Third 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 2007

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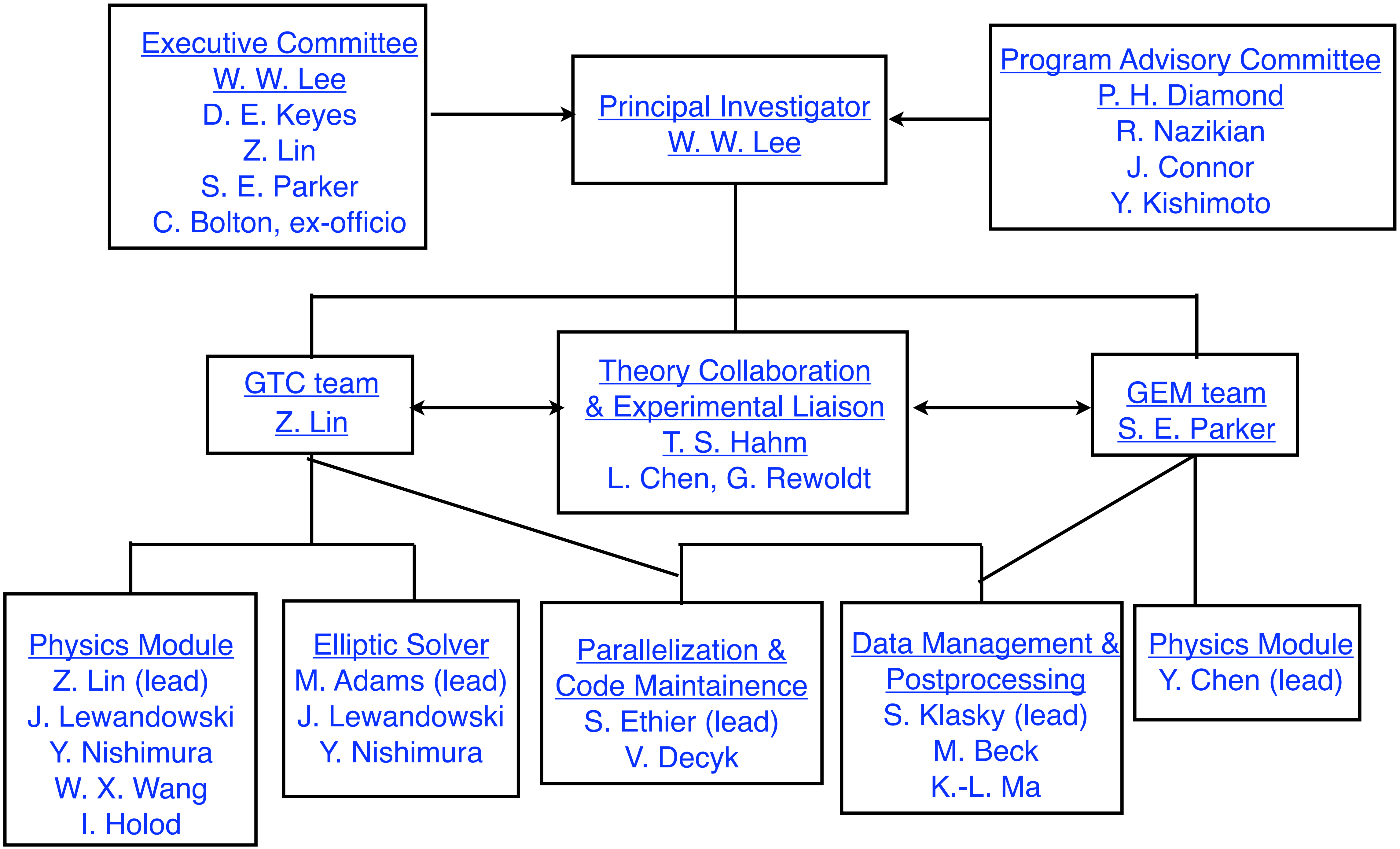
Outline

- Center Activities
  -- Fall Meeting
  -- Invited talks and Publications
- Code Development
- Code Validation
- Physics Investigations
- The noise and growing weight issues
- Conclusions

Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas



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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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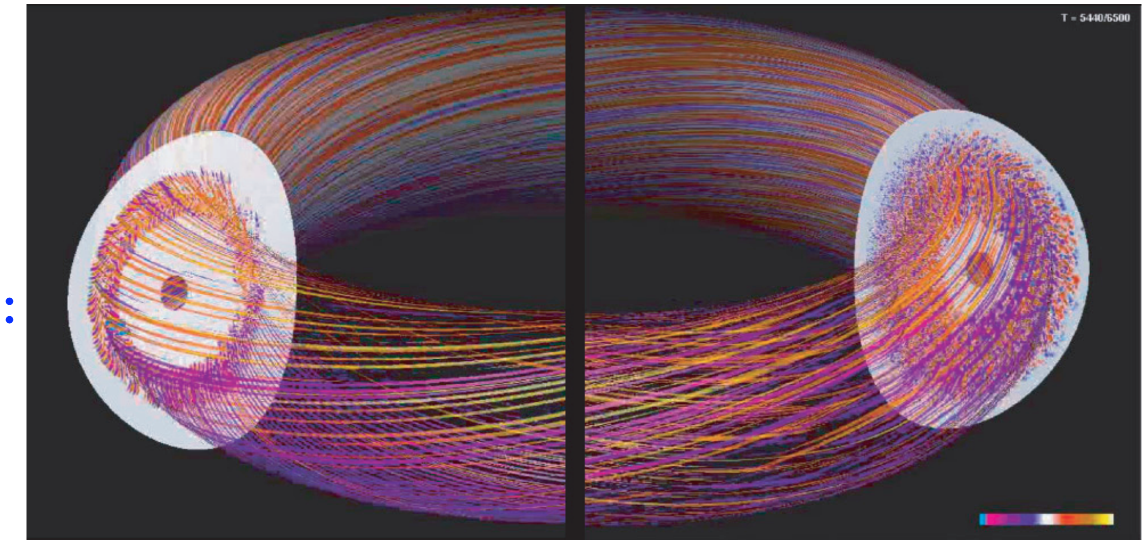
Code Development

- 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

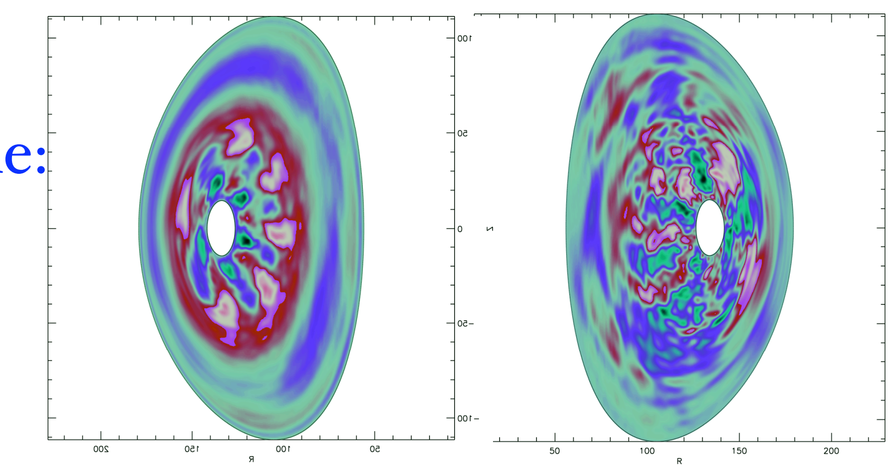


GTS

- 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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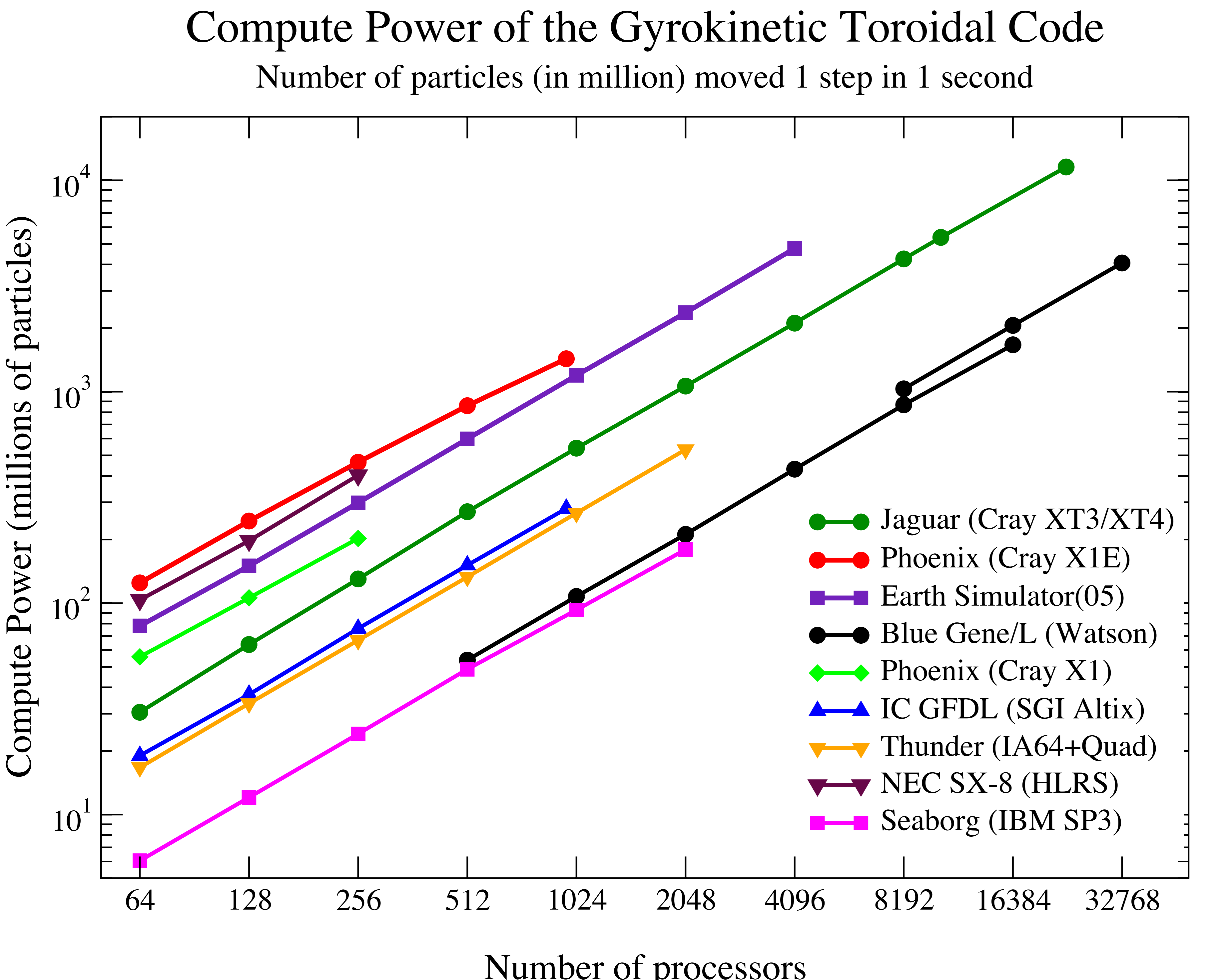
GTC performance on MPP platforms aiming for ITER-size Plasmas

- 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



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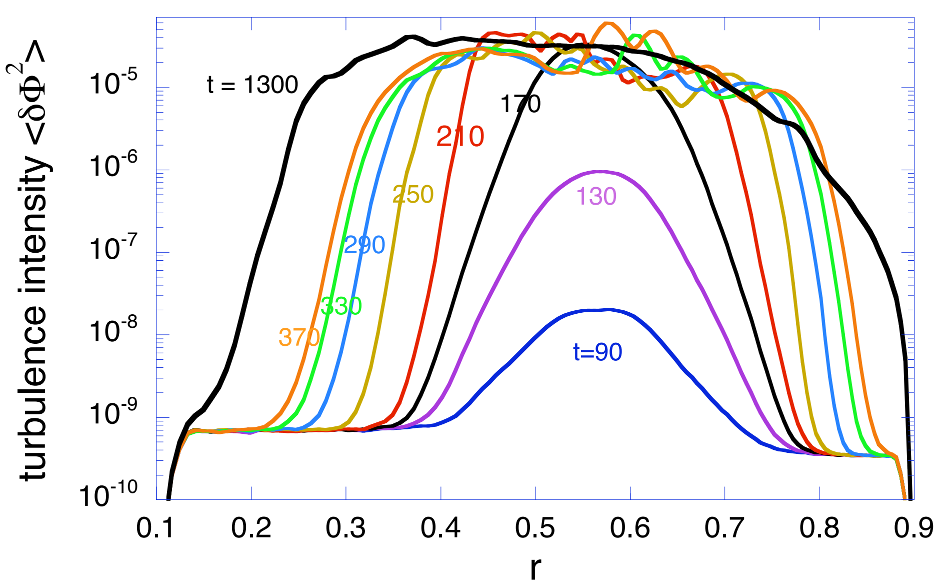
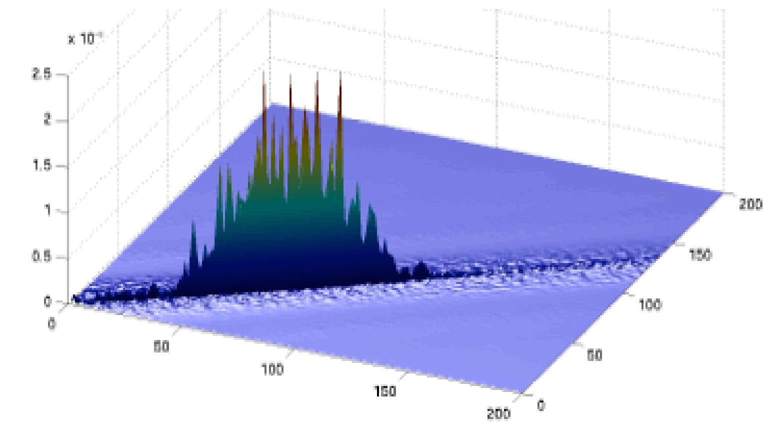
General Geometry GTS
W. X. Wang [PoP '06]

- **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



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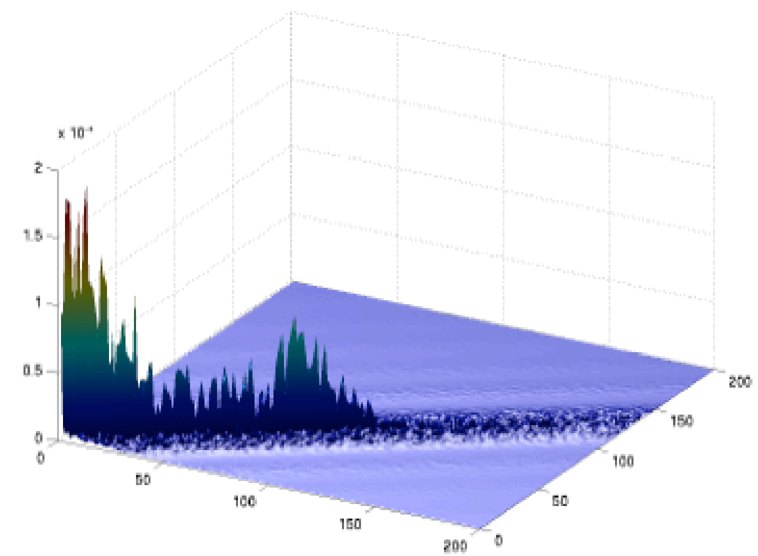

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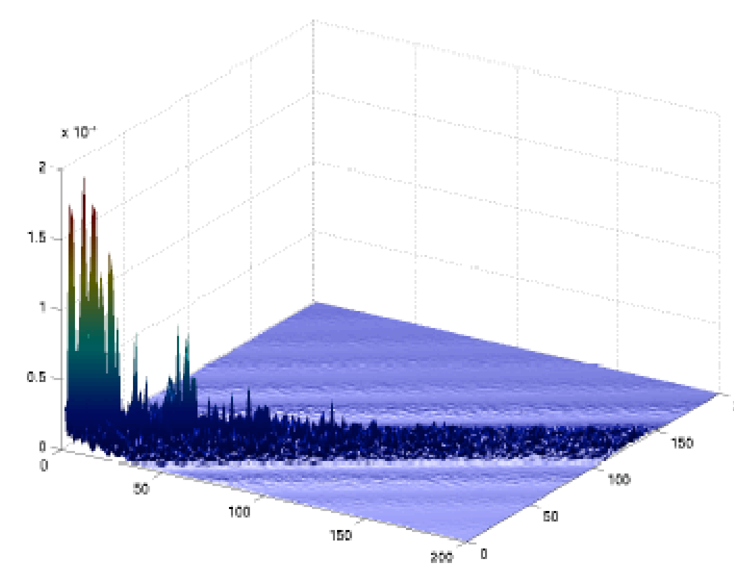

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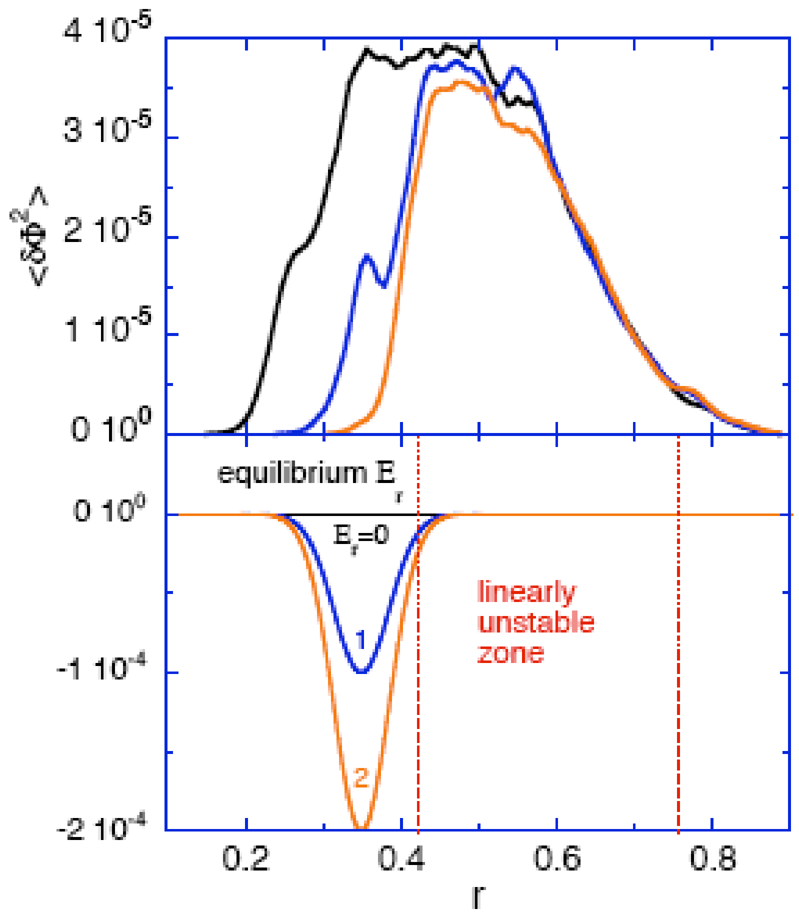
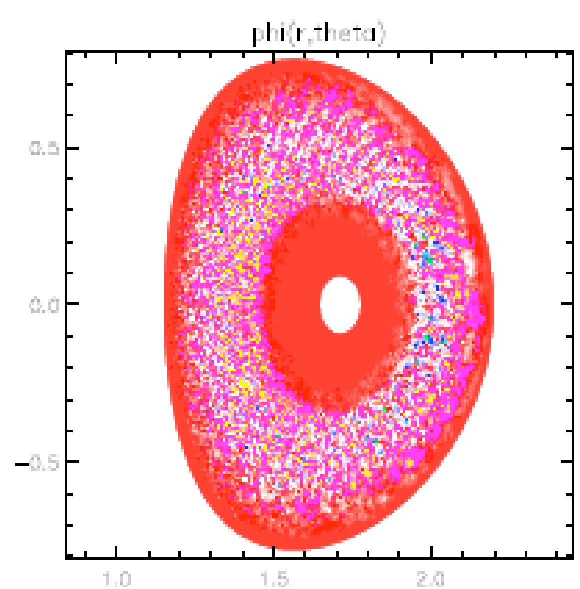
Turbulent transport is a global phenomena

$E \times B$ 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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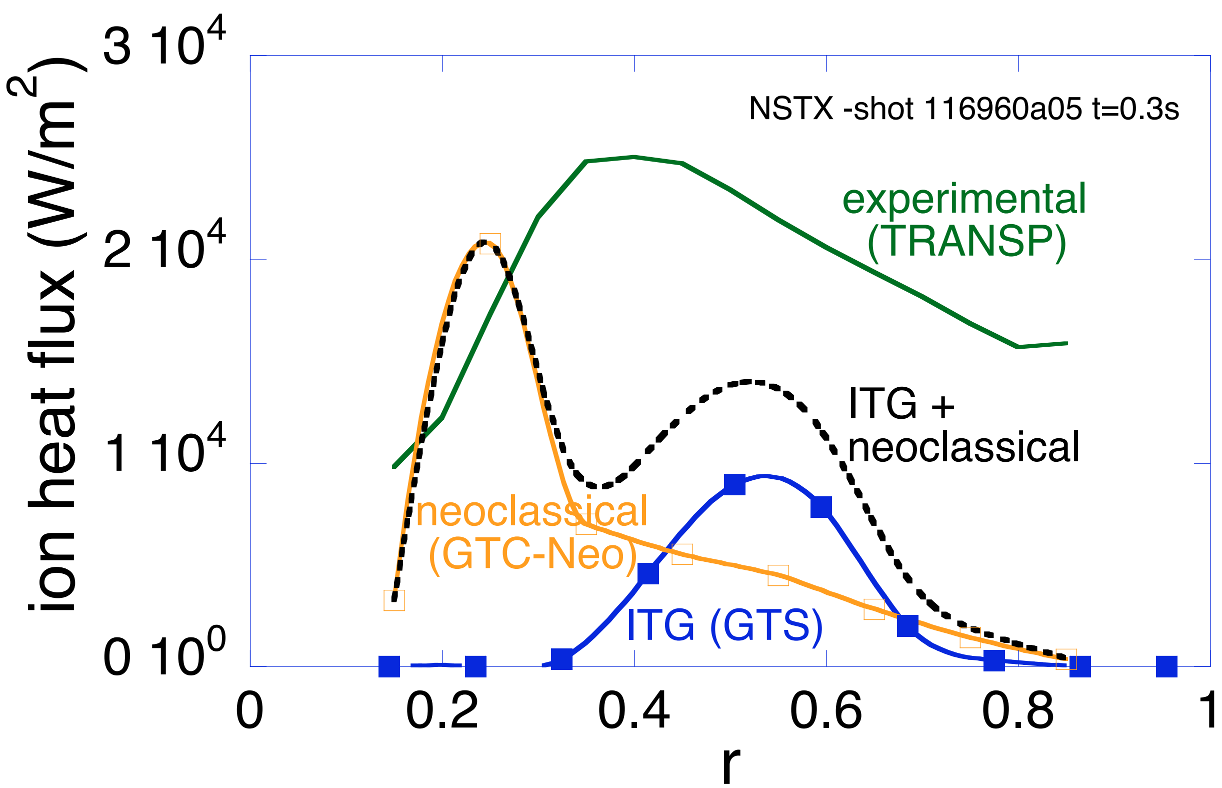
Recent Development of GTC-S and NSTX-physics-oriented Algorithm

- 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!



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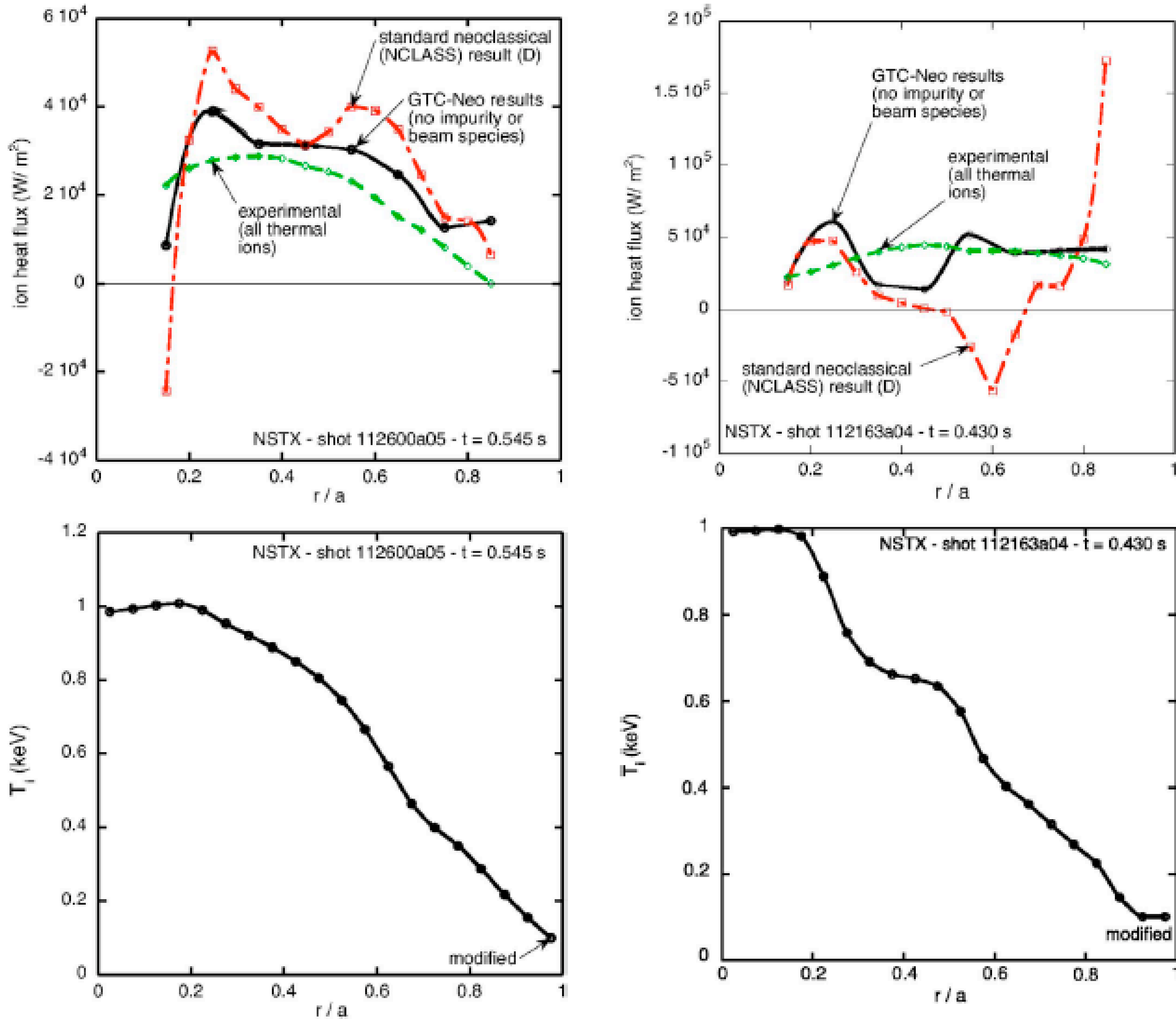
General Geometry GTC-neo

W. X. Wang [PoP, '06]



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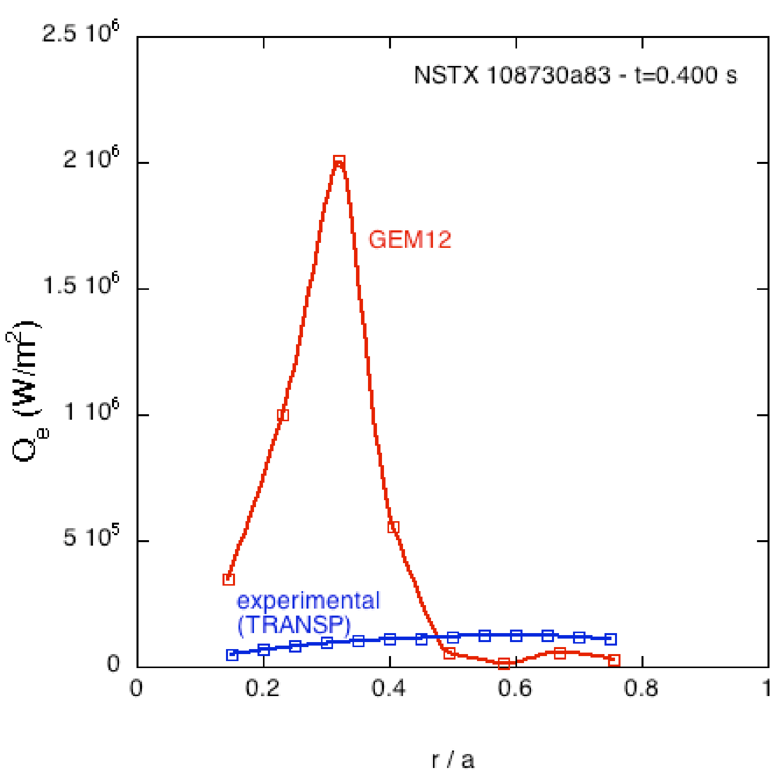
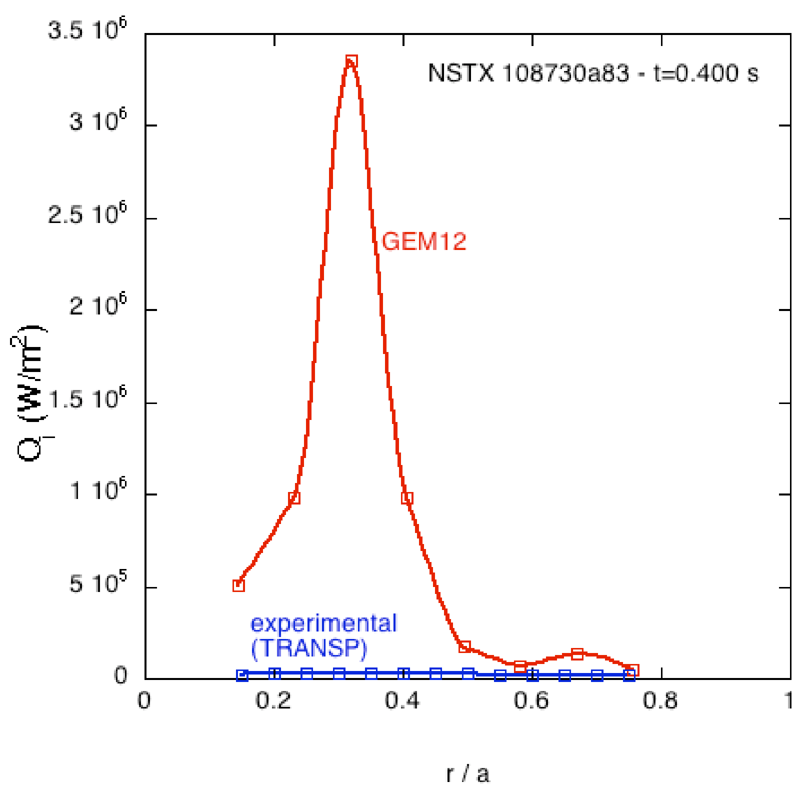
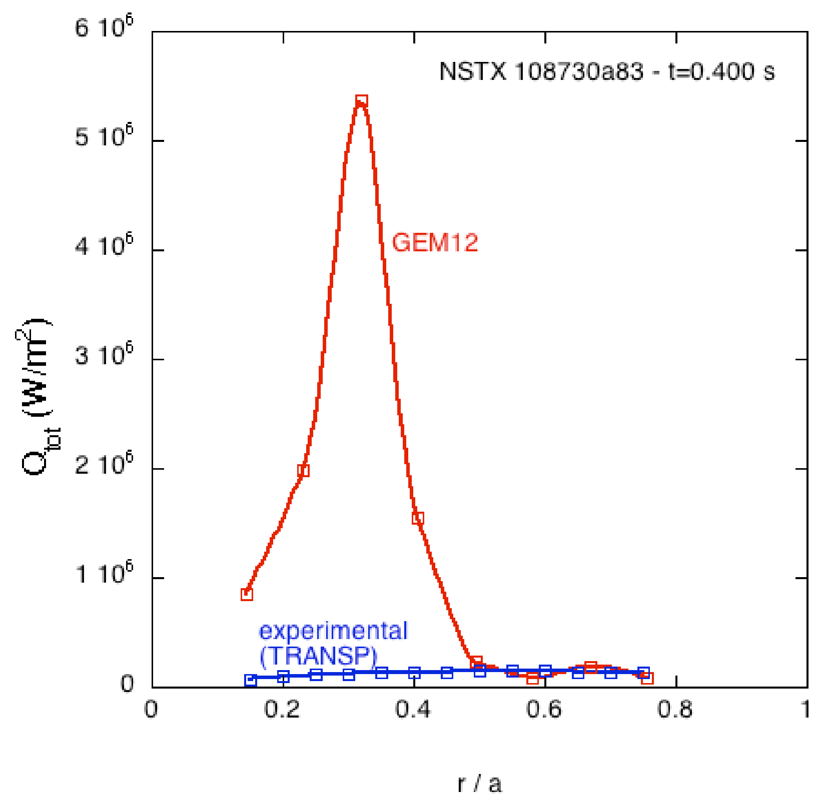
Comparisons of GEM with NSTX: Energy Flux Measurements

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







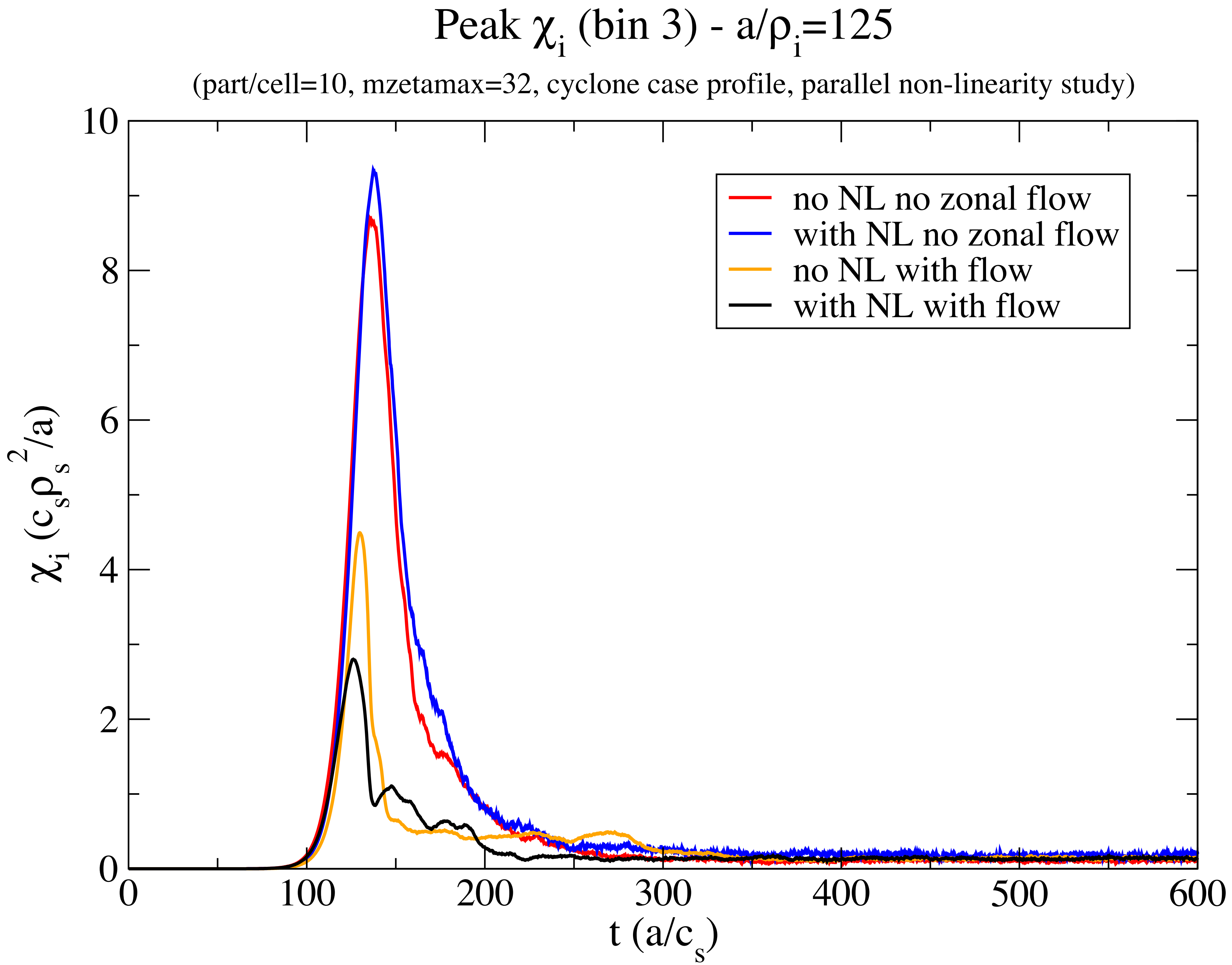
G. Rewoldt and Y. Chen

Colorado PPPL PRINCETON PLASMA PHYSICS LABORATORY

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



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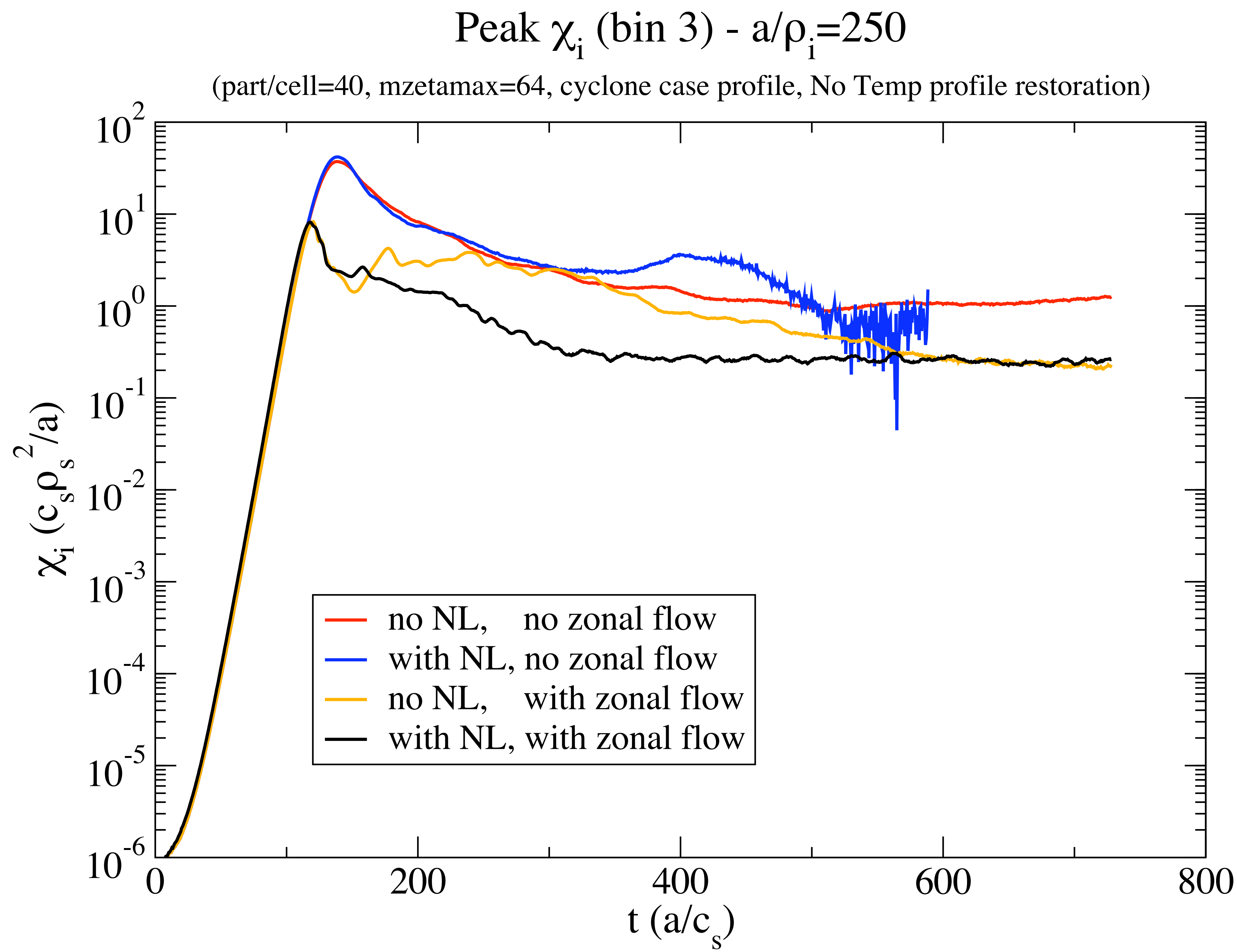
ITG simulations using GTC (cont.)

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



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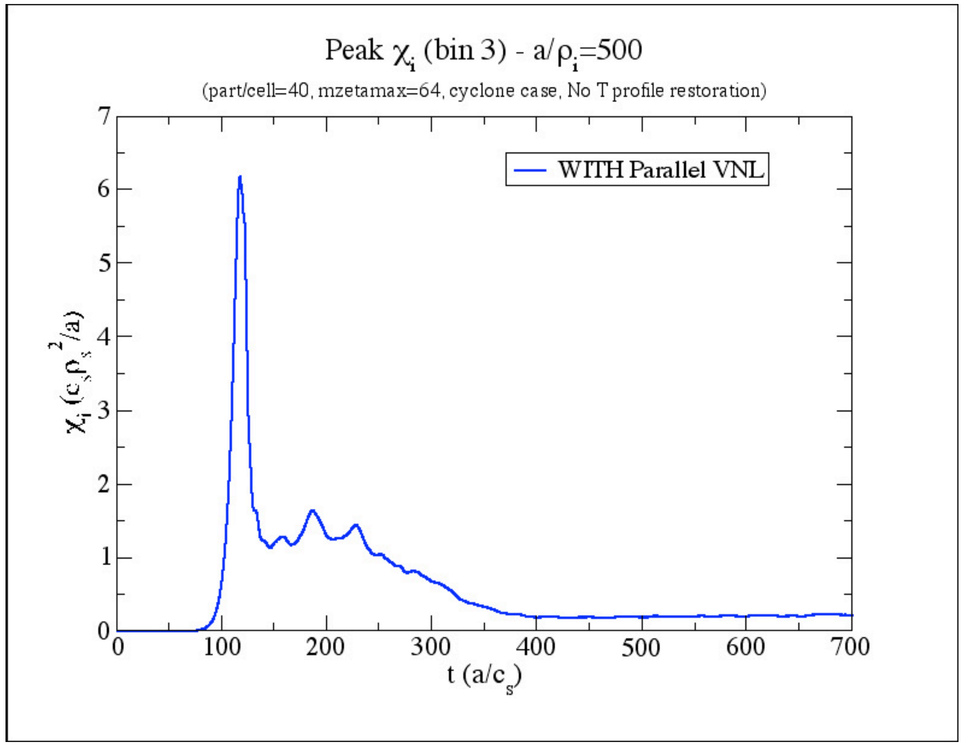
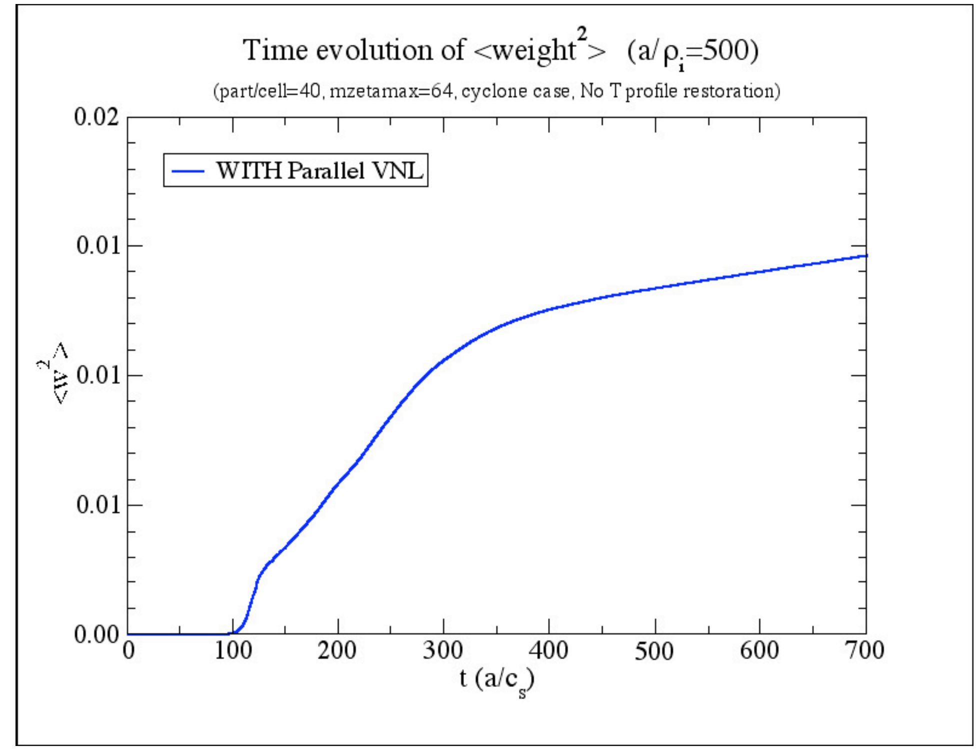
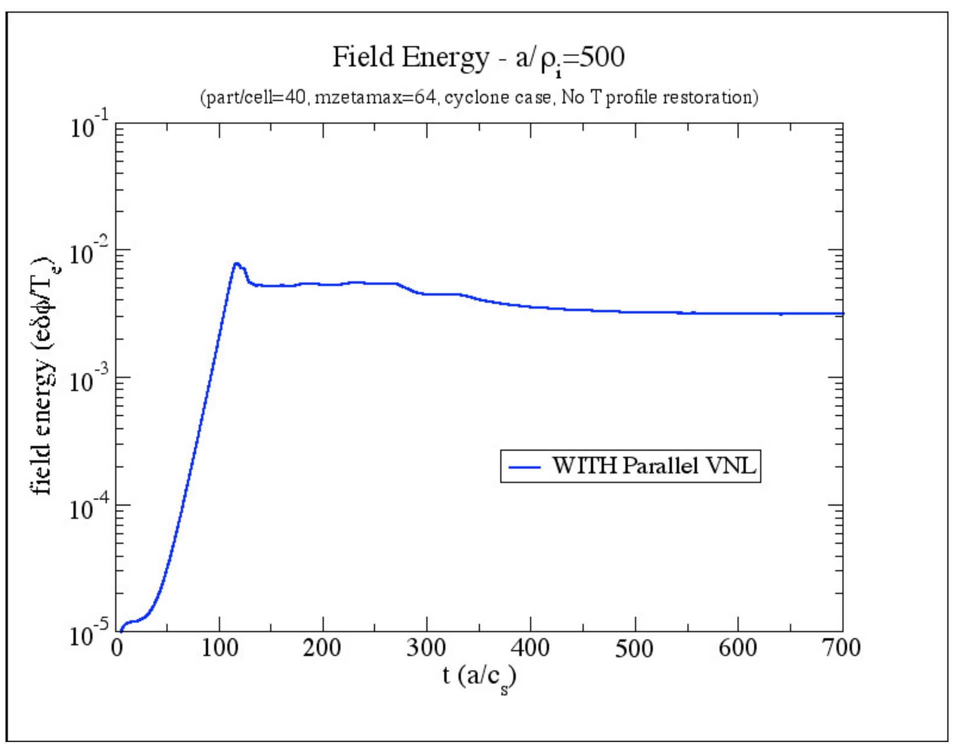
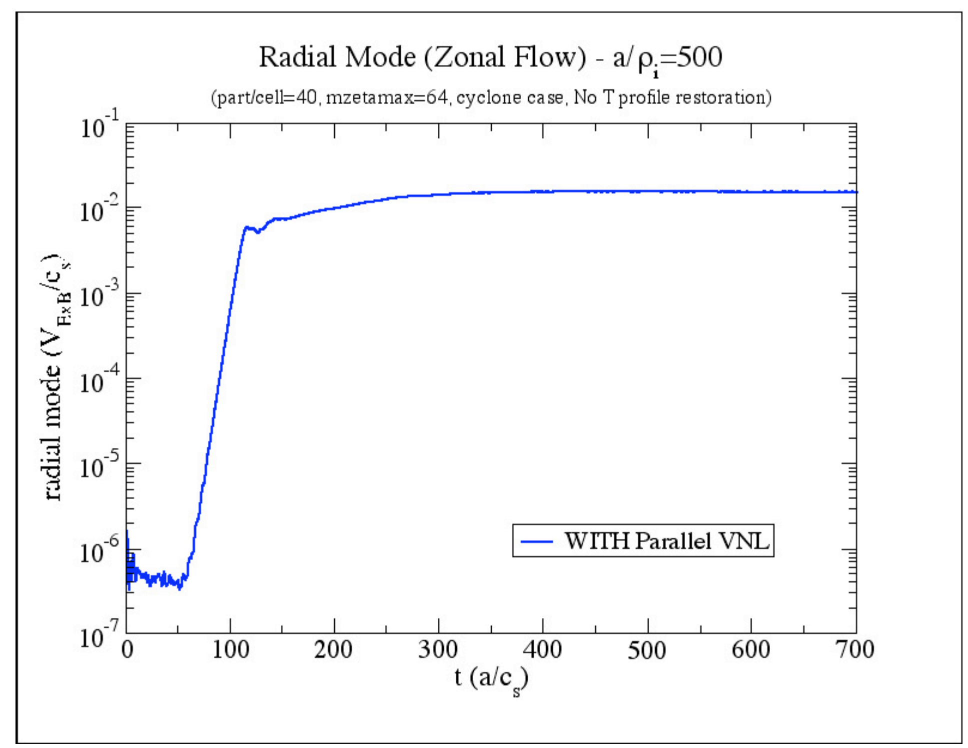
Both zonal flows and velocity-space nonlinearity are essential for maintaining steady state flux for an even larger system ($a/\rho = 500$).









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

Lee, Ethier and Kolesnikov

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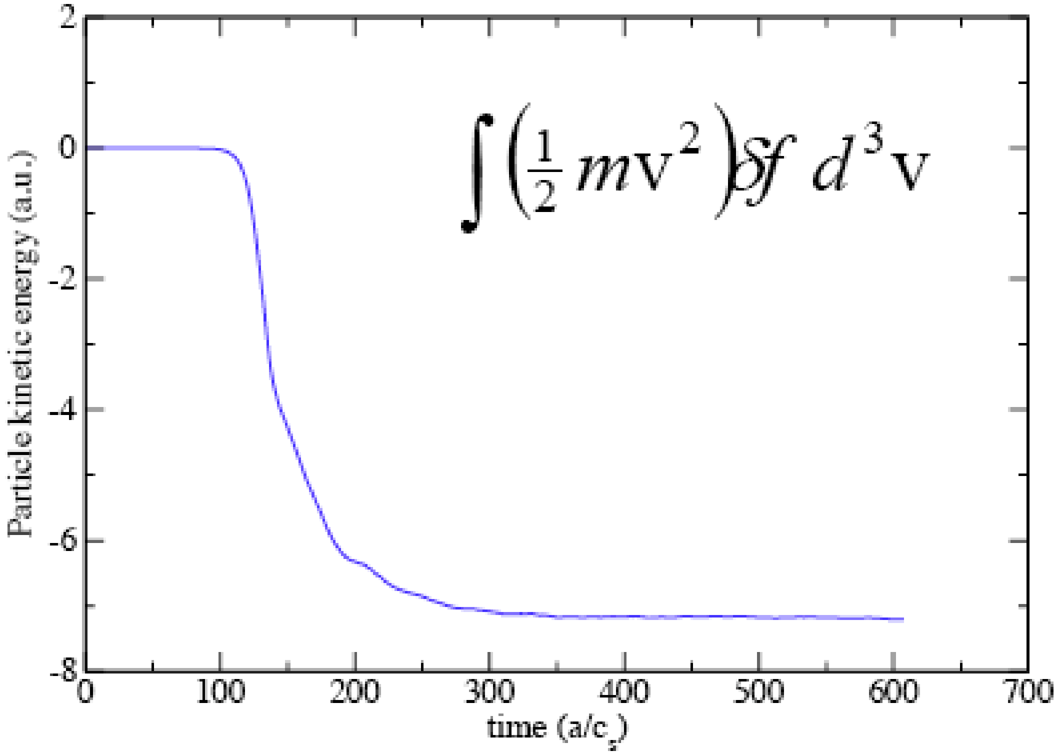
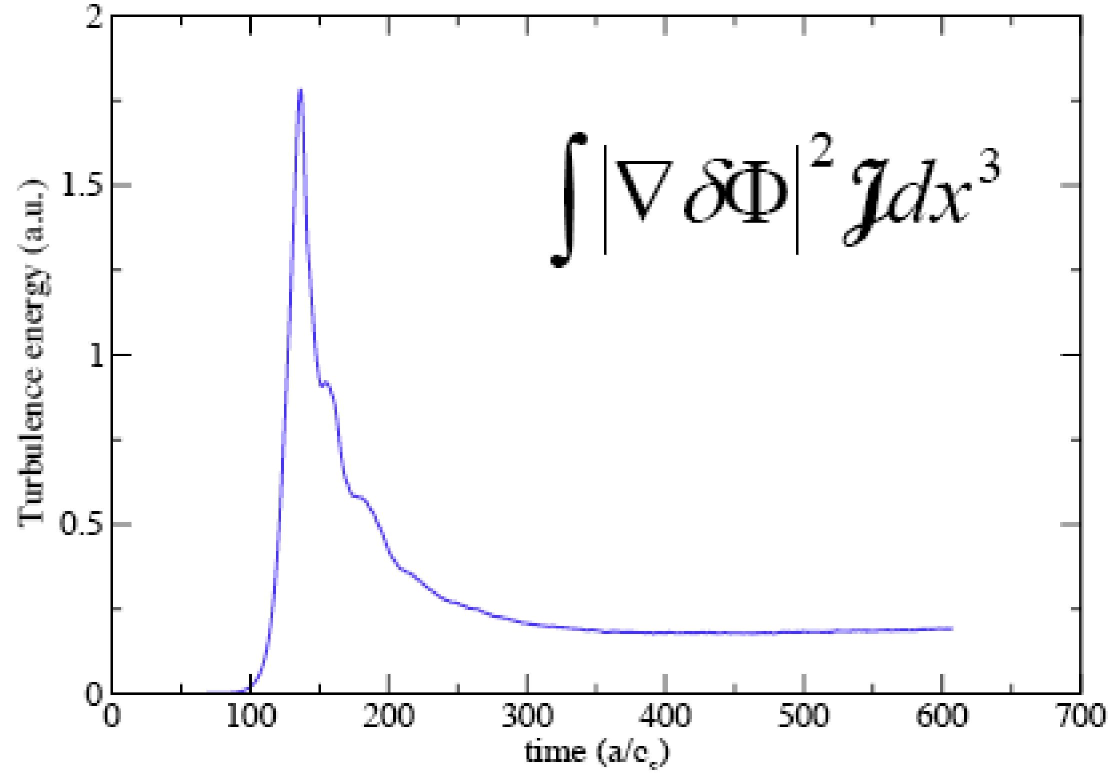
Conservation properties of ITG simulation (20 particles/cell)

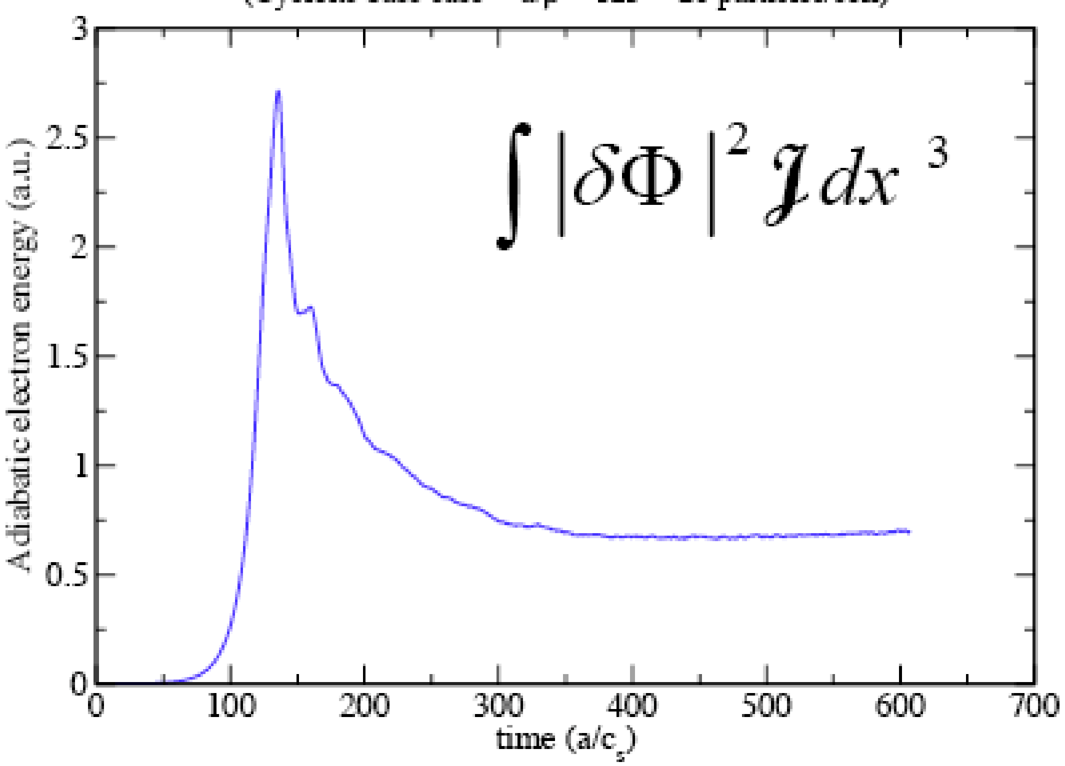
Time evolution of particle energy
(Cyclone base case -- a/ρ = 125 -- 20 particles/cell)



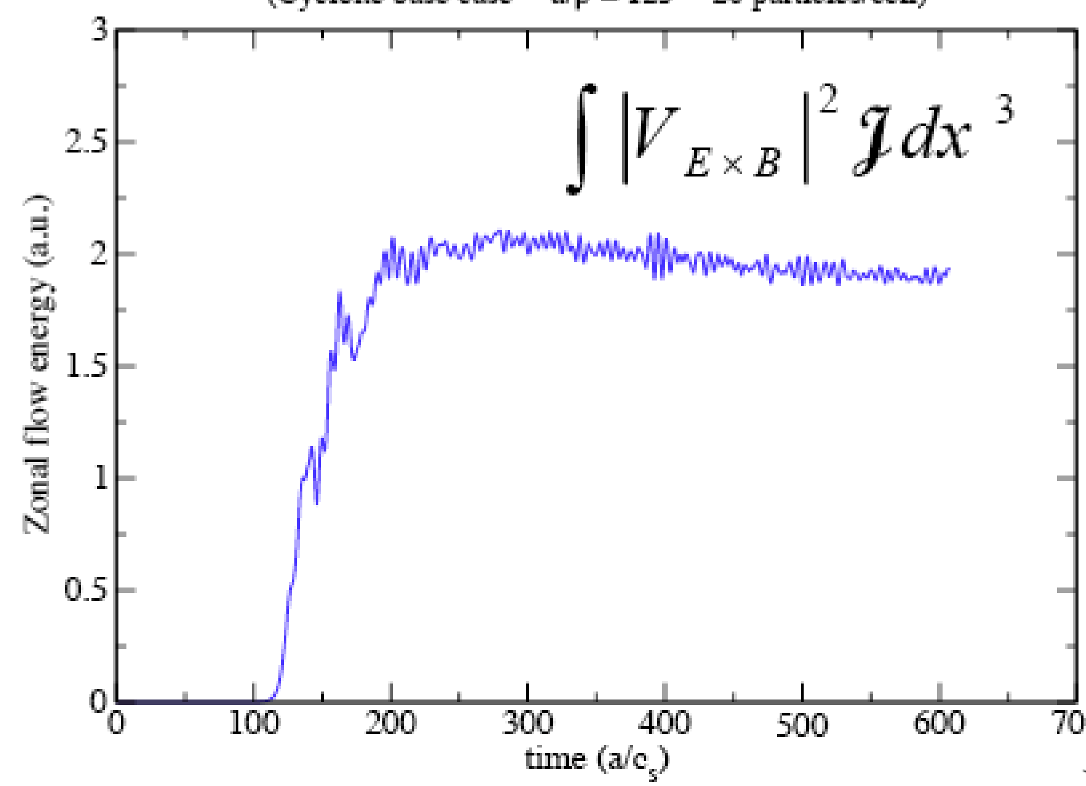
Time evolution of turbulence energy
(Cyclone base case -- a/ρ = 125 -- 20 particles/cell)



Time evolution of adiabatic electron energy
(Cyclone base case -- a/ρ = 125 -- 20 particles/cell)



Time evolution of zonal flow energy
(Cyclone base case -- a/ρ = 125 -- 20 particles/cell)



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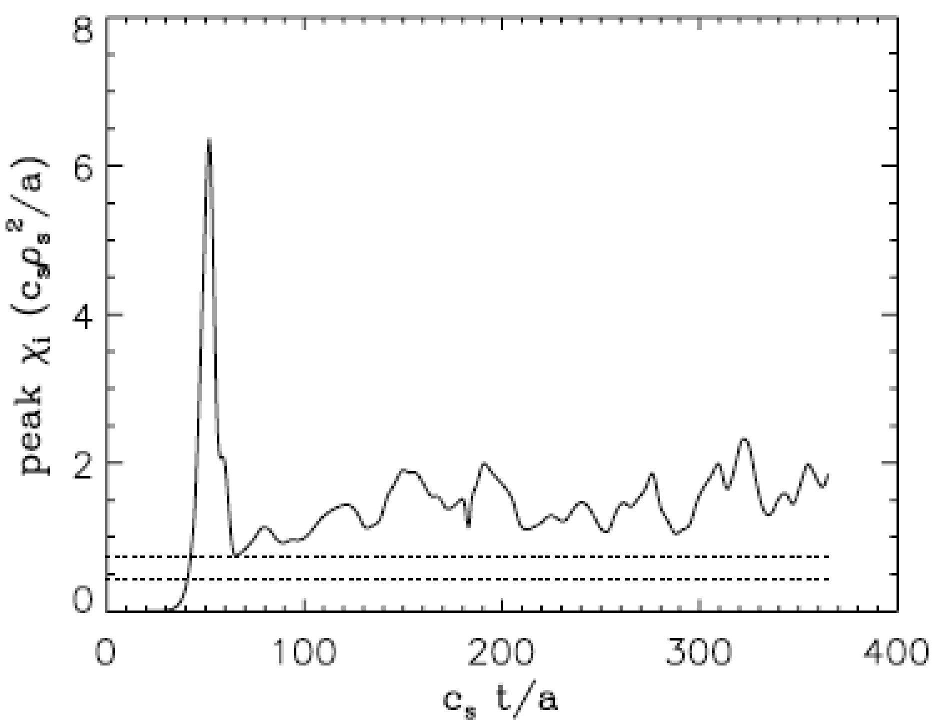
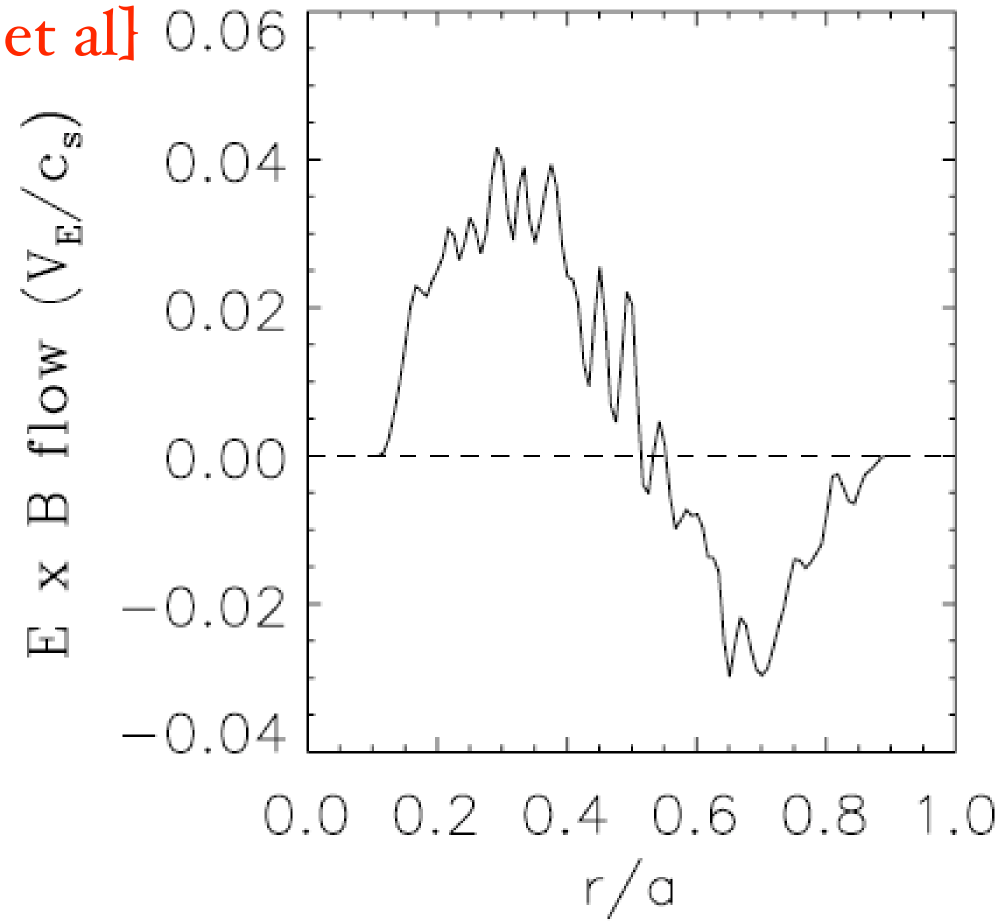
• ITG simulation with kinetic electrons using GTC with the split-weight scheme [Lewandowski et al]



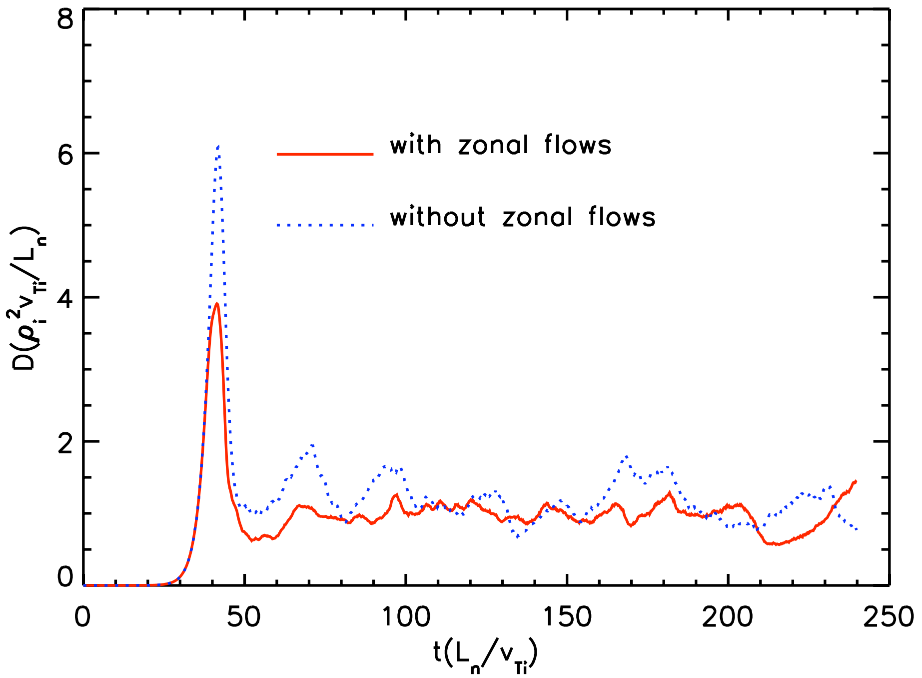


Zonal flows develop finer structures

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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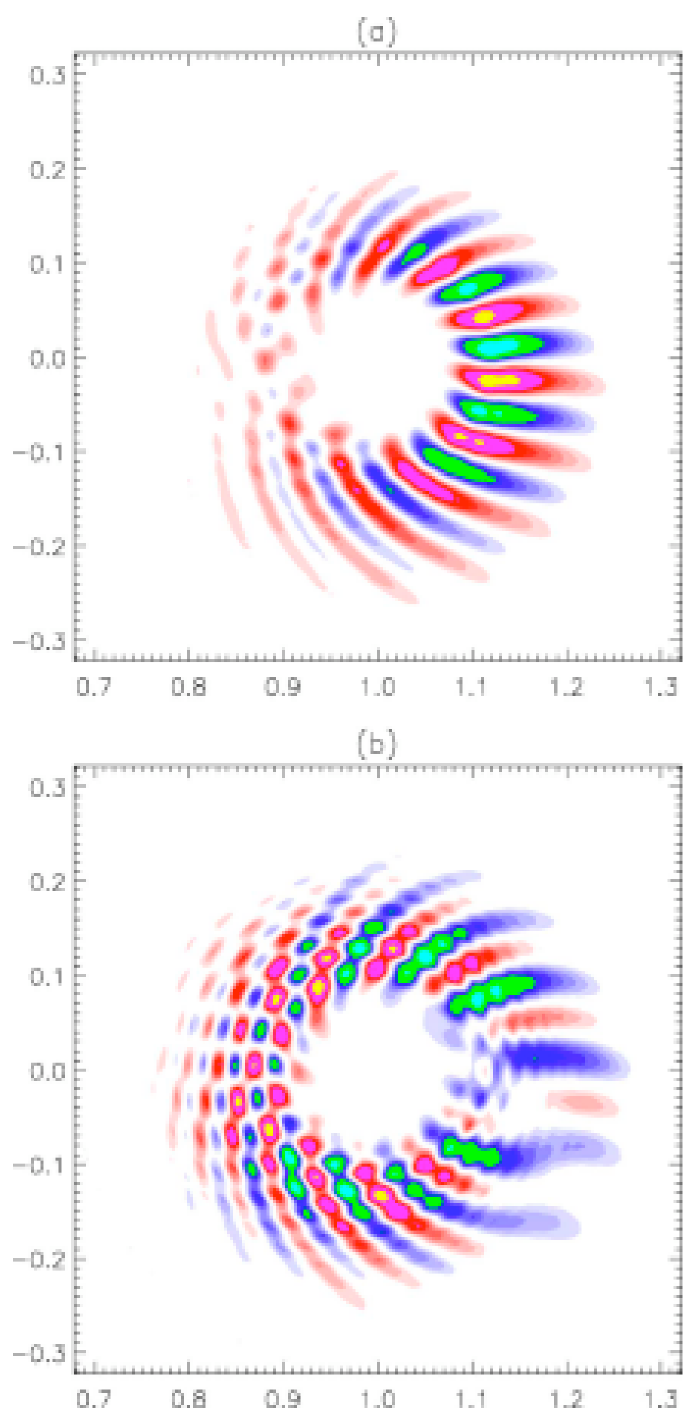
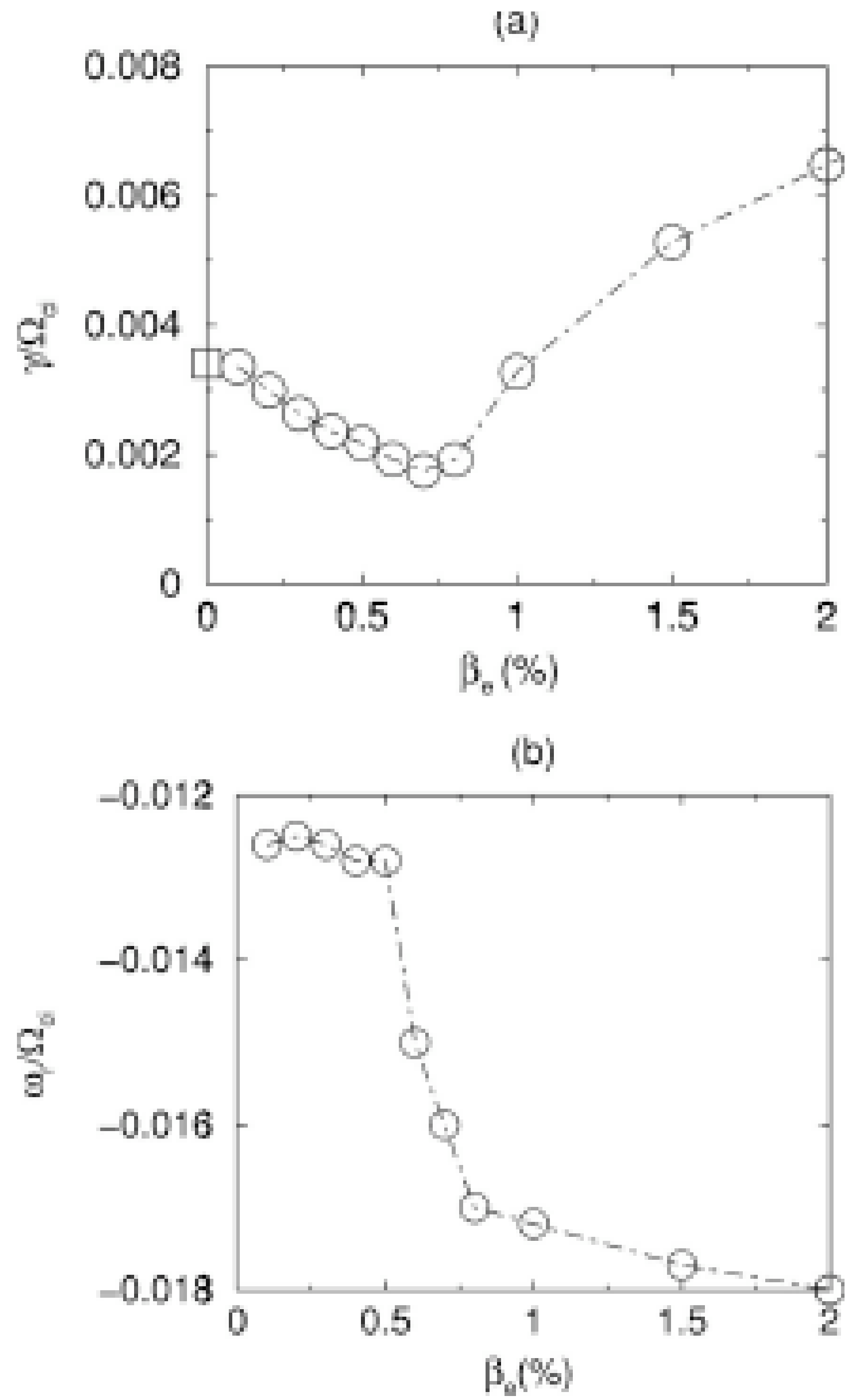
GTC-EM : fluid electron model





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 Magnetic Curvature

Two different mechanisms for non-diffusive momentum flux

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

	Gurcan, Diamond, Hahm, Singh [Phys. Plasmas 14, 042306 '07]	Hahm, Diamond, Gurcan, Rewoldt [Phys. Plasmas, June '07]
Net acceleration of parallel flow:	$-e_i B\nabla_{\|}\delta\phi$	$-m_i c\mathrm{v}_{\|}\nabla\times\hat{b}\cdot\nabla\delta\phi$
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

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

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

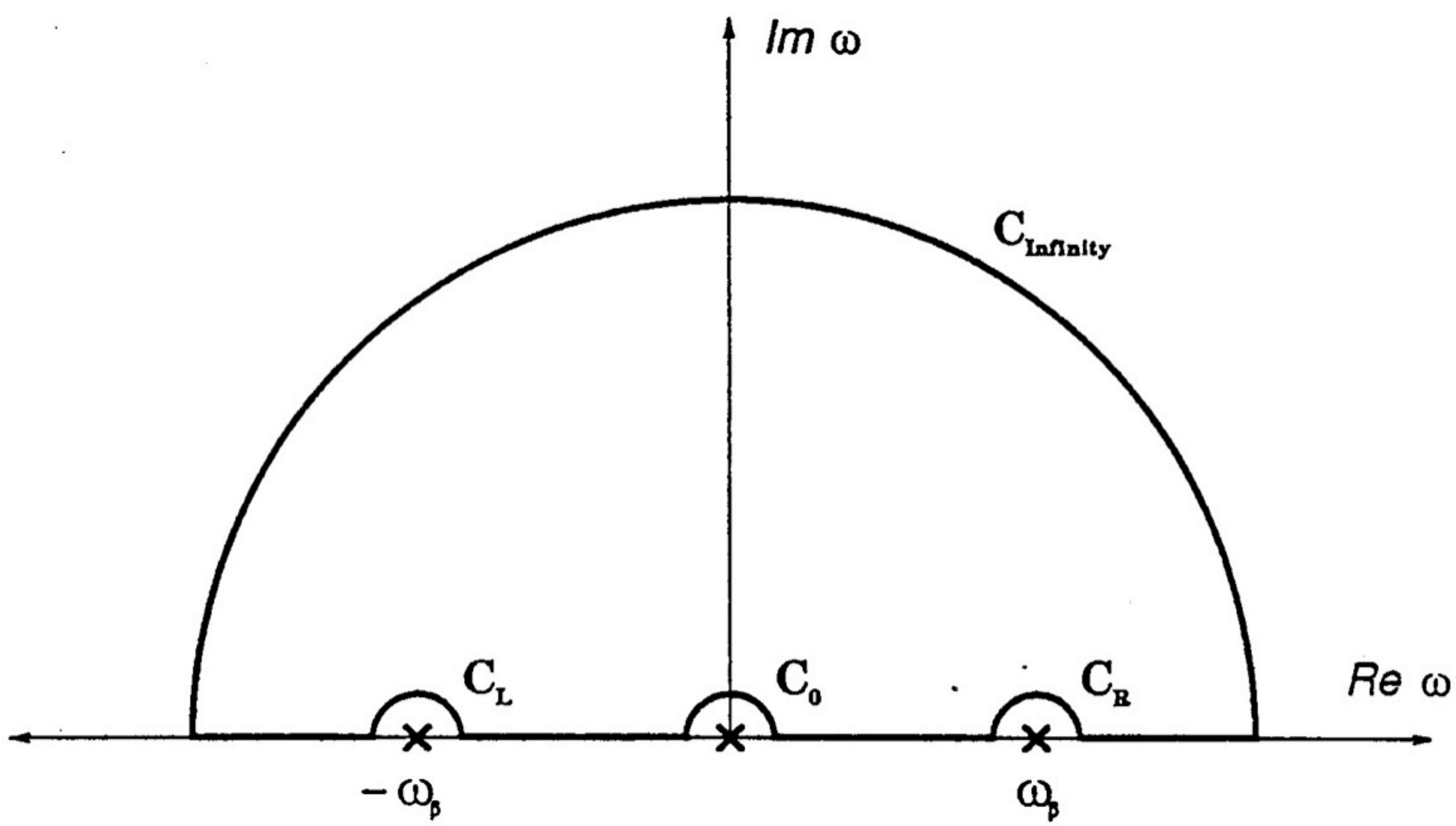


Figure 4.1: Contour integration

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

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

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

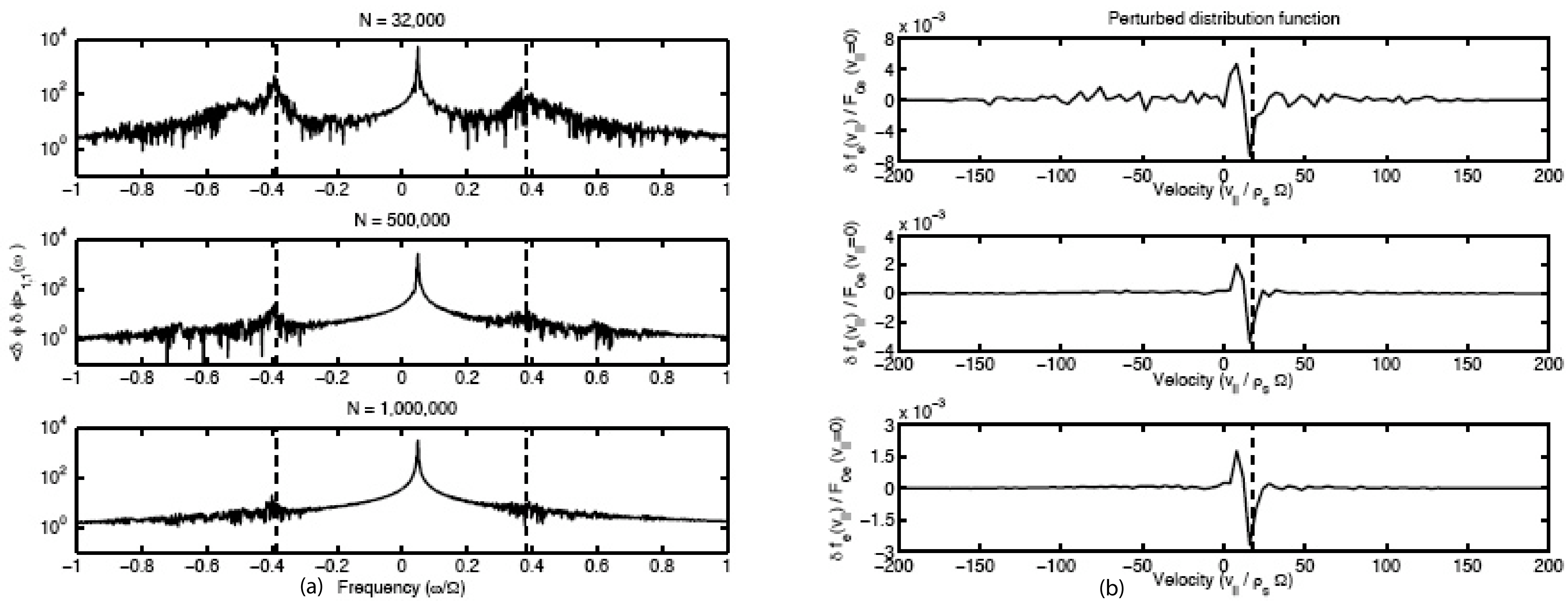
- Nonlinear saturation amplitude

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

[Jenkins and Lee, PoP ‘07]

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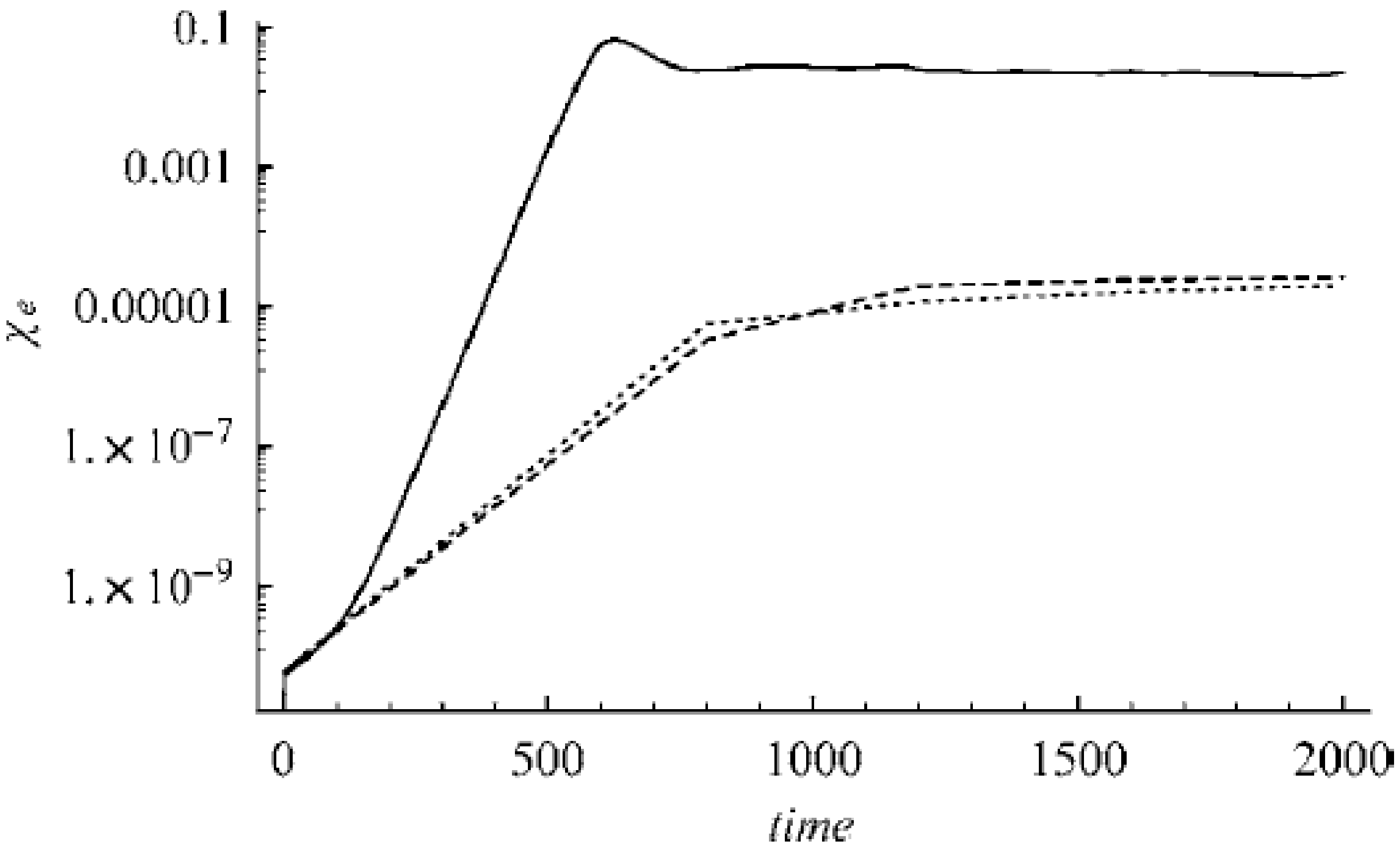
ETG simulation using GTC:
Noise-driven transport vs. fluctuation-driven transport



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]

UCIrvine

Entropy conservation in ITG turbulence:

velocity-space nonlinearity, collisions and numerical noise & dissipation in steady state

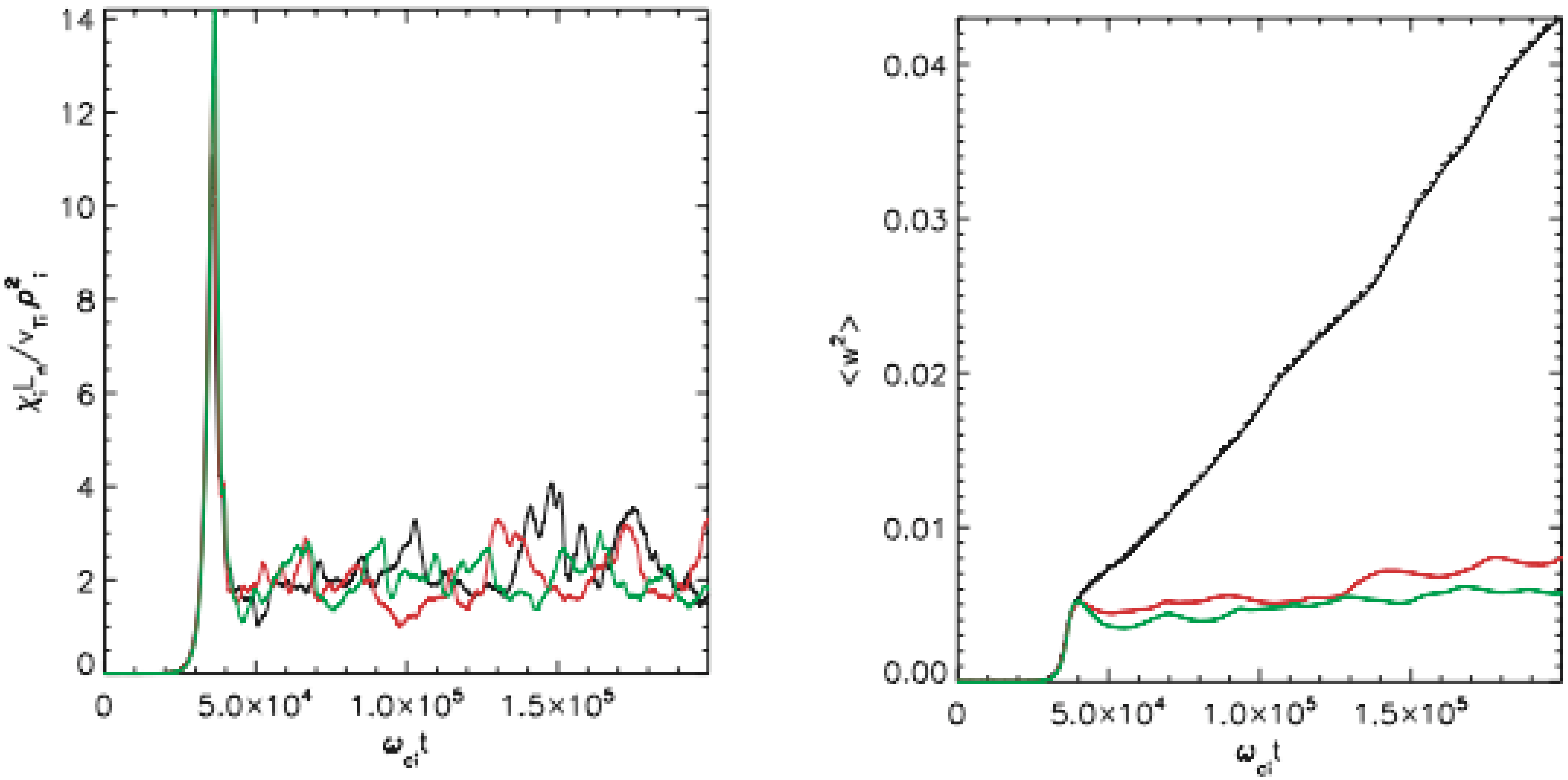
$$\underbrace{\frac{\partial}{\partial t}\langle\int \frac{\delta f_i^2}{F_{0i}}dv_\parallel}_{\text{Monotonic increase in time}}+\underbrace{\tau\phi^2+\tau|\nabla_\perp\phi|^2\rangle}_{\text{Vanishes in steady state}}+\underbrace{\langle\tau\frac{\partial\phi}{\partial x_\parallel}\int v_\parallel\frac{\delta f_i^2}{F_{0i}}dv_\parallel}_{\text{Velocity Space Nonlinearity}}+\underbrace{2\tau\nu\int\frac{dv_\parallel}{F_{0i}}\left(\frac{\partial\delta f_i}{\partial v_\parallel/v_{ti}}+\frac{v_\parallel}{v_{ti}}\delta f_i\right)^2}_{\text{Collisional and/or numerical dissipation}}\rangle=\underbrace{\kappa_{Ti}\langle Q_{ix}\rangle}_{\text{Entropy production}}$$

[Lee and Tang, '88]

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

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

The Growing Weight Problem?
and
The Particle-Continuum Method

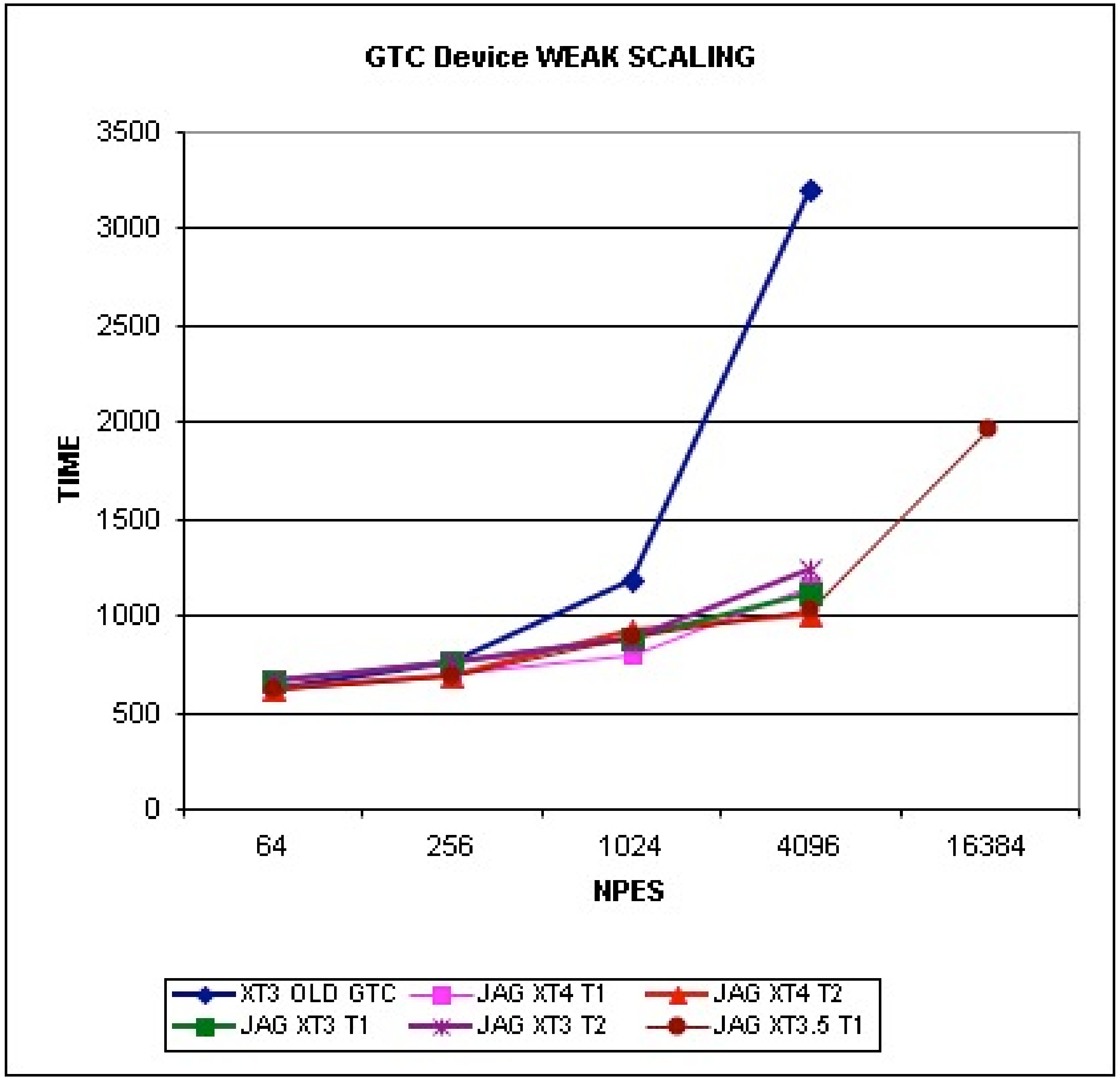


Resetting particle weights on a phase space grid periodically solves the so-called growing weight problem: no re-setting (black) vs. resetting (green and red)

[Chen and Parker]

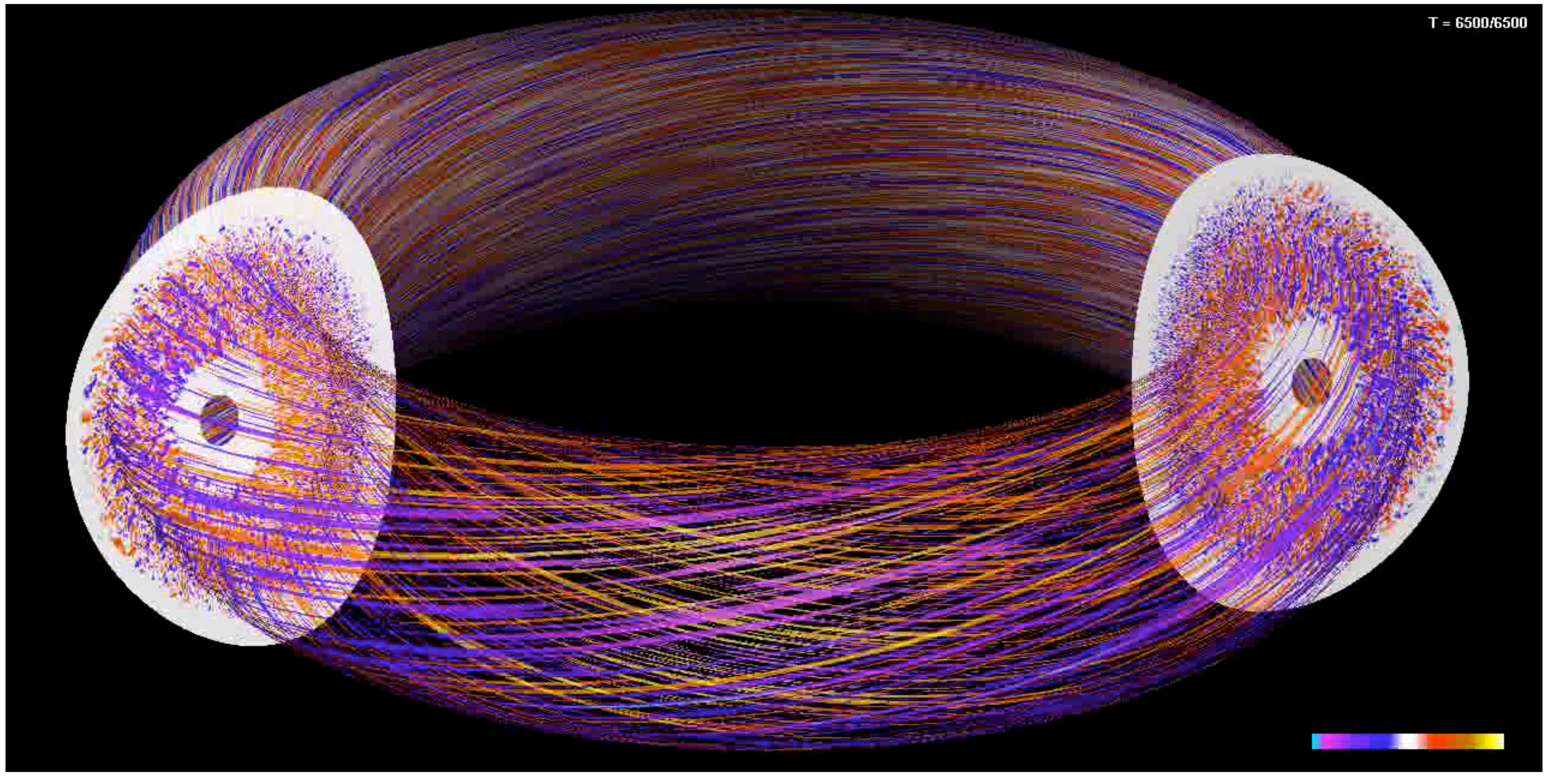
Colorado

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

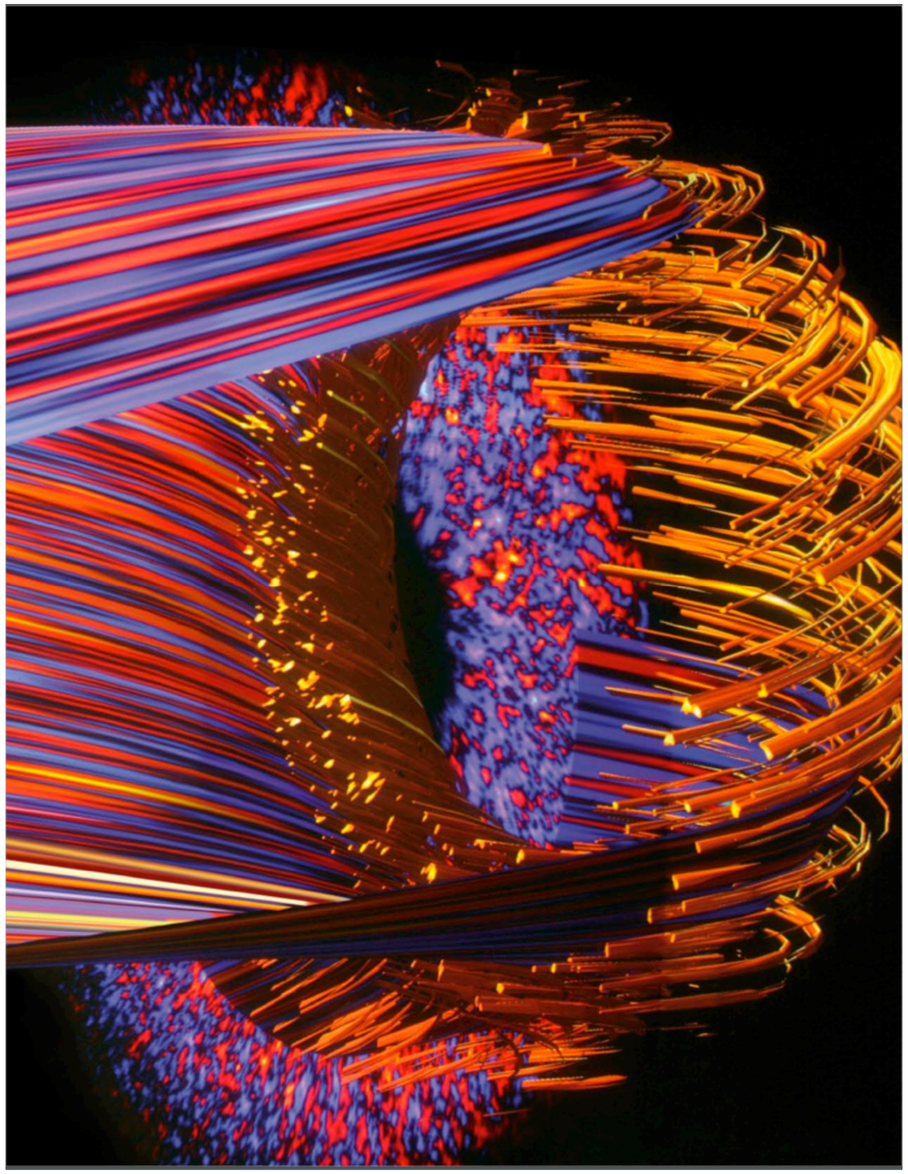


- It is important for simulating ITER-size devices
- Scaling inefficiencies point to large numbers of Translation Lookaside Buffer (TLB) misses on some processes on XT4/3 with larger grids.

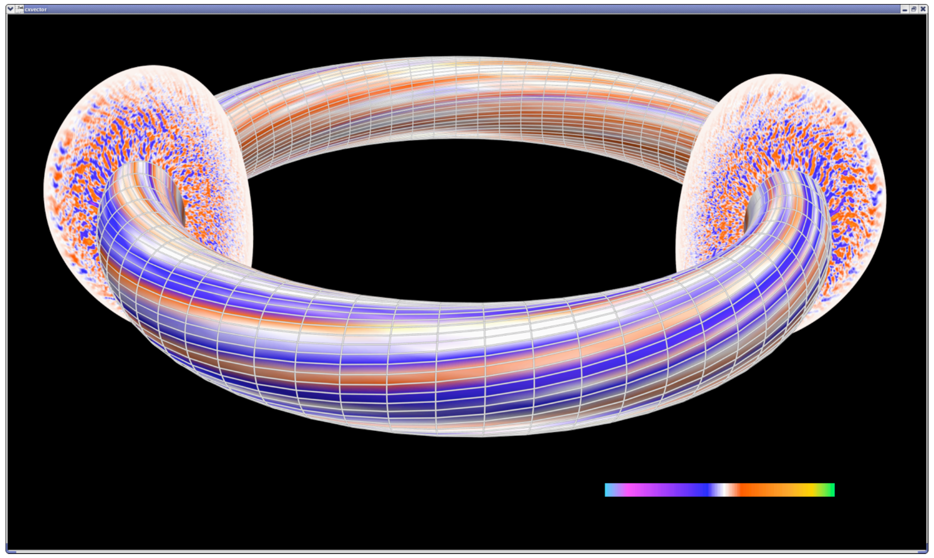
Visualization



[Klasky, ORNL; Ethier, Wang, PPPL]



[Klasky, ORNL; Ethier, Wang, PPPL]



[Ma, UC-Davis]

UCDAVIS

Oak Ridge National Laboratory

PPPL Princeton Plasma Physics Laboratory

Conclusions

- It has been an exciting three years

- Too bad that we can't keep the same team together for the next 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