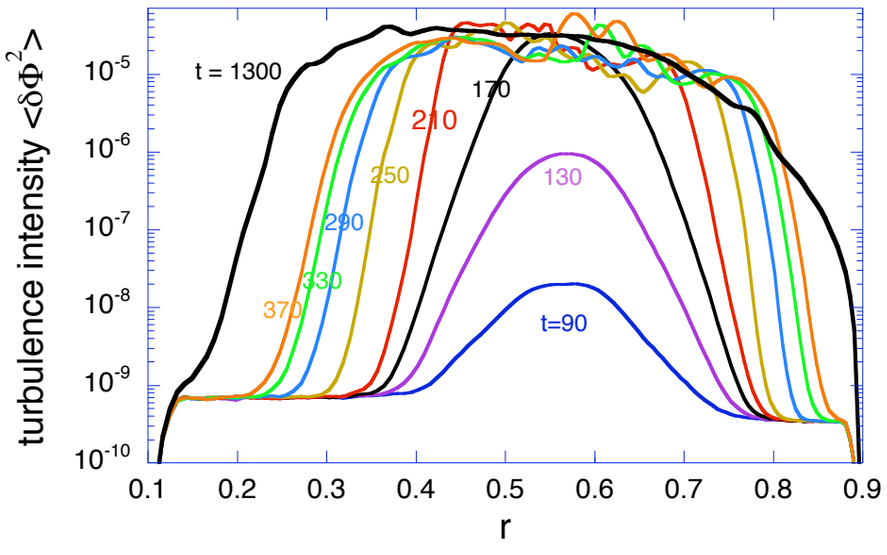
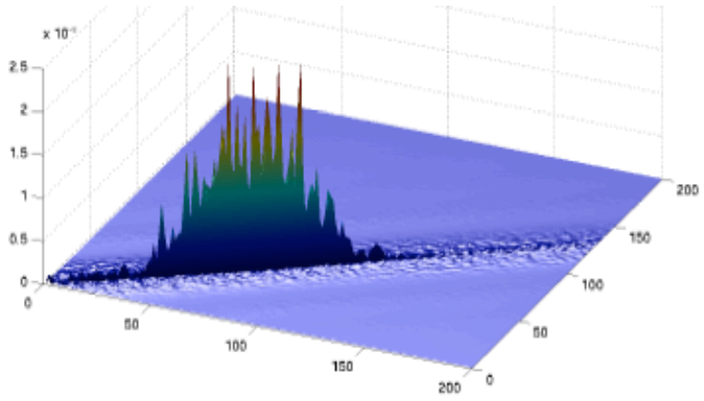
General Geometry GTS
W. X. Wang [PoP '06]

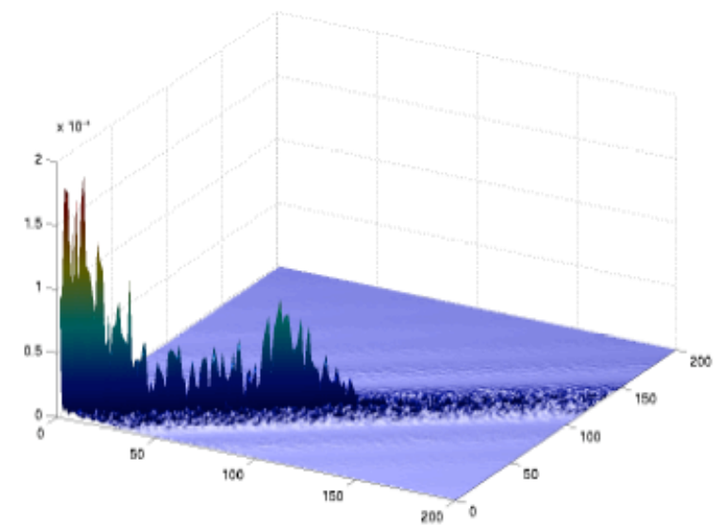
- **Global Turbulence Dynamics in Shaped Plasmas**
- **Interfaced with TRANSP and JSOLVER and ESC**
- **Re-Write of GTC**

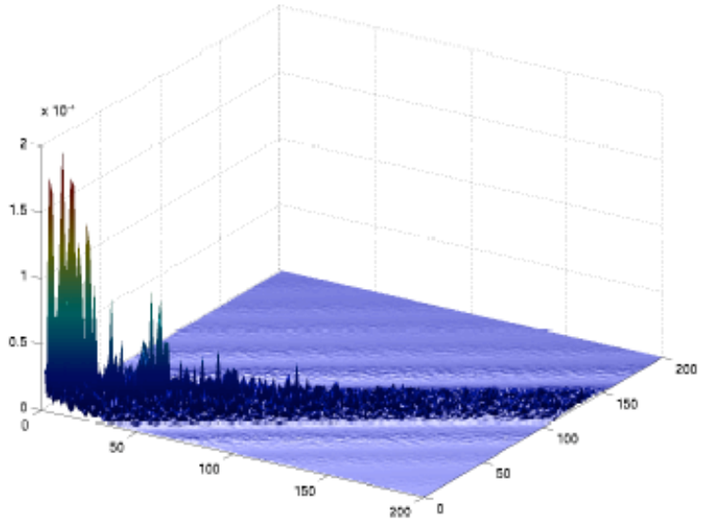
ITG Turbulence Spreading



ITG Energy Cascade to longer wavelength modes

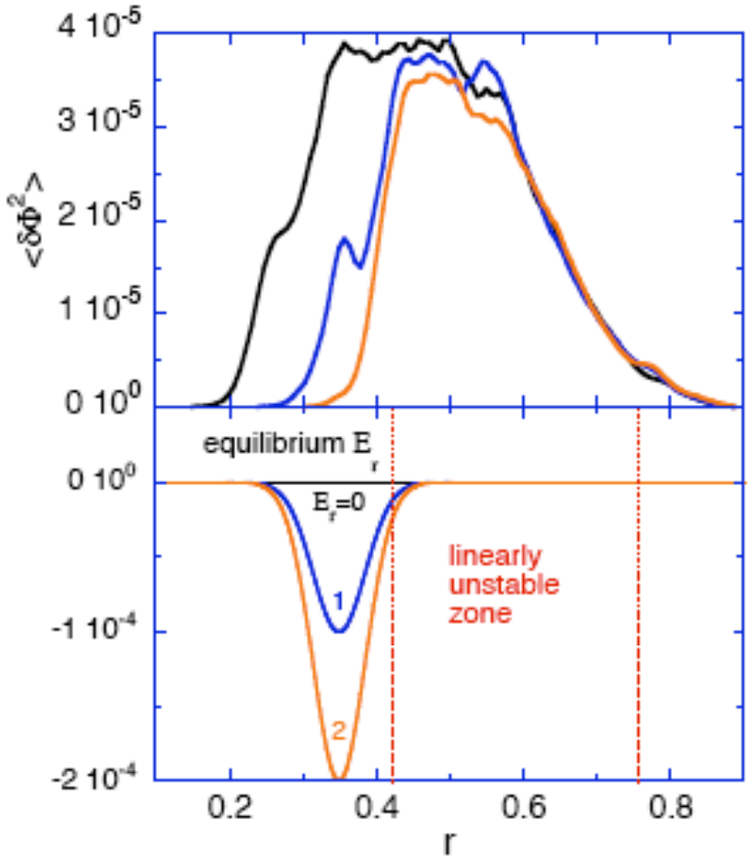


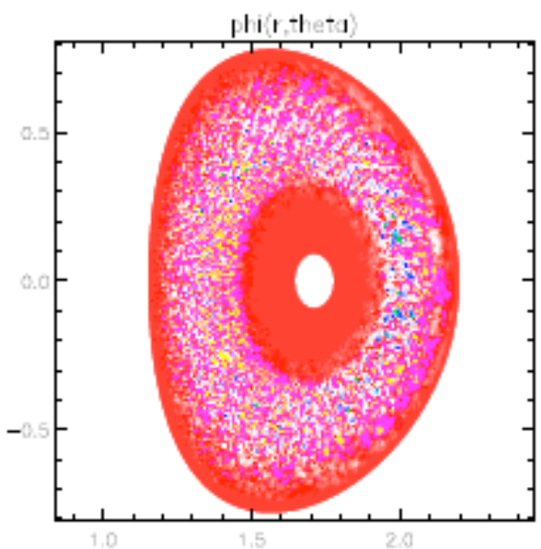




Turbulent transport is a global phenomena

$E \times B$ 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

W. X. Wang - GTS

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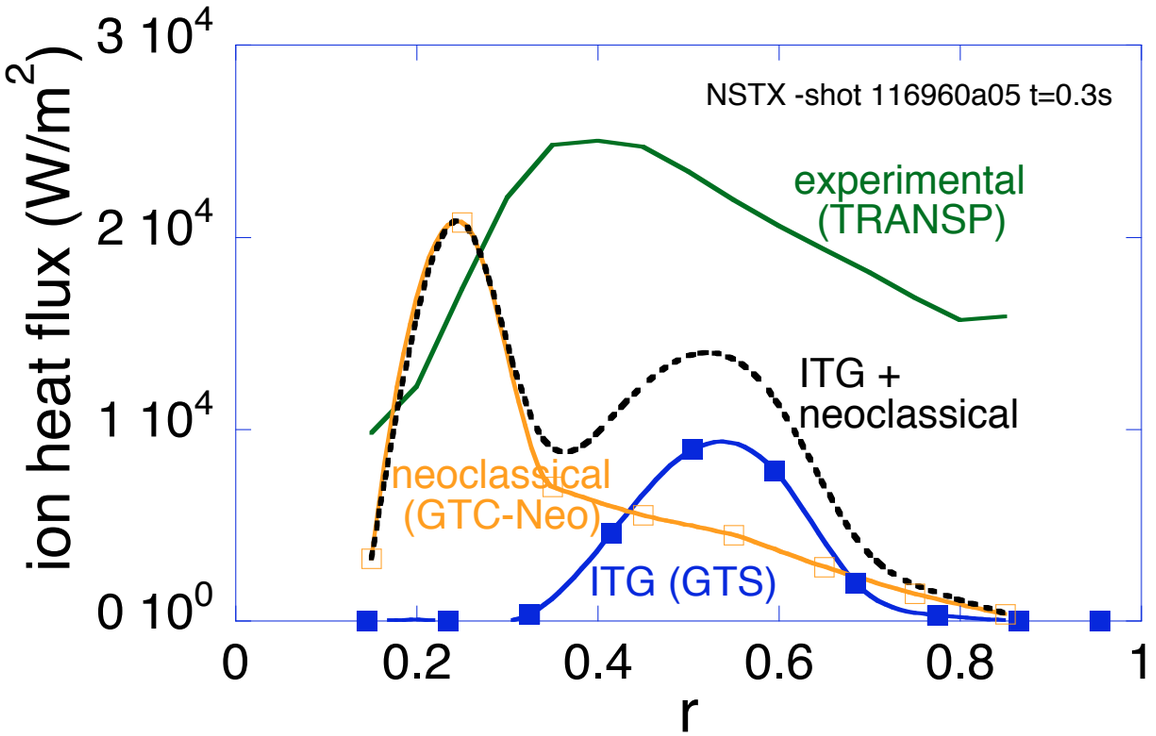
Recent Development of GTC-S and NSTX-physics-oriented Algorithm

- Generalized Poisson Solver to solve integral equation for total potential $\Phi = \delta\Phi + \langle\Phi\rangle$ using superLU/PETSc

  previous solver solves $\delta\Phi$ and $\langle\Phi\rangle$ separately using approximations:

  i) Pade approximation $\Gamma_0(b) \equiv I_0(b)e^{-b} \approx 1/(1+b)$ and

  ii) $\left\langle\tilde{\Phi}\right\rangle \approx \widetilde{\langle\Phi\rangle}$ – not justified for NSTX geometry!



W. X. Wang

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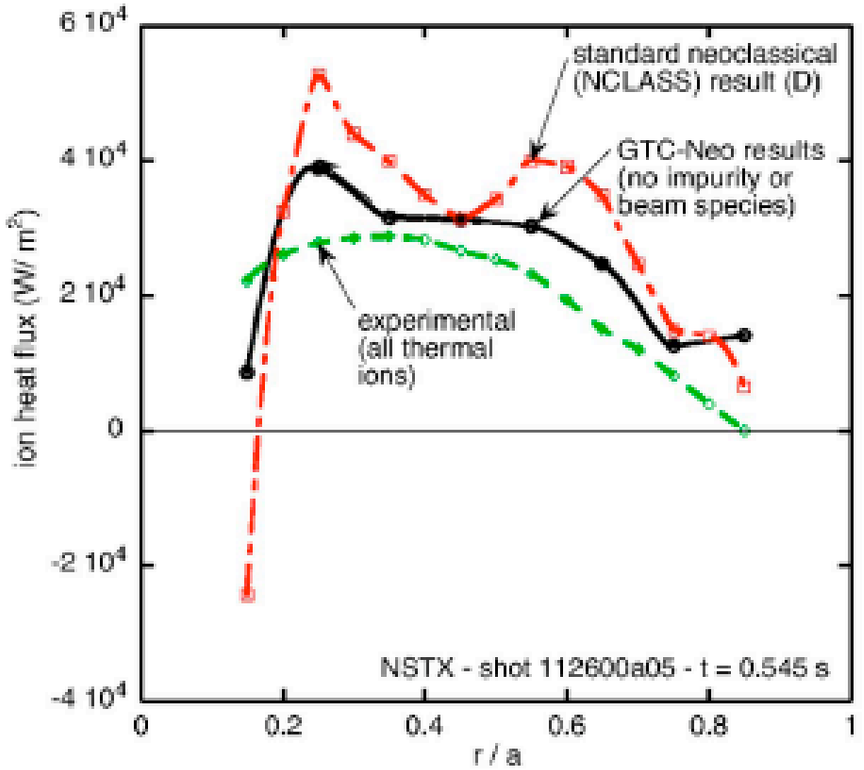
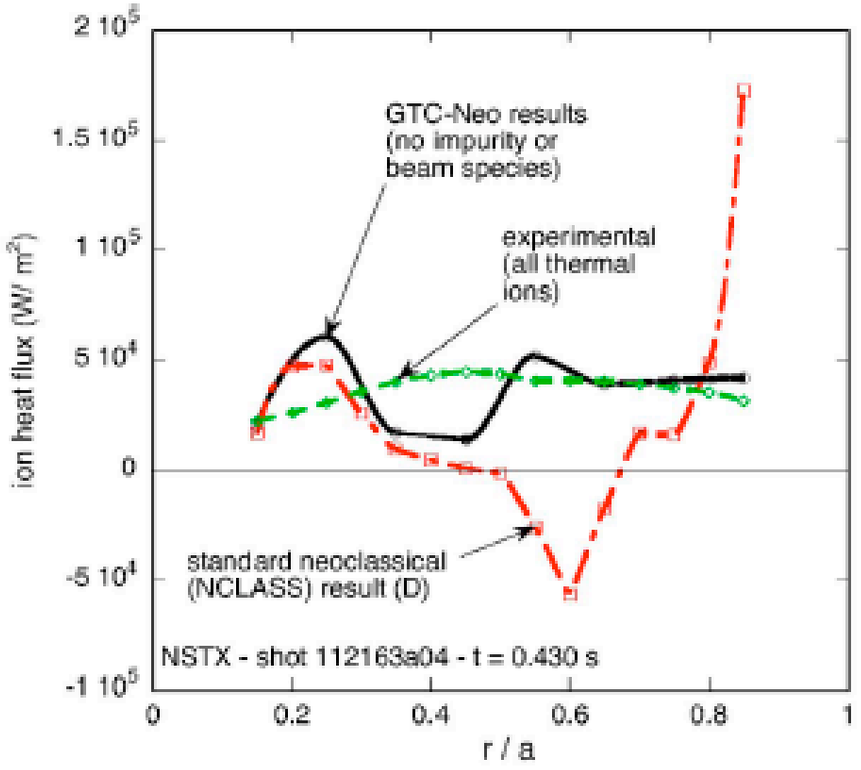
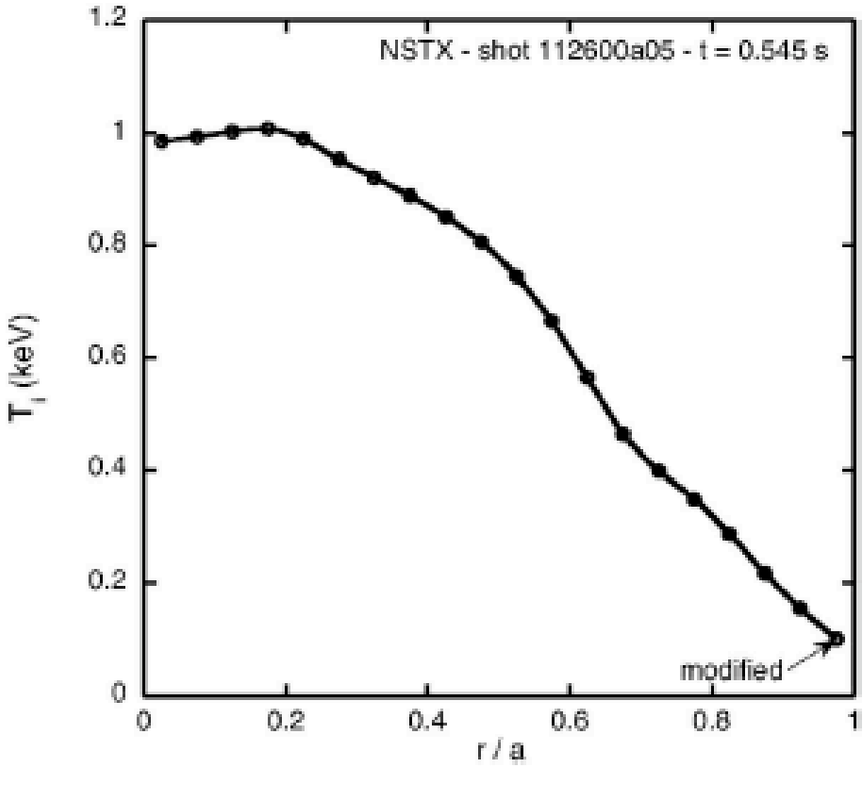
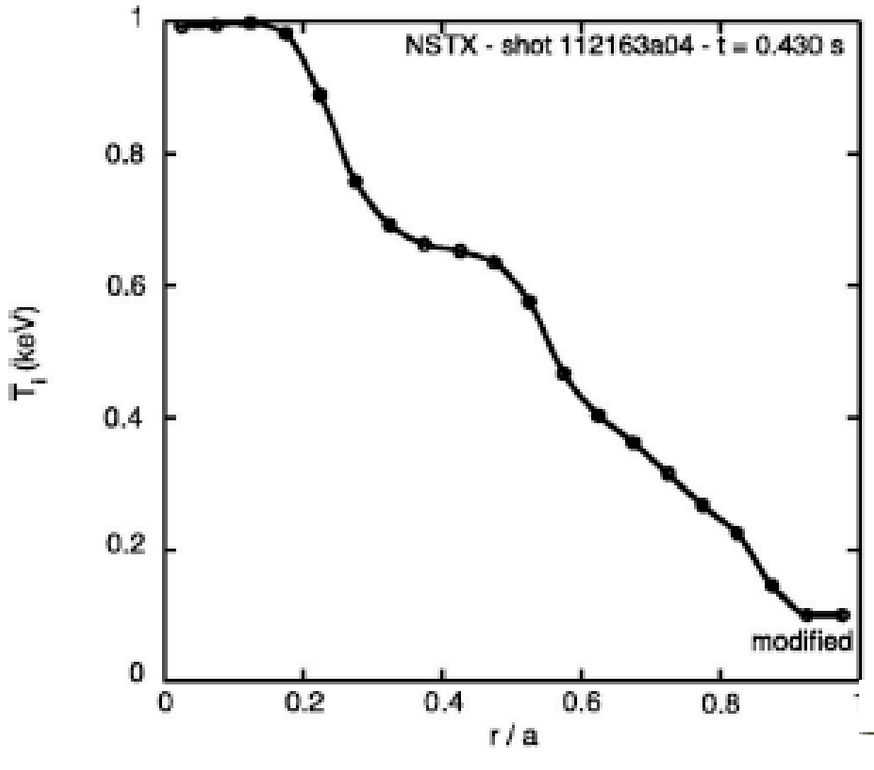
General Geometry GTC-neo

W. X. Wang [PoP, '06]









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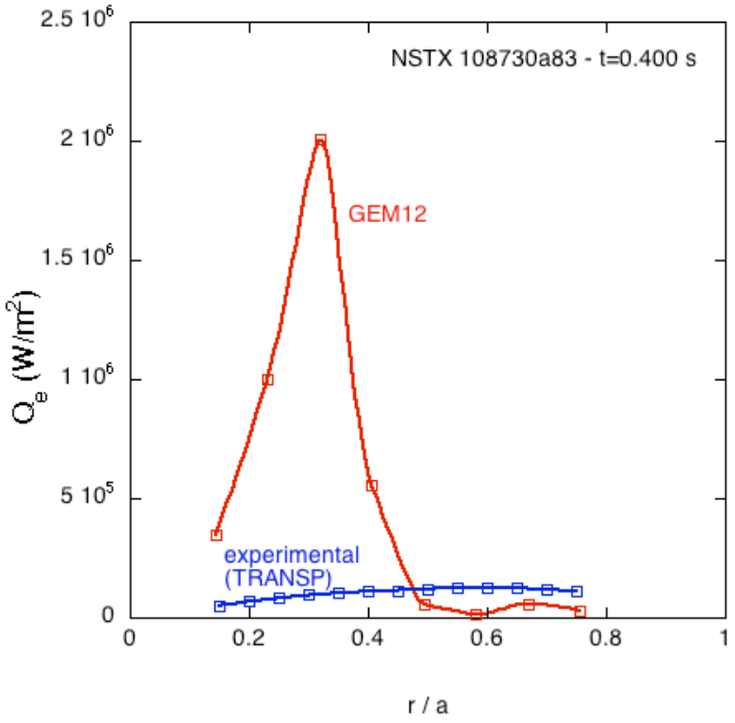
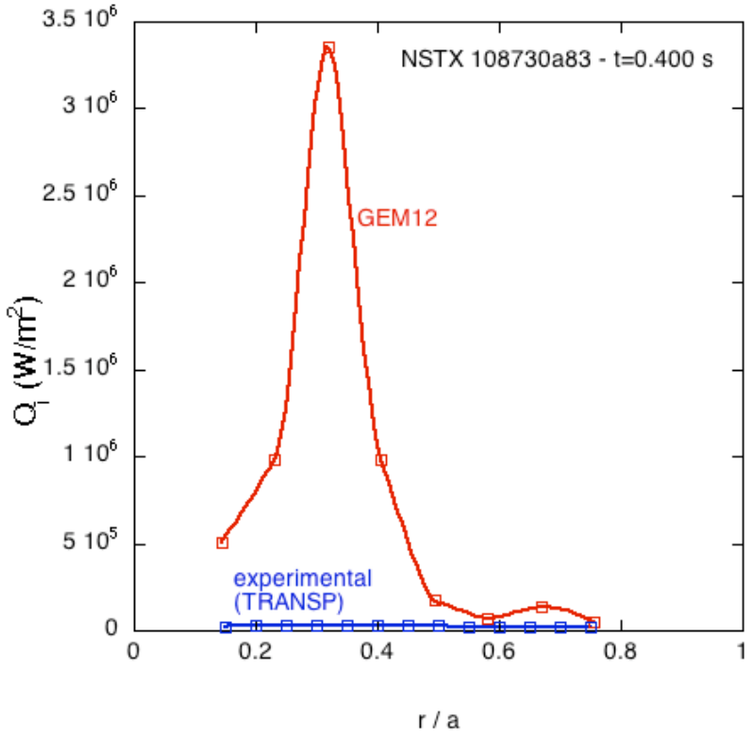
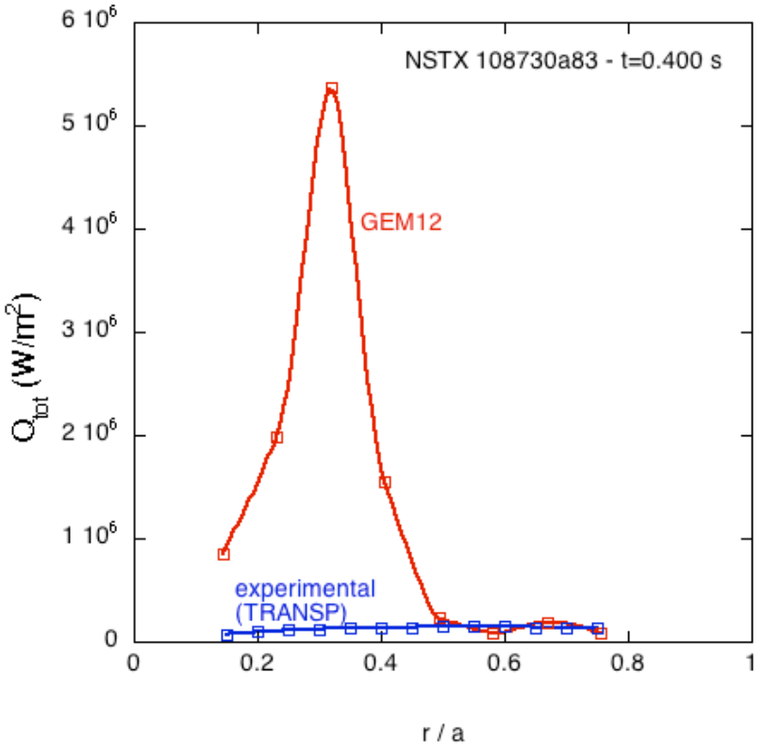
Comparisons of GEM with NSTX: Energy Flux Measurements

- First results - does not include parallel ion equilibrium flows! (which are transonic or supersonic)
- 128 particles / species / grid cell, 3 ion species, experimental β







G. Rewoldt and Y. Chen

Colorado

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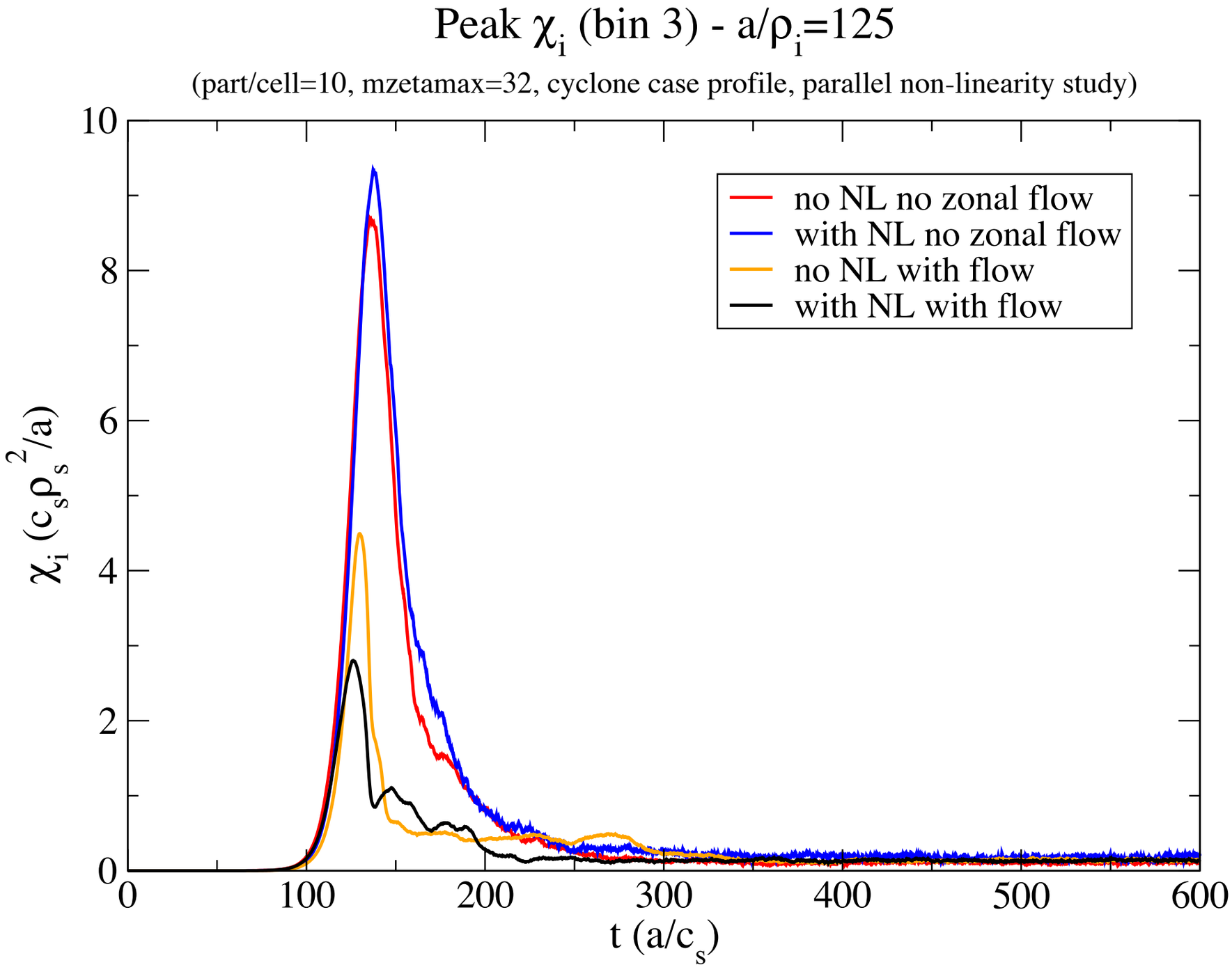
ITG simulations with for adiabatic electrons based on Cyclone-based parameters using GTC

- Steady state fluxes remain essentially the same with or without zonal flows and with or without parallel velocity space nonlinearity for a small simulation volume.

- But, these nonlinearities become progressively important for larger systems



Lee, Ethier and Kolesnikov

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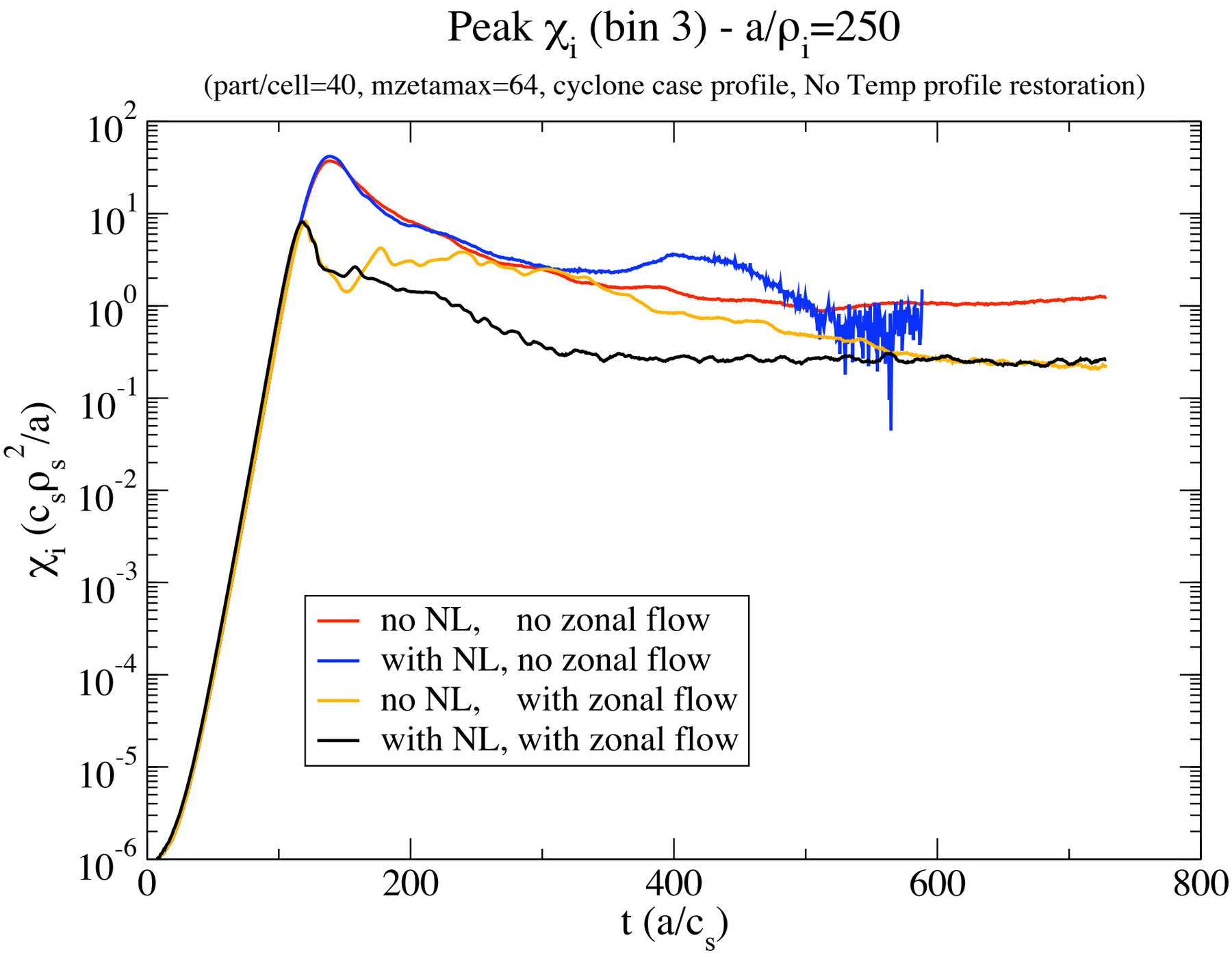
ITG simulations using GTC (cont.)

• For example, zonal flows are essential for maintaining steady state flux for a larger simulation volume.



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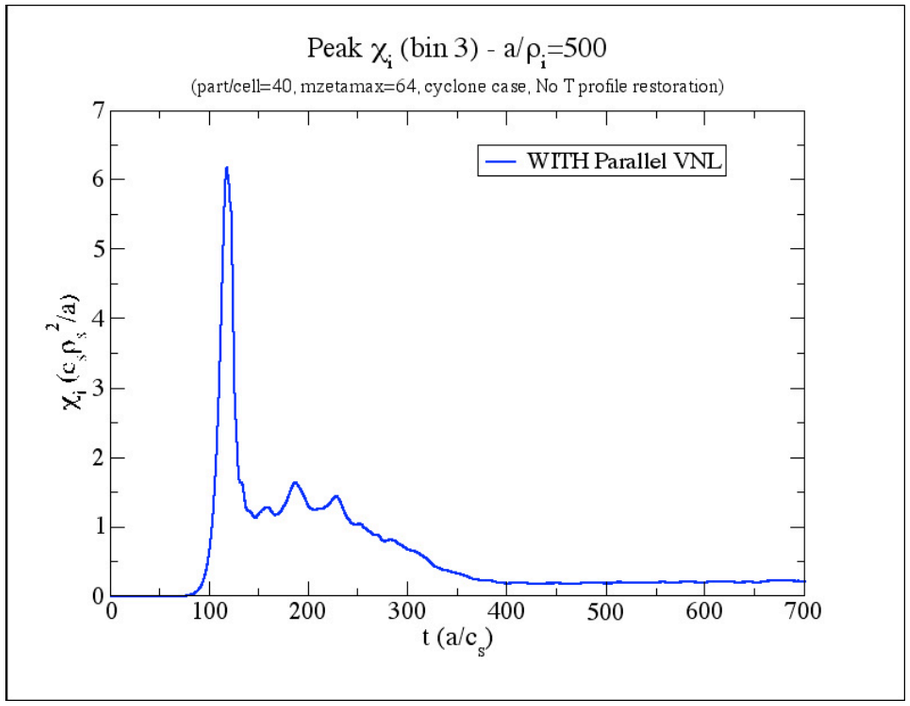
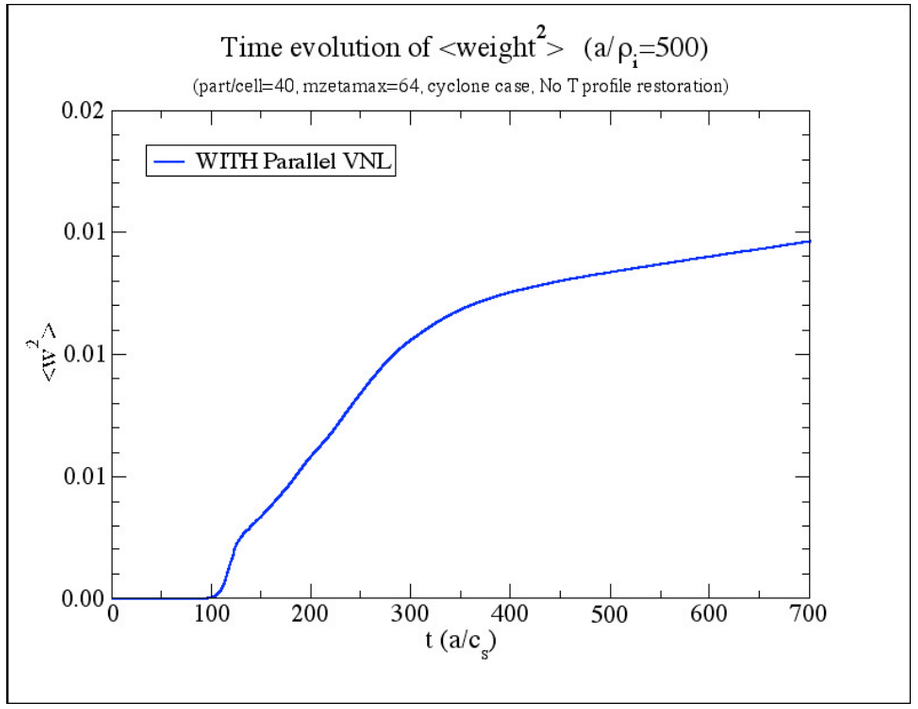
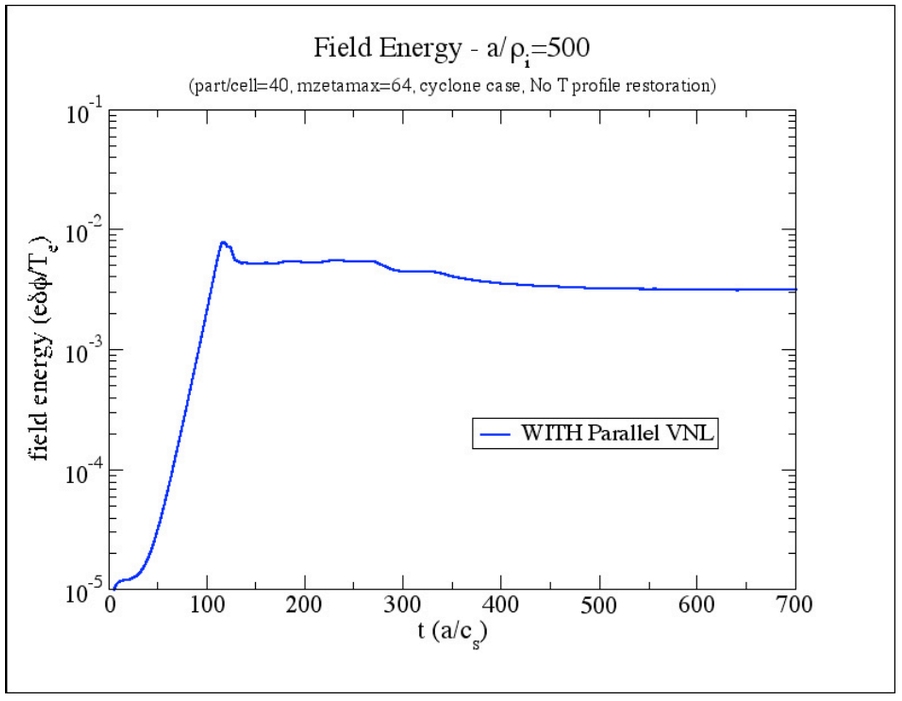
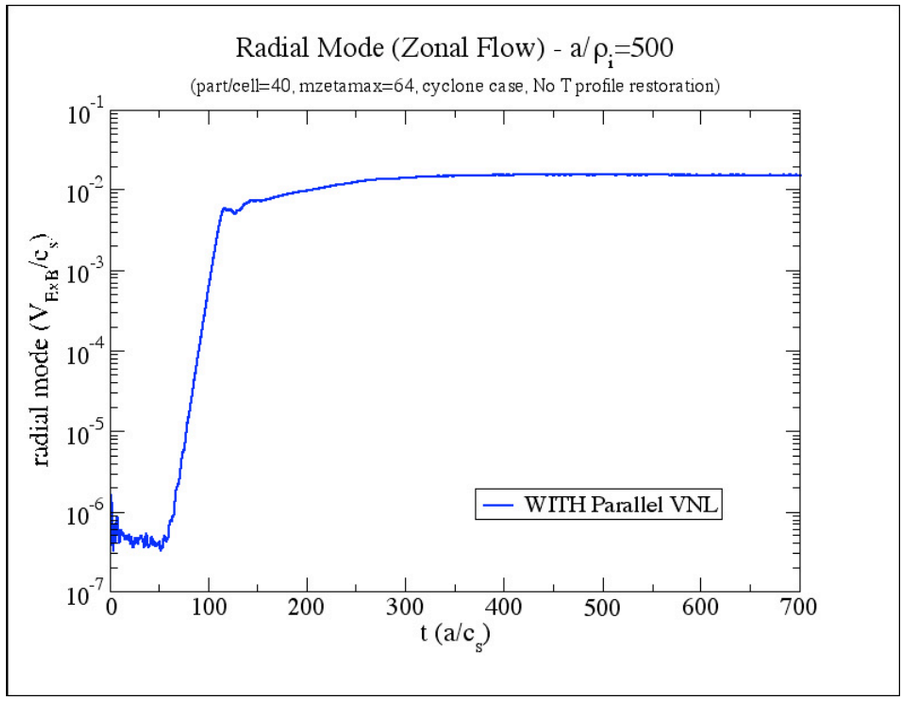
Both zonal flows and velocity-space nonlinearity are essential for maintaining steady state flux for an even larger system (a/ ρ = 500).









- There is no steady state without these nonlinearities in large scale global simulations.

Lee, Ethier and Kolesnikov

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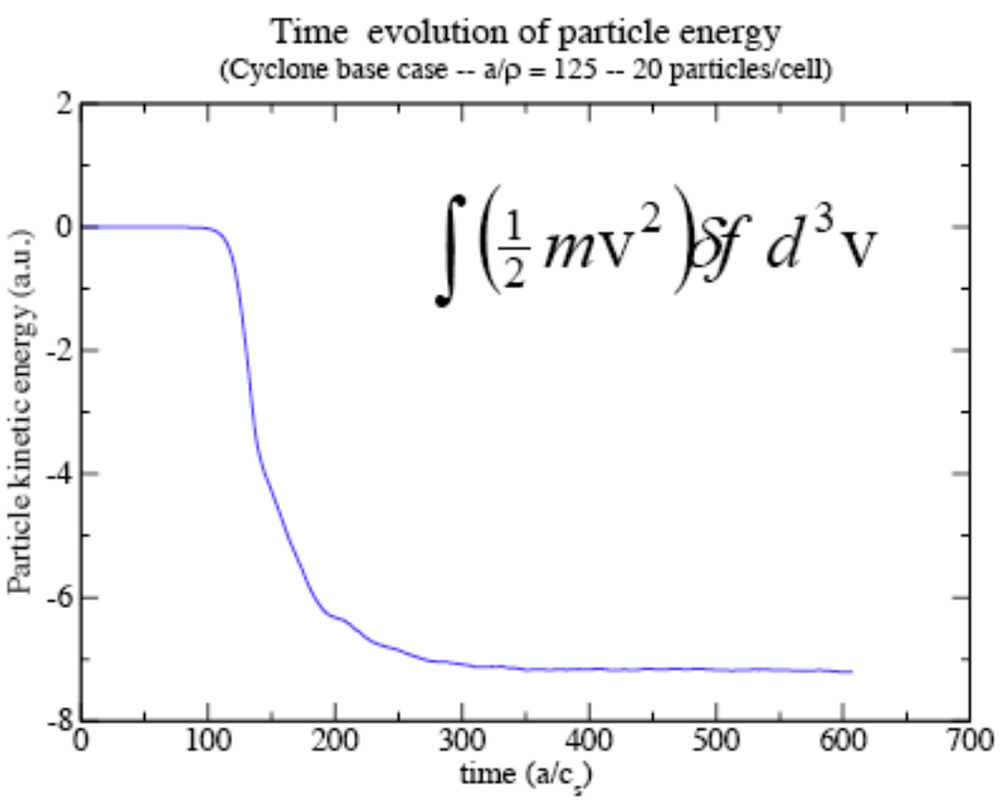
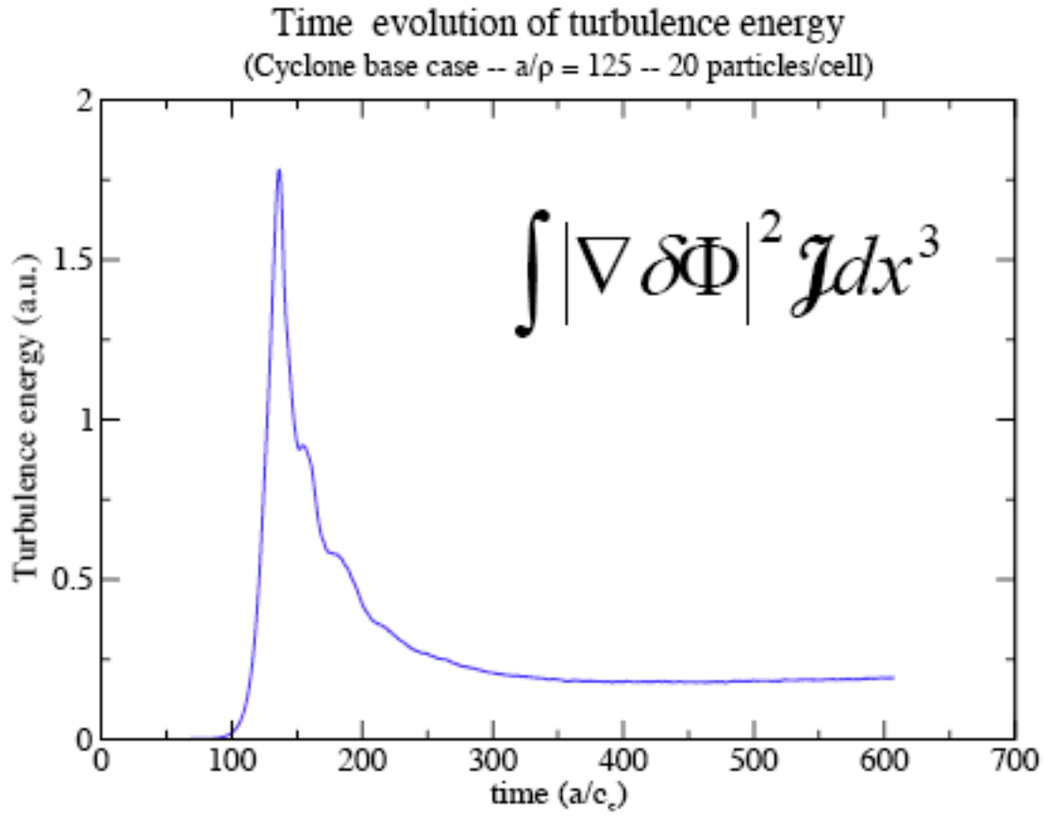
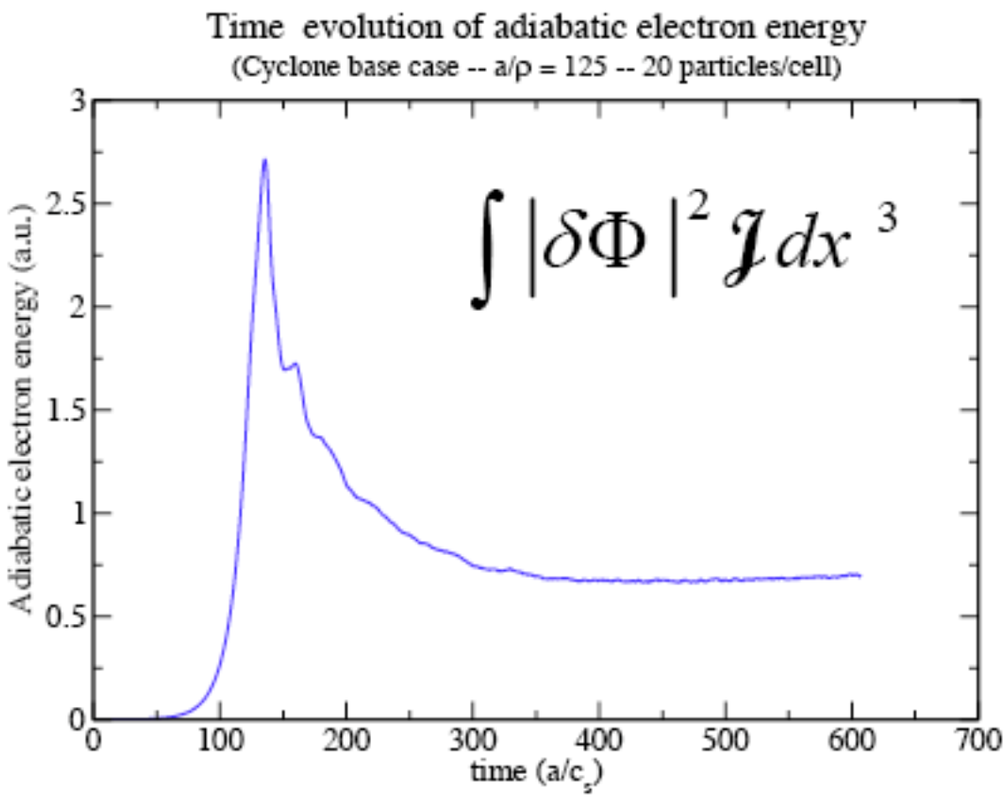
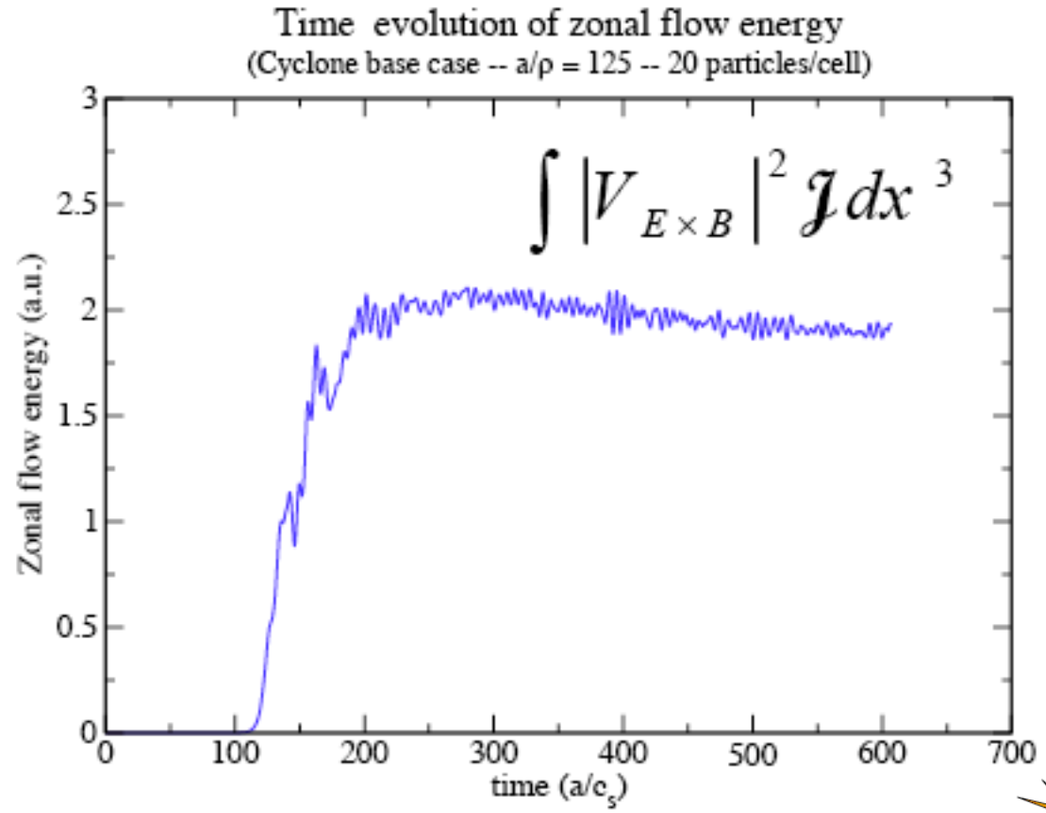
Conservation properties of ITG simulation (20 particles/cell)









Lee, Ethier and Kolesnikov

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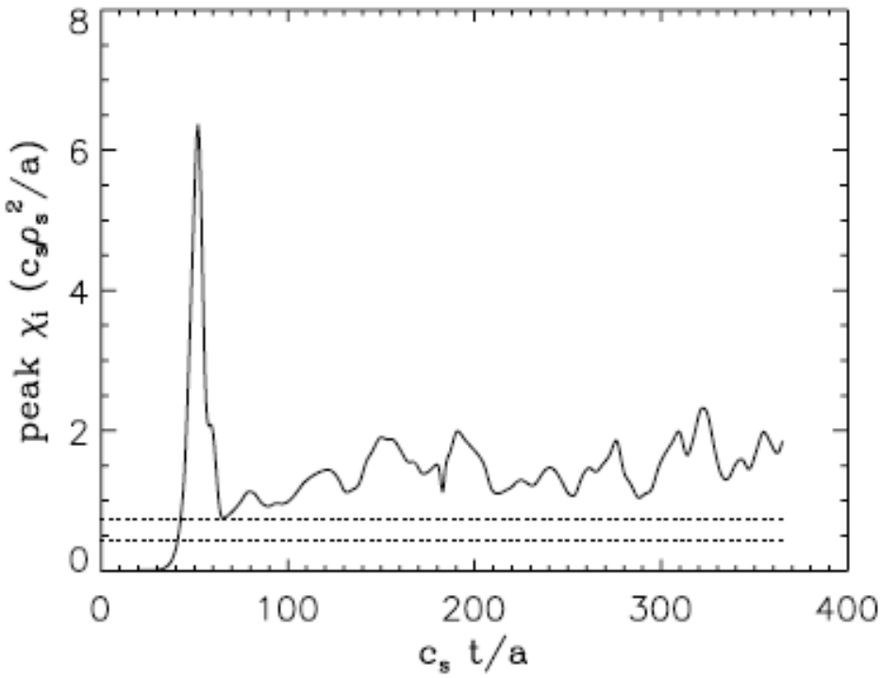
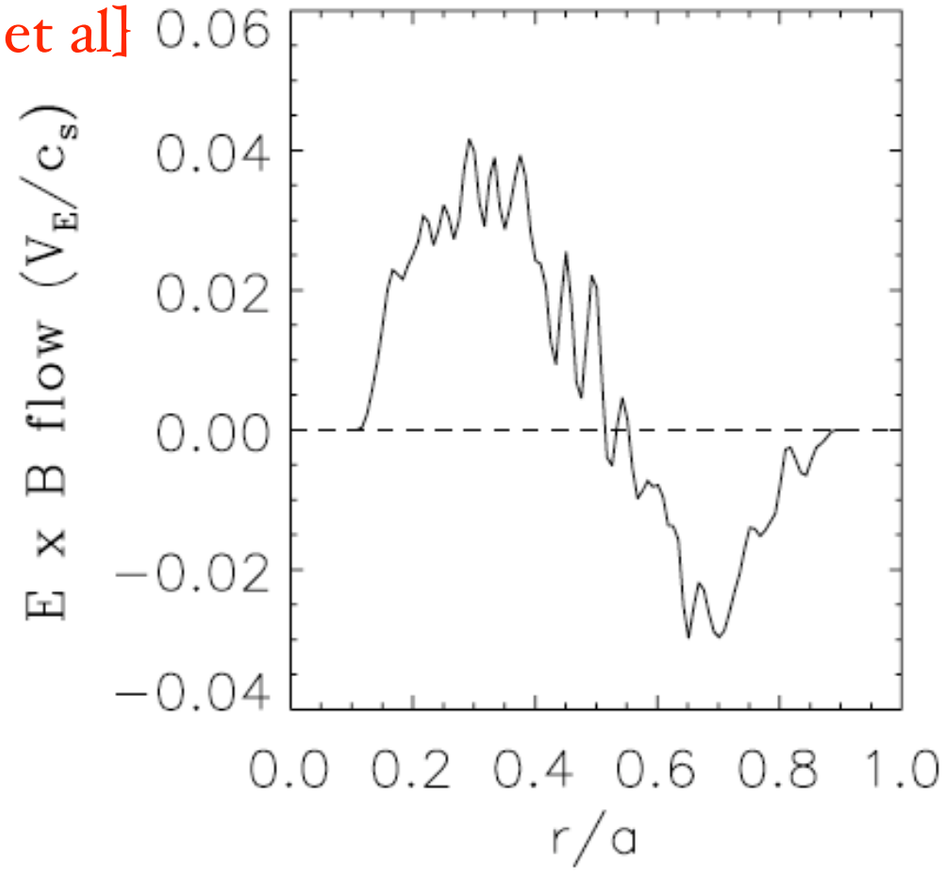
• ITG simulation with kinetic electrons using GTC with the split-weight scheme [Lewandowski et al]



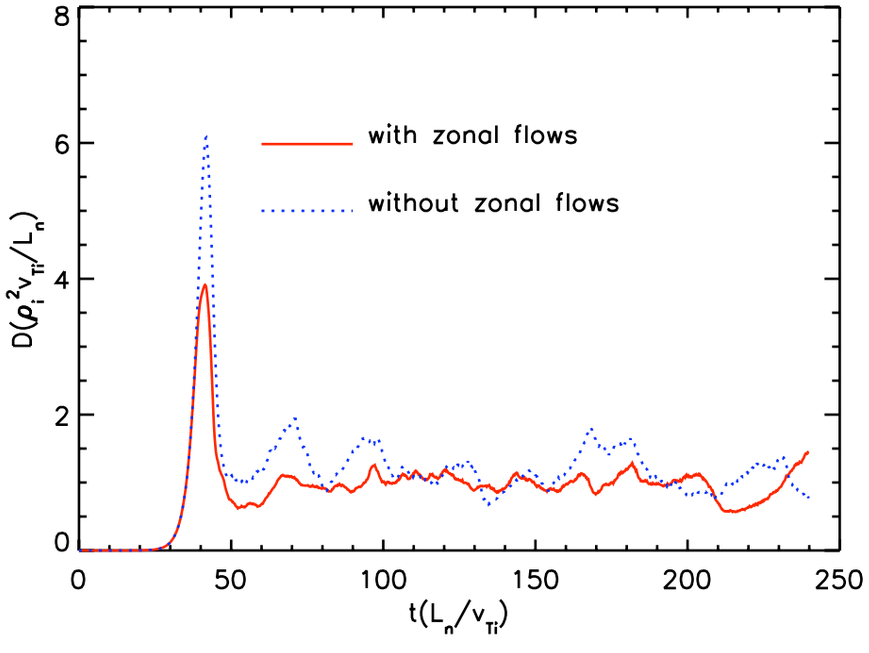


Zonal flows develop finer structures

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

• TEM simulation with collisionless electrons using GEM with the split-weight scheme [Lang, Parker and Chen]

Enhanced electron particle flux



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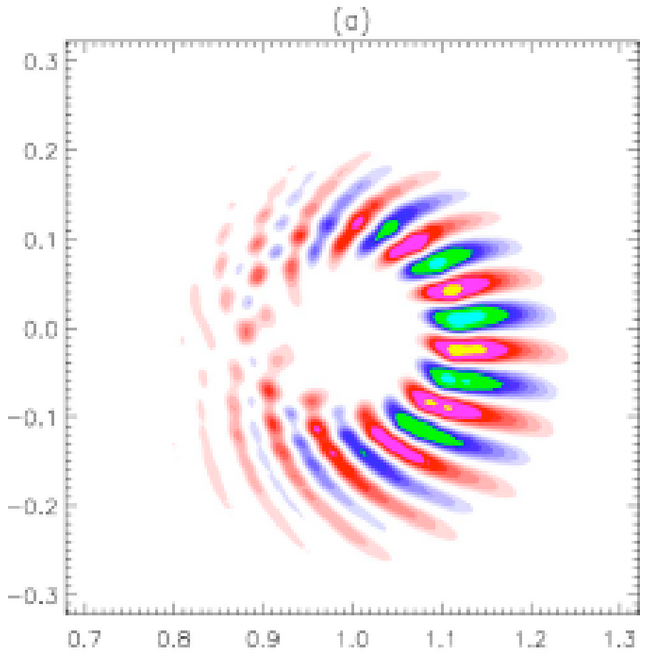
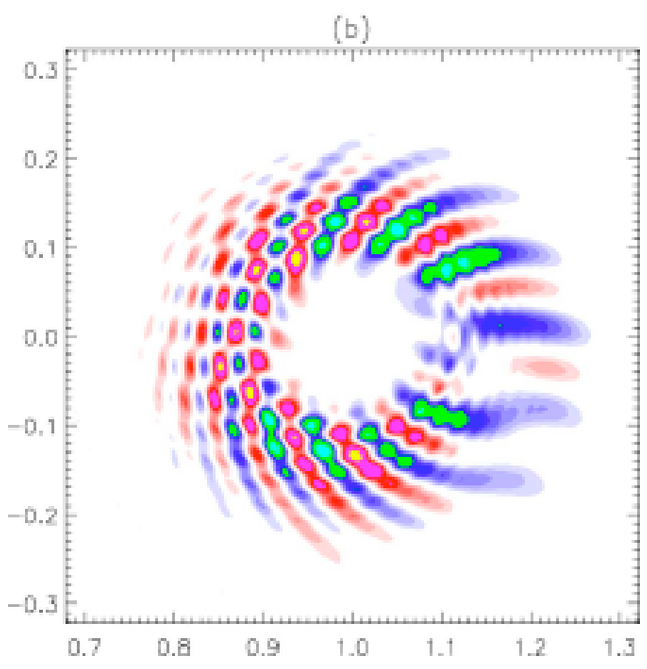
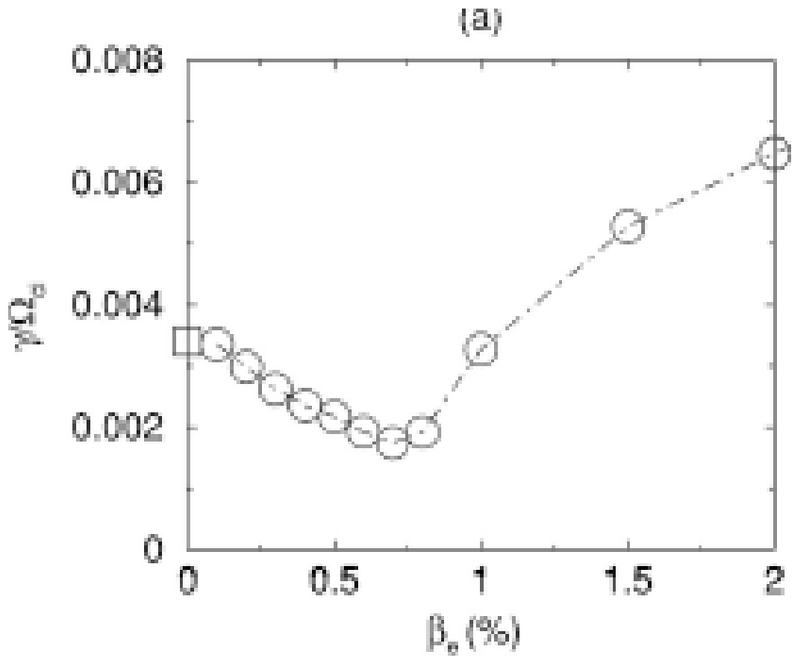
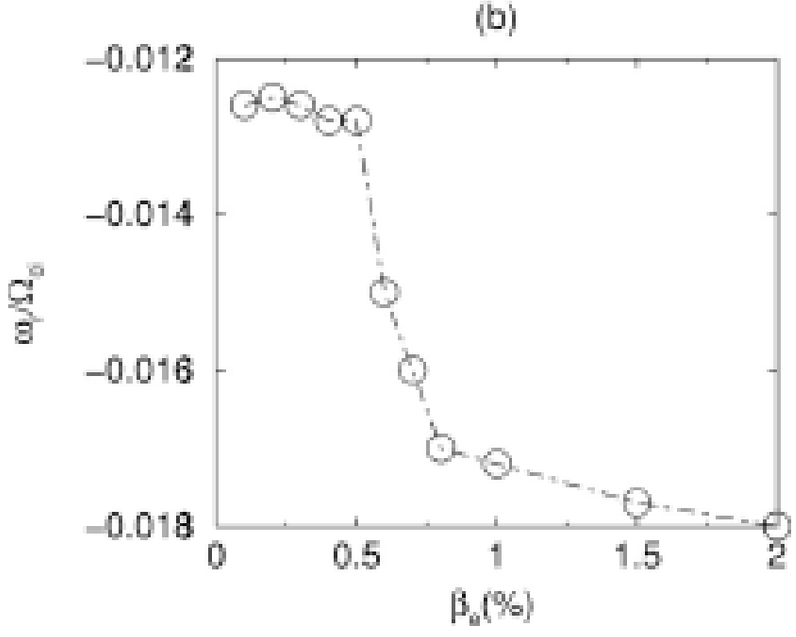
GTC-EM : fluid electron model





Mode structures for (a) the electrostatic potential and (b) the vector potential





Growth rates and real frequencies for finite-beta modified ITG modes

Nishimura, Lin and Wang

UCIrvine

Momentum Pinch from E x B shear and Magnetic Curvature

Two different mechanisms for non-diffusive momentum flux

$$m_i B^* dv_{||}/dt = -(eB + m_i c v_{||} \nabla \times \hat{b}) \cdot \nabla \delta\phi$$

	Gurcan, Diamond, Hahm, Singh [Phys. Plasmas 14, 042306 '07]	Hahm, Diamond, Gurcan, Rewoldt [Phys. Plasmas, June '07]
Net acceleration of parallel flow:	$-e_i B \nabla_{||} \delta\phi$	$-m_i c v_{||} \nabla \times \hat{b} \cdot \nabla \delta\phi$
Symmetry-breaking:	$k_{||}$ over the spectral width	curvature drift $\sim \hat{b} \times (\hat{b} \cdot \nabla)\hat{b}$ over the flux surface
Provided by:	mean **ExB** shear shifting fluctuations radially	ballooning mode structure causing finite net parallel acceleration over the flux surface
Main consequence:	residual stress driven by **ExB** shear (or $\nabla P_i/n_i$ and velocity shear via radial force balance)	convective pinch-like term (the TEP-like piece is insensitive to mode details)
Most likely to be relevant for:	plasmas with strong **ExB** shear, incl. H-mode, ITB's	pinch is likely to be inward for OH and electron-heated plasmas

Hahm et al.

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Discrete particle noise in particle-in-cell simulations of plasma microturbulence

[Nevins, Hammett, Dimits, Dorland, and Shumaker, PoP 12, 122305 (2005)]

$$\{1+[1-\Gamma_0(k_\perp^2\rho_e^2)]\}\frac{e\phi_{\mathbf{k}}}{T}=\frac{S_G(\mathbf{k})}{N_p}\sum_{\mathbf{p}}S(\mathbf{k_p})\sum_i w_i J_o(k_\perp\rho_i)$$
$$\times\exp(-i\mathbf{k_p}\cdot\mathbf{x}_i), \qquad (1)$$

$$\left\langle\left|\frac{e\phi}{T}\right|^2\right\rangle=\sum_{\mathbf{k}}\left\langle\left|\frac{e\phi_{\mathbf{k}}}{T}\right|^2\right\rangle=\frac{\langle w^2\rangle}{n_p V_{\text{shield}}}, \qquad (8)$$

$$V_{\text{shield}}^{(N)}\equiv\left\{\frac{1}{(2\pi)^3}\int d^3\mathbf{k}\frac{S_G^2\Gamma_0(k_\perp^2\rho_e^2)}{[2-\Gamma_0(k_\perp^2\rho_e^2)]^2}\right\}^{-1}, \qquad (9)$$

$$V_{\text{shield}}^{(H)}\equiv\left\{\frac{1}{(2\pi)^3}\int d^3\mathbf{k}\frac{S_G^2\Gamma_0(k_\perp^2\rho_e^2)}{(2-\Gamma_0)[2-(1-S_G d_\parallel)\Gamma_0]}\right\}^{-1}. \qquad (10)$$

- **Since dynamic plasma response is not included in the calculation, it is difficult to assess the effect of the shielding volume noise on long wavelength modes.**

Discrete Particle Noise for Equilibrium Plasmas

- Fluctuation-Dissipation Theorem

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

- Fluctuations per *k*-mode

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

$$\boxed{L|E(k)|^2/8\pi = (T/2)(\lambda_D^2/\rho_s^2)}$$

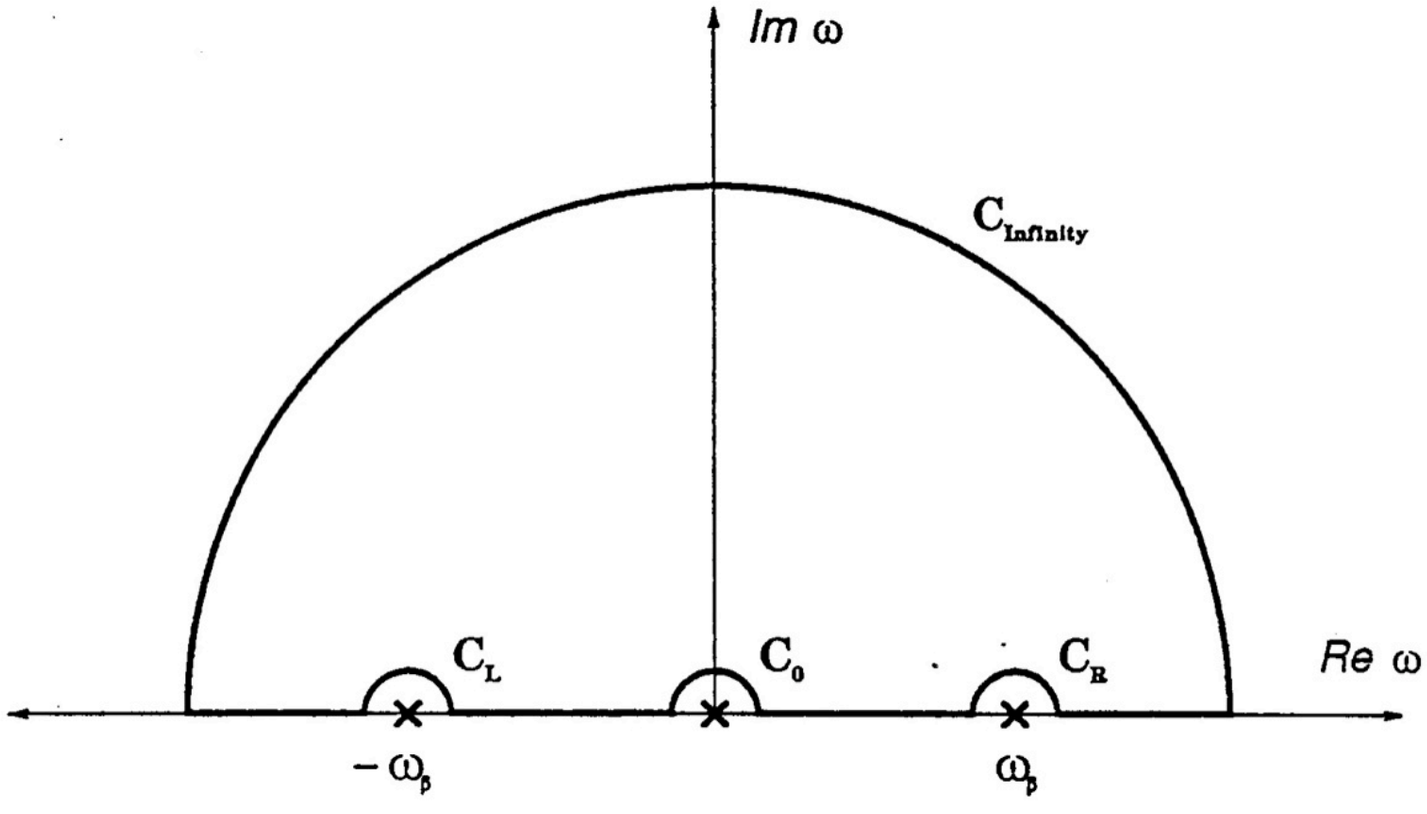

Figure 4.1: Contour integration

(John Reynders, PhD thesis, Princeton University, 1992)

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Fluctuation Dissipation Theorem applied to a nonlinearly saturated driven system

$$1 + k_\perp^2 - i\sqrt{\frac{\pi}{2}}\frac{\omega_* - \omega}{k_\parallel v_{te}}\left[1 - \frac{k_\perp^4}{\gamma_l^2}|\phi|^2\right] - \frac{\omega_*}{\omega} = 0$$

- Noise level for high frequency modes $\left|\frac{e\Phi}{T_e}\right|^2_{HF-noise} = \frac{< w^2 >}{N k_\perp^2 \rho_s^2},$

- Noise level for low frequency modes $\left|\frac{e\Phi}{T_e}\right|^2_{LF-noise} = \frac{< w^2 >}{N(1 + k_\perp^2 \rho_s^2)}$

- Nonlinear saturation amplitude $\left|\frac{e\Phi}{T_e}\right|^2_{NL} = \frac{\gamma_L/\Omega_i}{2k_x k_y \rho_s^2}$

[Jenkins and Lee, PoP '07]

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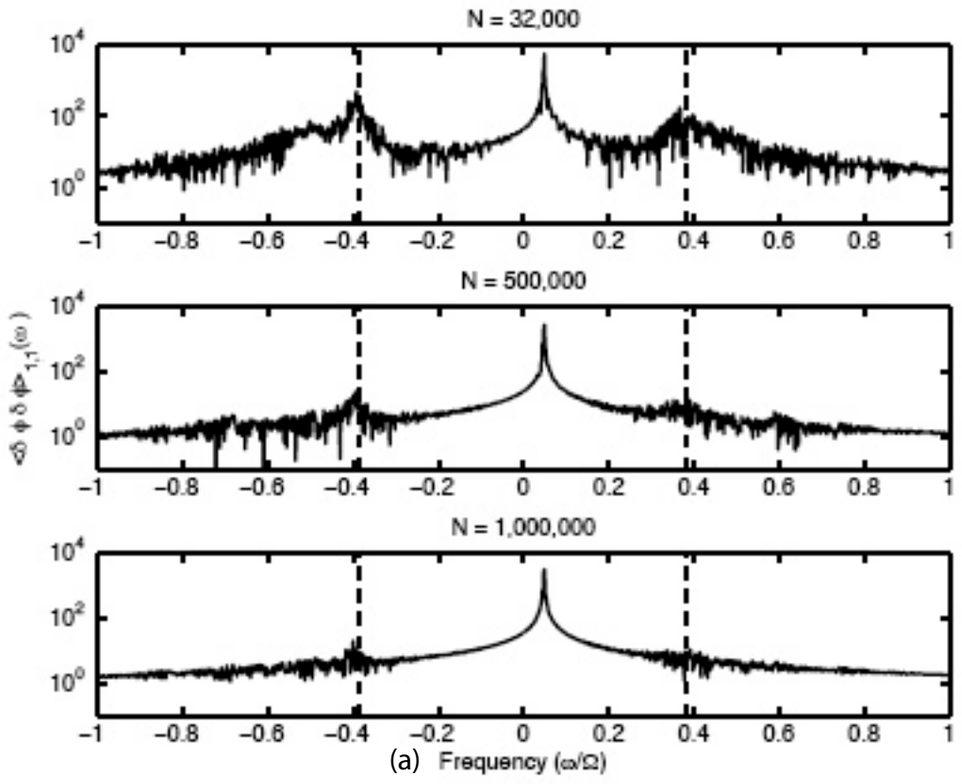
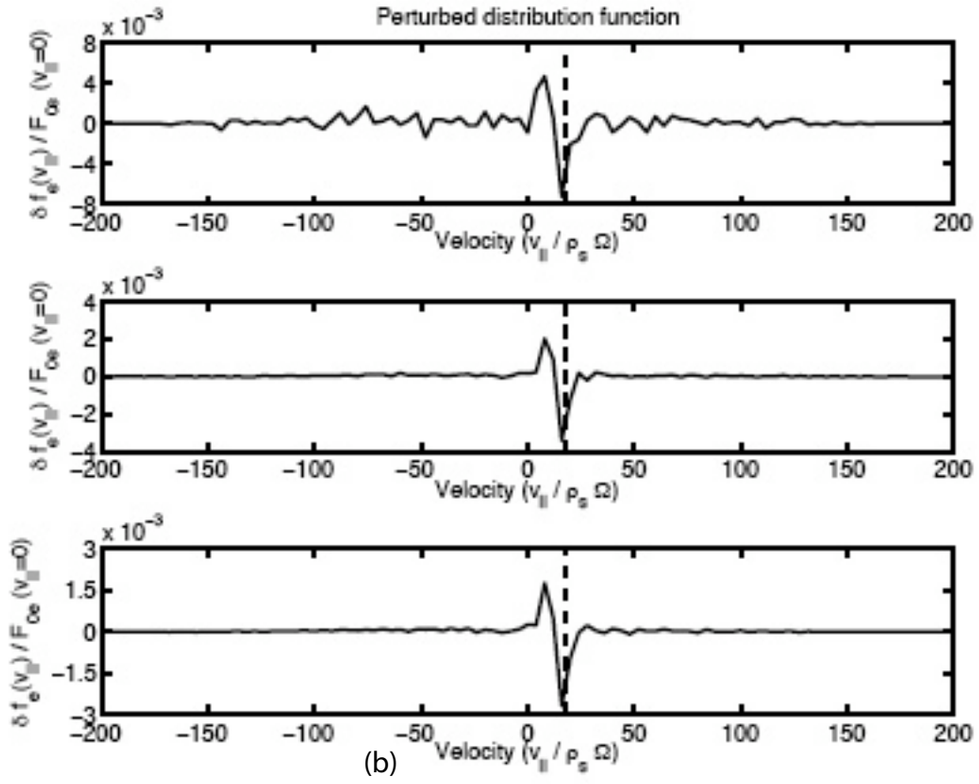
Discrete Particle Noise in Nonlinearly Saturated Plasmas

2D drift wave simulations
with
N = 32K, 500K, 1M





- high frequency noise decreases with particle number,
- saturation level is independent of particle number,
- background change is small.

[Jenkins and Lee, PoP '07]

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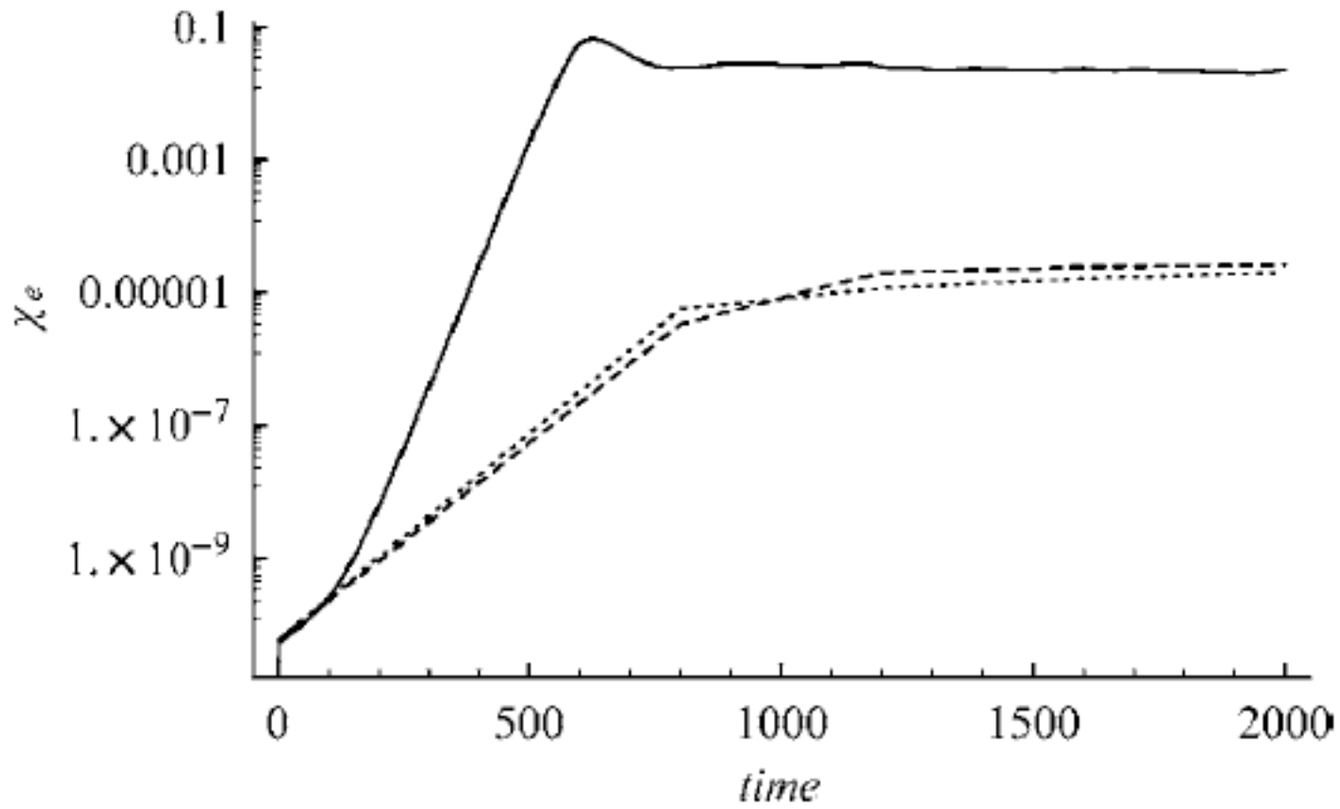
ETG simulation using GTC:
Noise-driven transport vs. fluctuation-driven transport



Electron transport in ETG simulation: total (solid line), noise driven contribution estimated by scramble test (dashed line) and estimated from δf weight (doted line).

[Holod and Lin, PoP '07]

Entropy conservation 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]

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

• Coarse graining in velocity space has to be taken with great care [Parker and Chen '06, Watanabe and Sugama '06]

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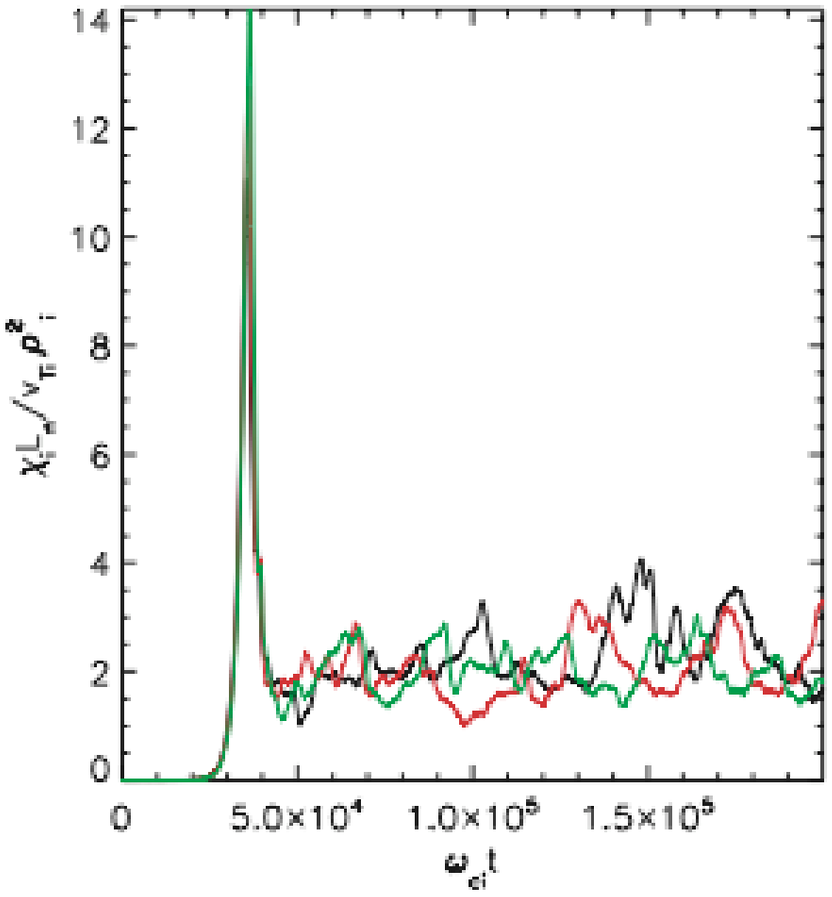
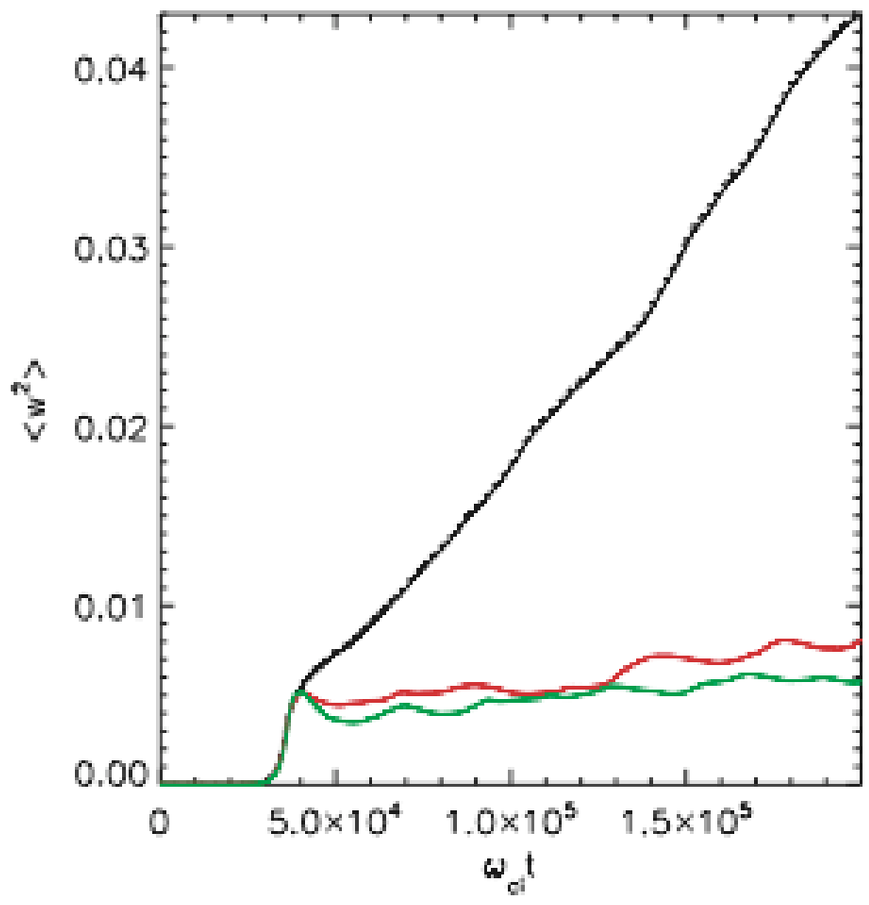
The Growing Weight Problem?
and
The Particle-Continuum Method

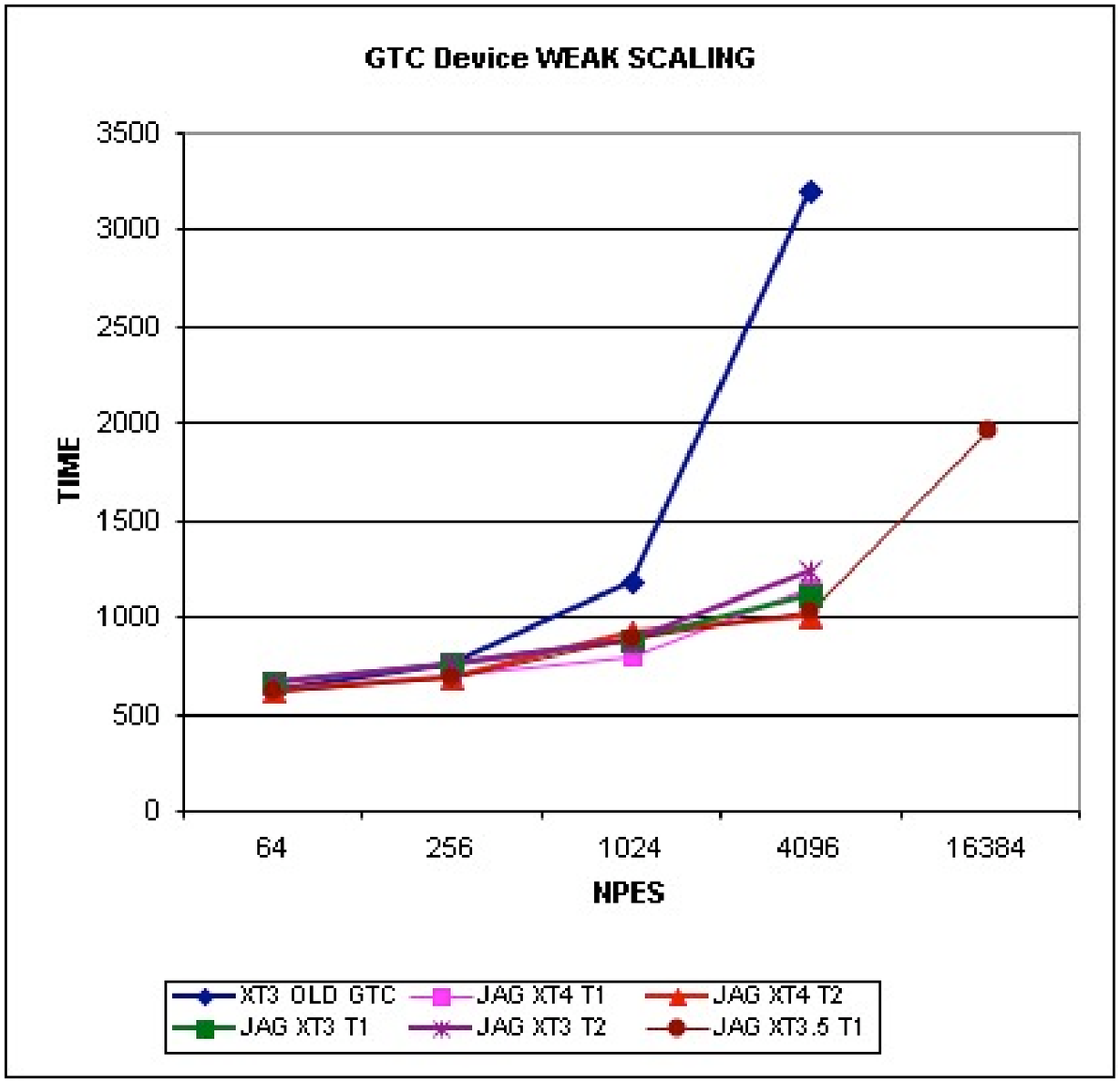




Resetting particle weights on a phase space grid periodically solves the so-called growing weight problem: no re-setting (black) vs. resetting (green and red)

[Chen and Parker]

Two dimensional grid domain decomposition on GTC [Adams, Ethier, Wichmann]



- It is important for simulating ITER-size devices
- Scaling inefficiencies point to large numbers of Translation Lookaside Buffer (TLB) misses on some processes on XT4/3 with larger grids.

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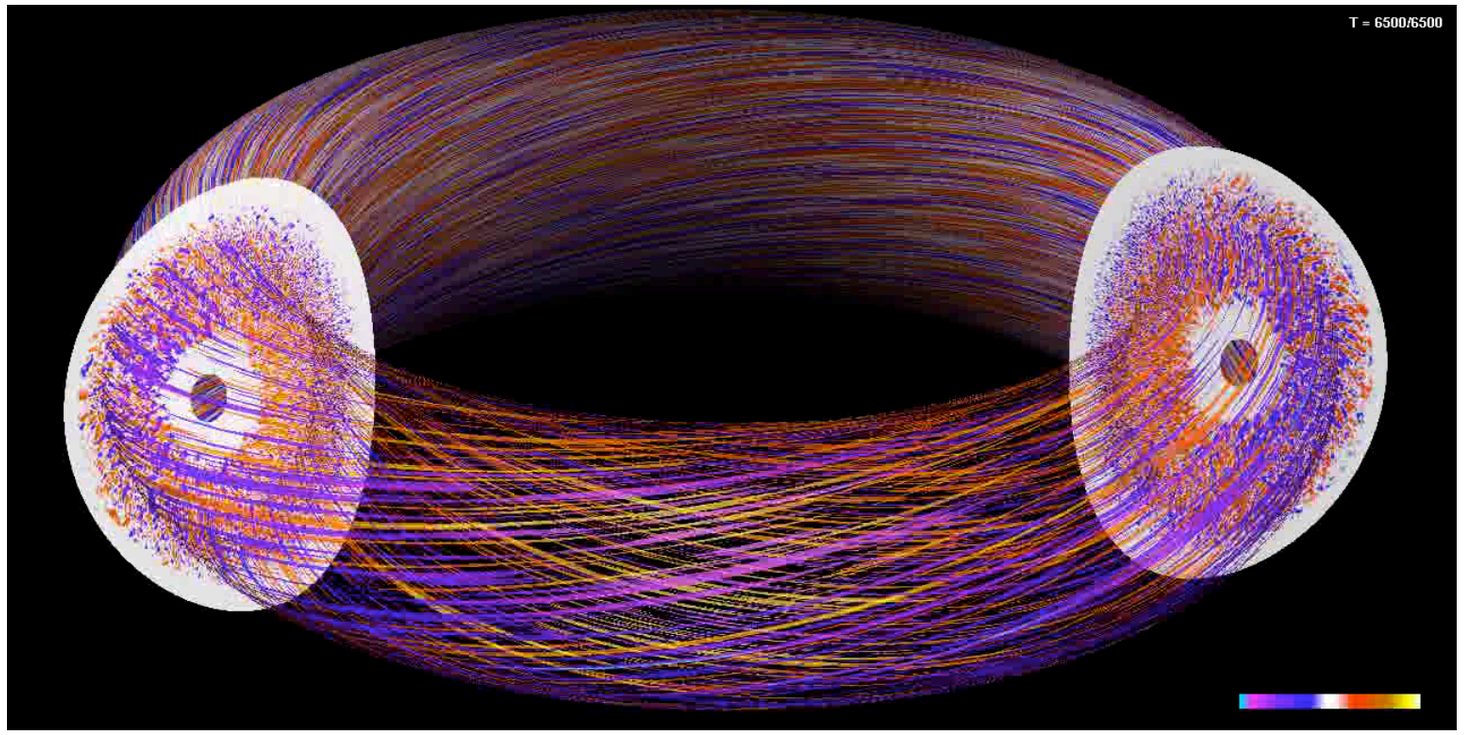
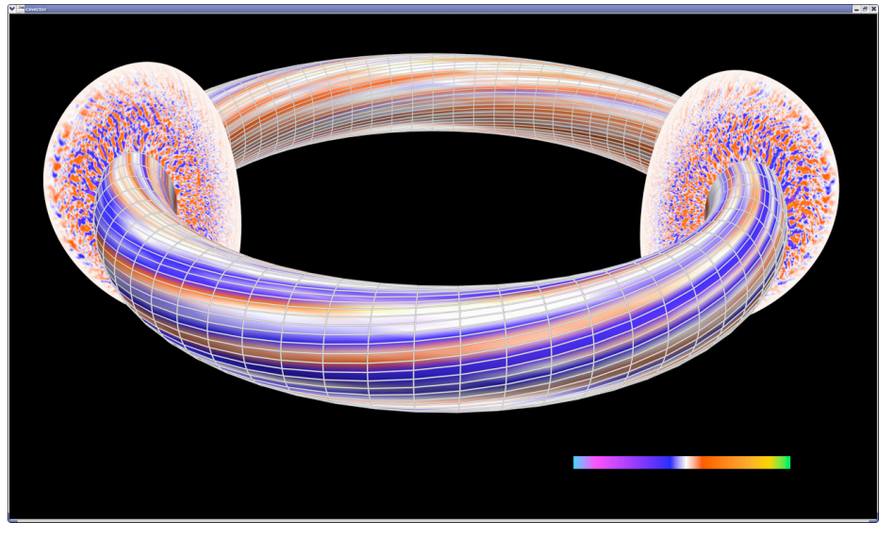
Visualization

[Klasky, ORNL; Ethier, Wang, PPPL]



[Klasky, ORNL; Ethier, Wang, PPPL]



[Ma, UC-Davis]

UCDAVIS ornl Oak Ridge National Laboratory PPPL Princeton Plasma Physics Laboratory

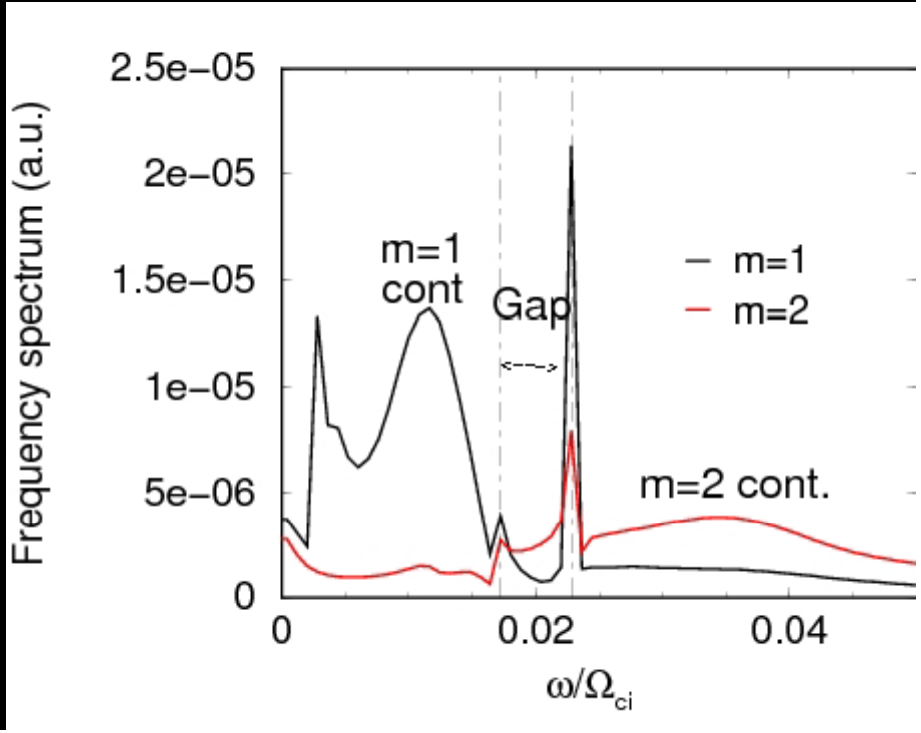
Electromagnetic GTC development at UCI

UCI

- **Kinetic electrons and electromagnetic fluctuations implemented using fluid-kinetic hybrid electron model**
- Enabled by a FEM field solver *[Nishimura, Lin, Lewandowski, Ethier, JCP2006]*
- FEM solver extension for edge geometry in collaboration with CPES *[Nishimura and Lin, CPP 2006]*
- A shaped version with 3D equilibrium is being applied for DIII-D resonant magnetic perturbation (RMP) experiments in collaboration with Evans and Joseph of GA
- Decyk of UCLA, in collaboration with Nishimura and Ethier, developed OO version for supporting multiple field solvers and multiple species (impurity and energetic particle), and for integrating with shaped version
- GTC selected for early application of 250TF ORNL computer

GTC electromagnetic simulation *UCI*

- Electromagnetic fluctuation via toroidal fluid-kinetic hybrid electron model
- Demonstrated finite-β stabilization of ITG mode
- Demonstrated Alfven wave propagation in tokamak, damping via phase mixing, and existence of toroidal frequency gap
- [*Nishimura, Lin, and Wang, PoP2007*]



GTC nonlinear convergence in ETG simulation

UCI

Convergence from 400 to 2000 particles per cell

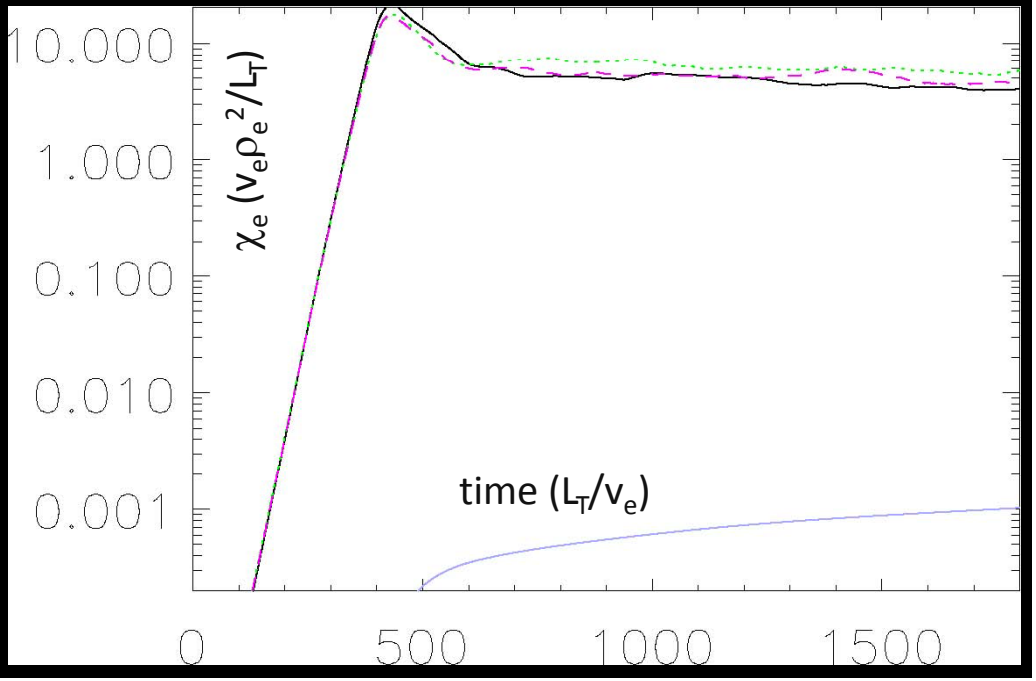
- Weak Cyclone case: R/L_T=5.3, s=0.78, q=1.4, a/ρ_e=500, $\gamma \sim \omega_r/4$

Noise driven flux is 4000 times smaller than ETG driven flux

Noise spectrum in ETG simulation measured. Noise driven flux calculated & measured, both in good agreement

ORNL Cray XT3, 6400 PE, 4×10^{10} particles

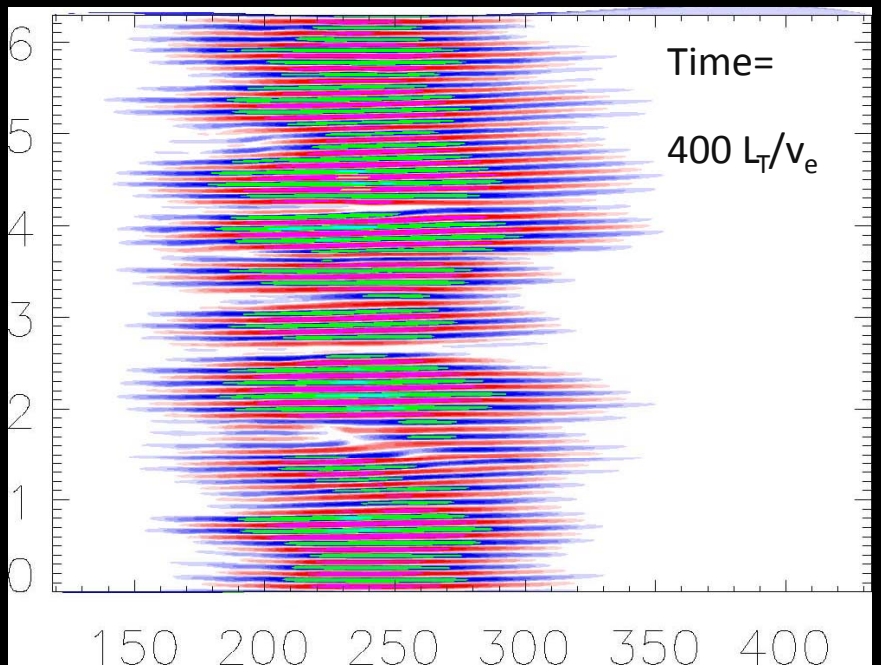
[Holod and Lin, PoP2007]

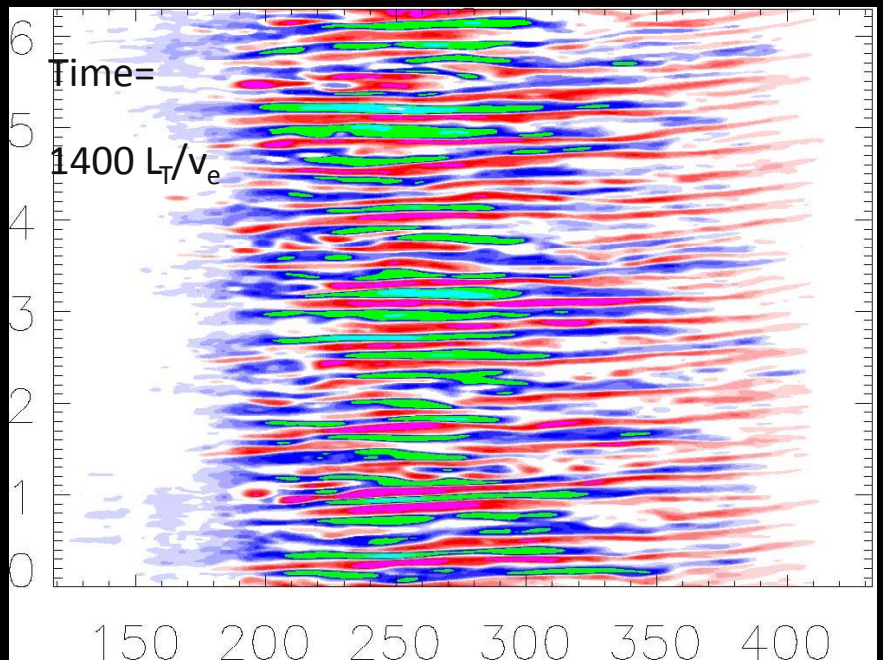


Electron transport via wave-particle decorrelation

UCI

- Time scale separation between kinetic and fluid processes
  $\tau_{auto} >> 1/\gamma >> \tau_{wp} \sim 1/\Delta k_{||} v_e$
- Electron heat transport dominated by wave-particle decorrelation of parallel resonance $\delta(\omega - k_{||} v_{||})$
- Quasilinear calculation agrees well with GTC simulation
- *[Lin et al, EPS2007 invited]*

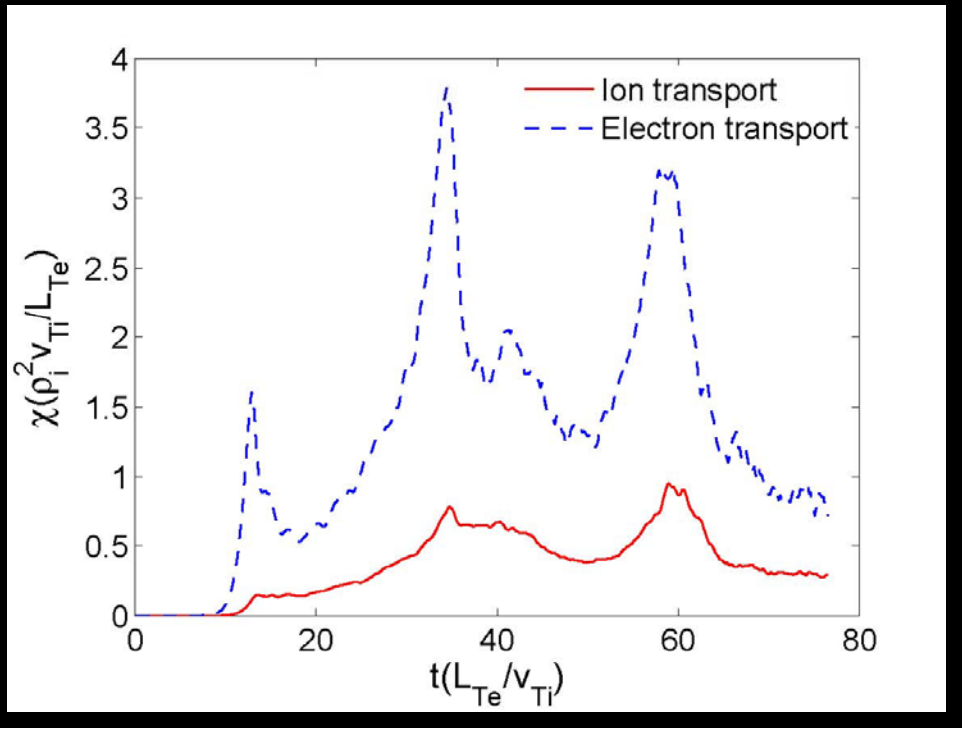




GTC Simulation of CTEM turbulence *UCI*

- CTEM turbulence: electron transport dominant & bursty, zonal flows dominate saturation mechanism but not regulate the bursting.
- In collaboration with CPES *[Xiao and Lin, CPES spring meeting, 2007]*
- A kinetic theory was developed for radial propagation and damping of kinetic GAM mode [*Chen and Zonca, TTF2007*]

CTEM: $R/L_n=R/L_{Ti}=2.2$, $R/L_{Te}=6.9$, $s=0.78$, $q=1.4$



Conclusions

- It has been an exciting three years

- The PPPL team's work on
  -- GTC performance on MPP
  -- GTS and GTC-Neo and their V&V work
  -- PNL and noise
  -- Theory

- The UCI team's work on
  -- ETG, TEM and noise using GTC
  -- EM capability for GTC

- The Colorado team's work on
  -- GEM for TEM
  -- Particle continuum method
  -- EM capability in GEM and the V&V work

- The SAPP team on
  -- Solvers
  -- Visualization
  -- Data management

Future Directions

- Verification and & Validation
- Electromagnetic physics in GTS
- ITER simulation capabilities
- Integrated simulation: Heating, Turbulence, MHD, Transport