Gyrokinetic Simulations of Kinetic-MHD Processes in Fusion Plasmas

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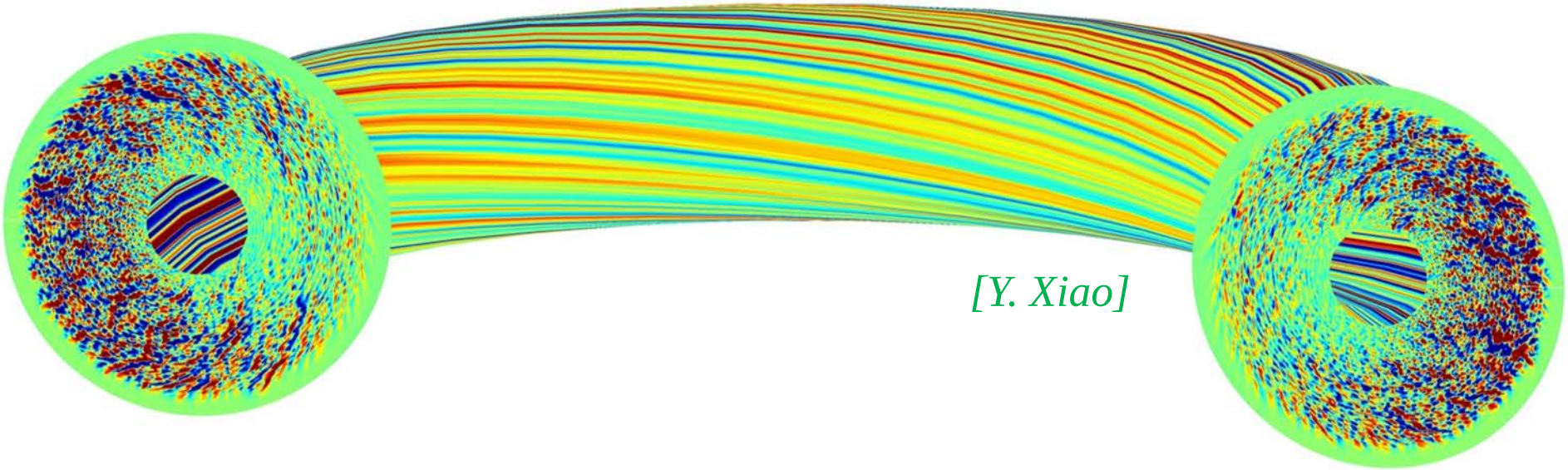
Outlines

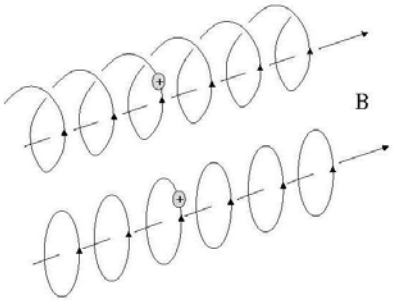
- GTC development strategy
  - Comprehensive simulation platform
  - Collaborative code development
  - Code capability driven by application requirement
- Capability for simulation of microturbulence
- Capability for simulation of kinetic-MHD
- Capability for simulation of RF heating & current drive



Gyrokinetic Simulation of Plasma Turbulence

- Nonlinear gyrokinetic equation (GKE) in 5D phase space (**R**, $v_{||}$,μ) for low frequency driftwave turbulence *[Lee, PoF1983]*

$$\frac{\partial F}{\partial t} + (v_{||}\mathbf{b} + \mathbf{v}_d) \cdot \frac{\partial F}{\partial \mathbf{R}} + \dot{v}_{||} \frac{\partial F}{\partial v_{||}} = 0$$

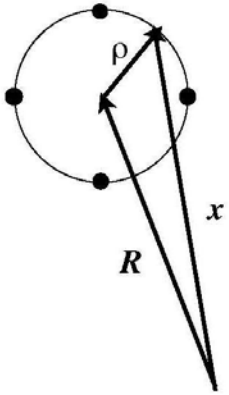


- Poisson equation in long wavelength limit

$$\frac{\rho_s^2}{\lambda_D^2} \nabla_\perp^2 \phi = 4\pi e (n_e - Z\overline{n}_i)$$

- Ampere's Law

$$\nabla_\perp^2 A_{||} = \frac{4\pi e n_0}{c} (u_e - Z\overline{u}_i)$$



- Particles (kinetic): electrons, thermal ions, fast ions etc

- Fields (fluid): density, temperature, electromagnetic fields etc

Magnetic Coordinates for Toroidal Geometry

- Magnetic coordinate (ψ, θ, ζ)

$$\mathbf{B} = \nabla\psi \times \nabla\theta + \frac{1}{q}\nabla\zeta \times \nabla\psi$$

$$\mathbf{B} = B_\psi \nabla\psi + B_\theta \nabla\theta + B_\zeta \nabla\zeta$$

- Flux surface: $\mathbf{B} \cdot \nabla\psi = 0$

- Straight field line: $\dfrac{\mathbf{B}\cdot\nabla\zeta}{\mathbf{B}\cdot\nabla\theta} = q$

  - Efficient for integrating particle orbits & discretizing field-aligned mode

- Boozer coordinates *[Boozer, PoF1981]*: $J=(gq+I)/B^2 \sim X^2$

Guiding Center Equation of Motion

- Gyrocenter Hamiltonian *[White & Chance, PF1984]*

$$H = \frac{1}{2}\rho_{\parallel}^{2}B^{2} + \mu B + \bar{\phi}$$

- Canonical variables in Boozer coordinates

$$P_{\theta} = I\rho_{\parallel} + \psi$$
$$P_{\zeta} = g\rho_{\parallel} - \psi_{p}$$

- Equation of motion

$$\frac{dP_{\theta}}{dt} = -\frac{\partial H}{\partial \theta}, \frac{d\theta}{dt} = \frac{\partial H}{\partial P_{\theta}}$$
$$\frac{dP_{\zeta}}{dt} = -\frac{\partial H}{\partial \zeta}, \frac{d\zeta}{dt} = \frac{\partial H}{\partial P_{\zeta}}$$

- Only scalar quantities needed, conserve phase space volume

Collisions: Monte-Carlo Method

- Electron-ion pitch angle $\xi = v_{\|}/v$ scattering in ion frame: Lorentz operator

$$C_{ei}(\delta f_e) = \upsilon_0 \frac{1}{2}\frac{\partial}{\partial \xi}(1-\xi^2)\frac{\partial}{\partial \xi}\delta f_e$$

$$\xi = \xi_0(1-\upsilon\Delta t) + (r-0.5)[12(1-\zeta_0{}^2)\upsilon\Delta t]^{1/2}$$

- Linear like-species guiding center collision operator *[Xu & Rosenbluth, PFB1991]*

$$C(\delta f) = C(\delta f, F_0) + P(F_0, \delta f) = P(F_0, \delta f) + \frac{\partial}{\partial v_{\|}}(\upsilon_{s\|}\delta f) + \frac{\partial}{\partial v_{\perp}{}^2}(\upsilon_{s\perp}\delta f)$$
$$+ \frac{\partial^2}{\partial_{\|}\partial v_{\perp}{}^2}(\upsilon_{\|\perp}\delta f) + \frac{1}{2}\frac{\partial^2}{(\partial v_{\|})^2}(\upsilon_{\|}\delta f) + \frac{1}{2}\frac{\partial^2}{(\partial v_{\perp}{}^2)^2}(\upsilon_{\perp}\delta f)$$

- Conserve momentum and energy [Dimits & Cohen, PRE1994], preserve Shifted Maxwellian *[Lin et al, PoP1995]*

$$\Delta w = -3\sqrt{\frac{\pi}{2}}\phi(x)(\frac{v_{th}}{v})^3 v_{\|}\delta P - 3\sqrt{\frac{\pi}{2}}[\phi(x) - \frac{d\phi(x)}{dx}]\frac{v_{th}}{v}\delta E$$

- Application for effects of finite orbit size in neoclassical transport: resolving an discrepancy between standard neoclassical theory and DIII-D experiment *[Lin et al, PRL1997]*

Toroidal Perturbative Method

- Perturbative method: discrete particle noise reduced by $(\delta f/f)^2$
  [Dimits & Lee, PF1993; Parker & Lee, PF1993; Hu & Krommes, PoP1994]

- ES GK equation: $Lf(\mathbf{R}, v_{||}, \mu)=0$

$$L = \frac{\partial}{\partial t} + (v_{||}\mathbf{b} + \mathbf{v}_d + \mathbf{v}_{E\times B})\cdot\frac{\partial}{\partial \mathbf{R}} - \mathbf{b}^*\cdot\nabla(\mu B + \Phi)\frac{\partial}{\partial v_{||}}$$

- Define $f=f_0+\delta f$, $L=L_0+\delta L$, $L_0 f_0=0$,
  then $L\delta f=-\delta L f_0$

$$L_0 = \frac{\partial}{\partial t} + (v_{||}\mathbf{b} + \mathbf{v}_d)\cdot\frac{\partial}{\partial \mathbf{R}} - \mathbf{b}^*\cdot\nabla(\mu B)\frac{\partial}{\partial v_{||}}$$

- F_0: arbitrary function of constants of motion in collisionless limit.

  Canonical Maxwellian *[Idomura, PoP2003]*

- Neoclassical δf simulation *[Lin et al, PoP1995]*
  $f_0=f_M+f_{02}$, $L_0=L_{01}+L_{02}$, $L_{01}f_M=0$, $L_0 f_{02}=-L_{02}f_M$

$$L_{01} = \frac{\partial}{\partial t} + v_{||}\mathbf{b}\cdot\frac{\partial}{\partial \mathbf{R}} - \mathbf{b}^*\cdot\nabla(\mu B)\frac{\partial}{\partial v_{||}} - C$$

Poisson Solver

$$\frac{\tau}{\lambda_D^{\,2}}(\phi-\tilde{\phi})=4\pi e(\delta\overline{n}_i-\delta n_e)$$

- Gyrokinetic Poisson equation *[Lee, JCP1987]*
- Polarization density

$$\tilde{\phi}(\mathbf{x})=\overline{<\bar{\phi}(\mathbf{R})F_{\mathbf{M}}>}$$
$$\tilde{\phi}_k=\Gamma_0\phi_k$$

- Solve in *k*-space: Pade approximation

$$\Gamma_0\approx 1/[1+(k_\perp\rho_i)^2]$$

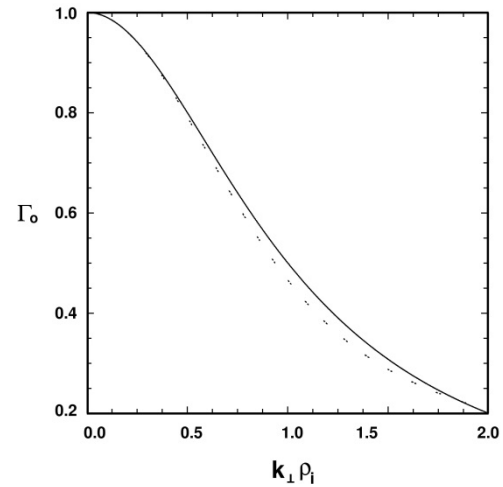
- Solve in real space *[Lin & Lee, PRE1995]*

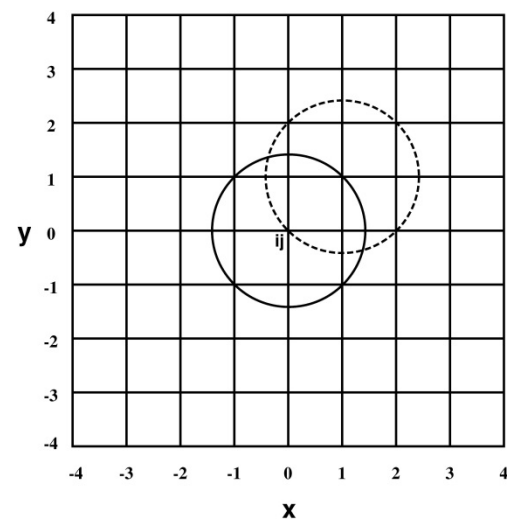
$$\Gamma_0(k_\perp\rho_i)=\int J_0^{\,2}(\frac{k_\perp v_\perp}{\Omega})F_{\mathbf{M}}(\mu)d\mu\approx\sum_j c_j J_0^{\,2}(\frac{k_\perp v_{\perp j}}{\Omega})$$

- Need to invert extremely large matrix

$$\sum_{m,n}c_{mnij}\phi_{mn}=(\delta n_i-\delta n_e)_{ij}$$

- Iterative method: good for electrostatic
- Electromagnetic: PETSc





Numerical Methods

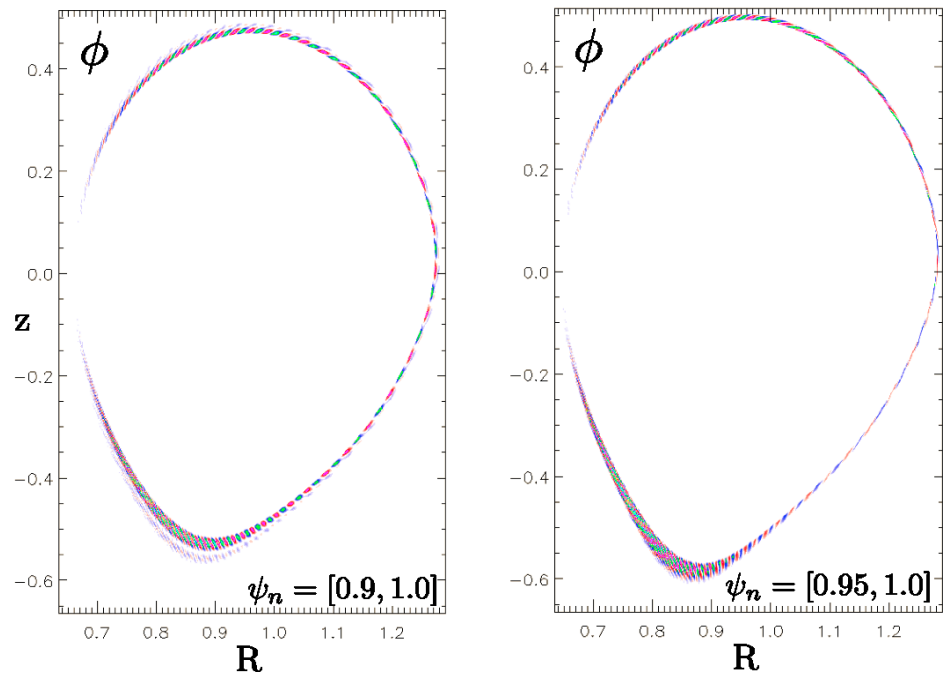
- 2D spline function for equilibrium data from EFIT etc [*Xiao, BOUT++ workshop*]
- Gyroaveraging: performed on poloidal plane (ζ=*constant*)
  - Assuming $k_{\parallel} << k_{\perp}$
  - Gyro-orbit elliptic
  - Linearized

$$\bar{\phi}(\mathbf{R}) = \overline{\phi(\mathbf{x}+\boldsymbol{\rho})}$$

$$\boldsymbol{\rho} = \frac{v}{v_{th}}\boldsymbol{\rho}_{th}$$

- No fluctuation at radial boundary
- Numerical filter

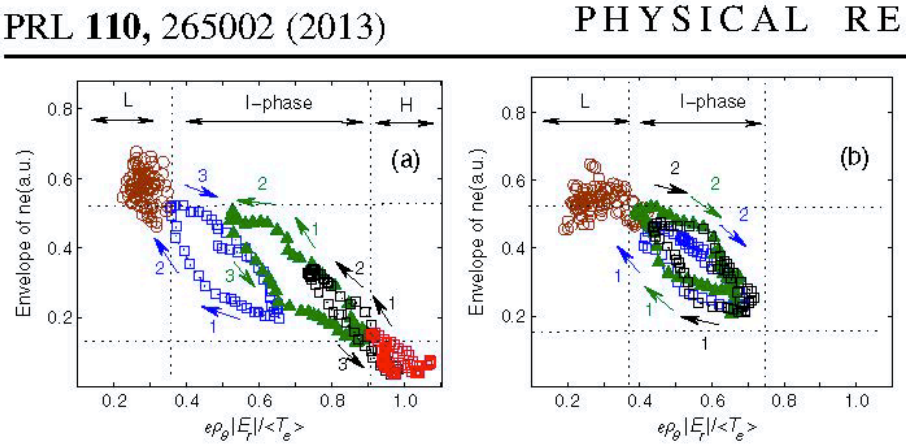
DIII-D shot # 131997

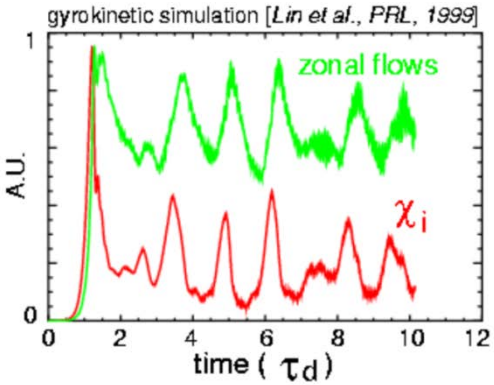


Application: Turbulence Self-regulation by Zonal Flows

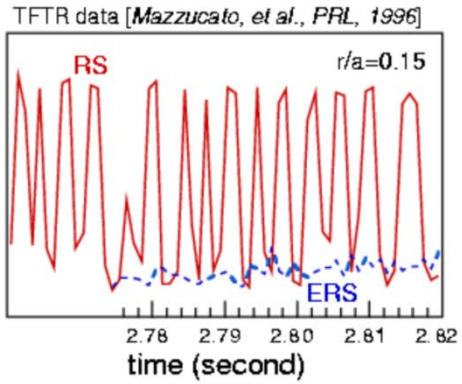
- GTC global gyrokinetic simulation finds self-regulation of turbulence by zonal flow (ZF) [*Lin et al, Science1998*]
- GTC finds that ZF collisional damping induces oscillation of ZF and turbulence intensity with 90° phase shift [*Lin et al, PRL1999*]
- Limit cycle oscillation (LCO) observed in TFTR RS to ERS transition [*Mazzucato et al, PRL1996*]
- LCO with a phase shift observed in HL-2A L-I-H transition [*Cheng et al, PRL2013*]

HL-2A L-I-H





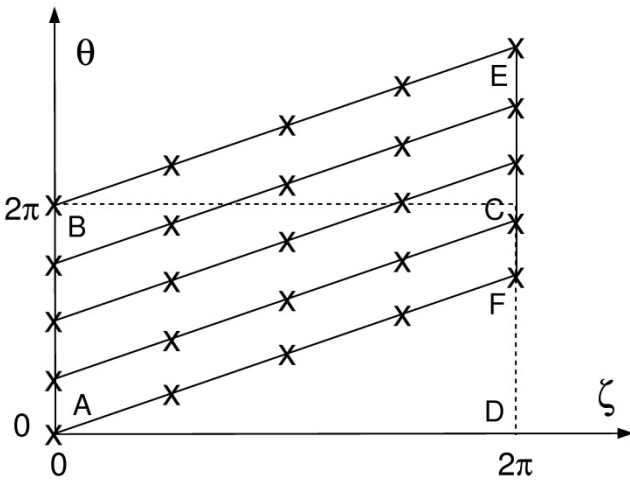
GTC simulation

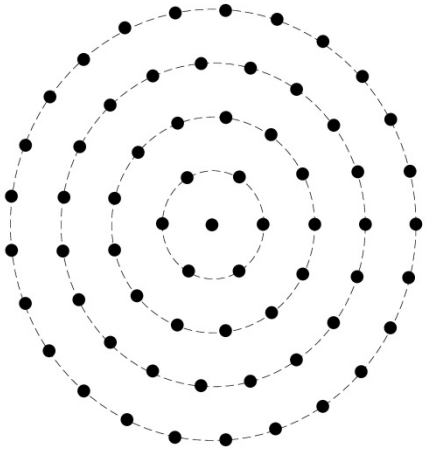


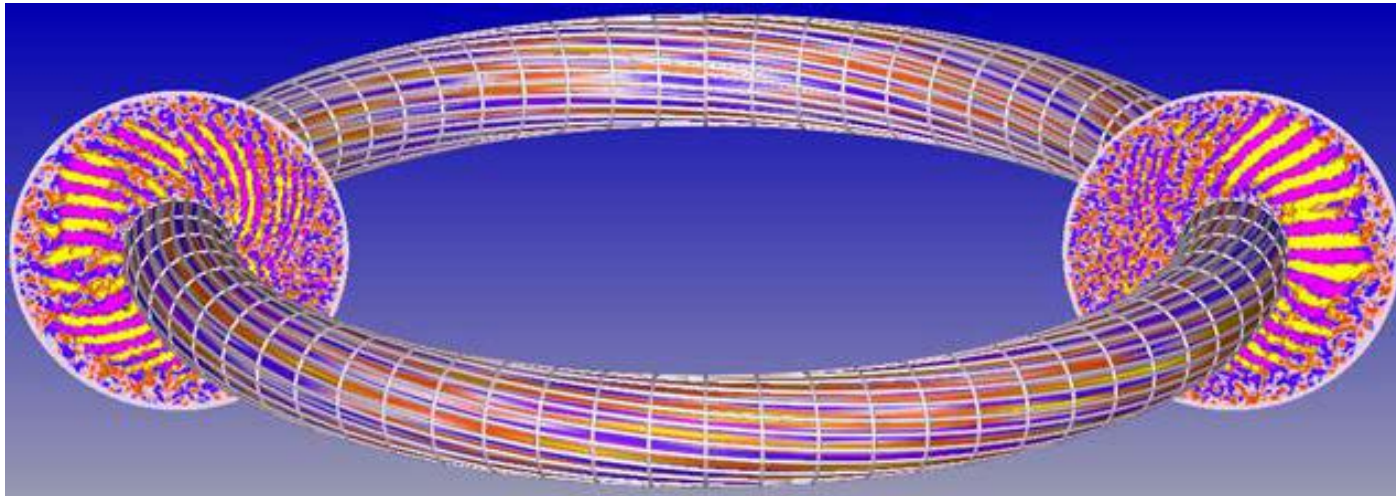
TFTR RS-ERS

Global Field-aligned Mesh in GTC

- Discretization in (ψ,α,ζ)), rectangular mesh in (α,ζ), $\alpha=\theta-\zeta/q$
  - # of computation ~ $(a/\rho)^2$, reduce computation by n
  - No approximation in geometry, loss of ignorable coordinate
  - Twisted in toroidal direction: periodicity preserved
- Decomposition in toroidal mode? ~ $(a/\rho)^3$

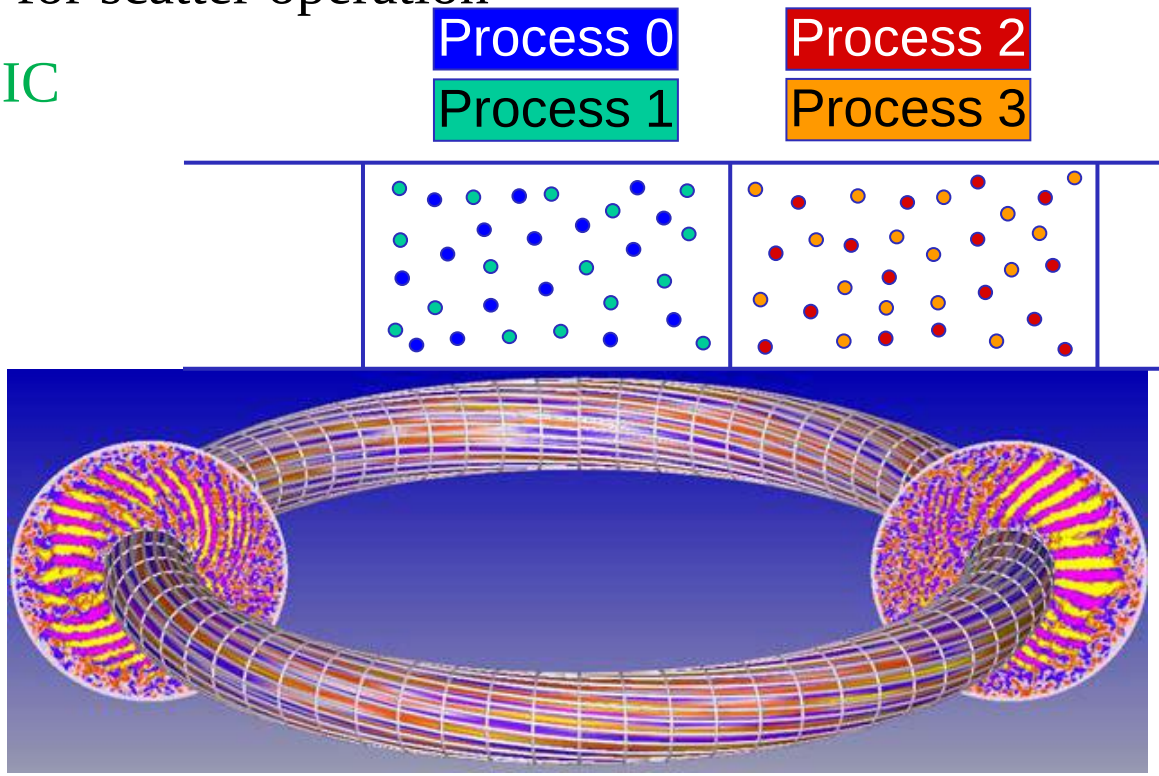






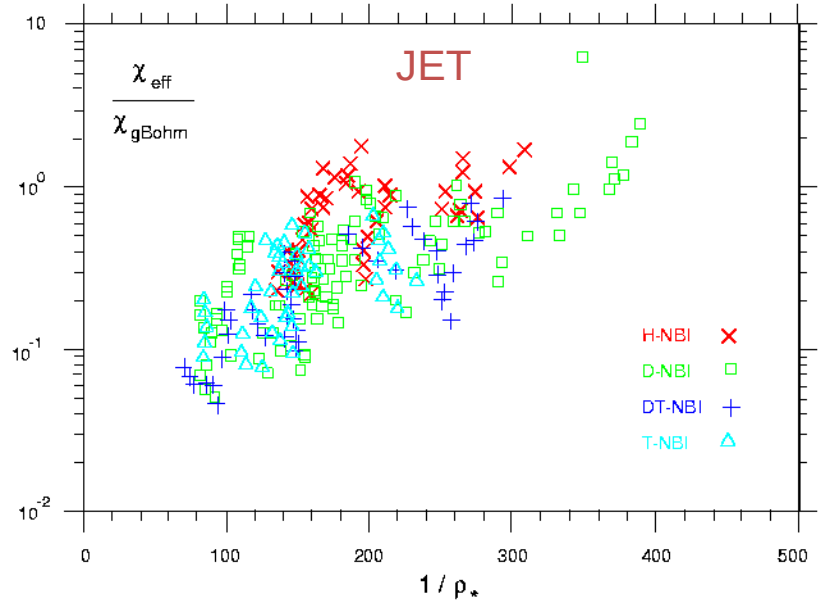
Multi-level Parallelization

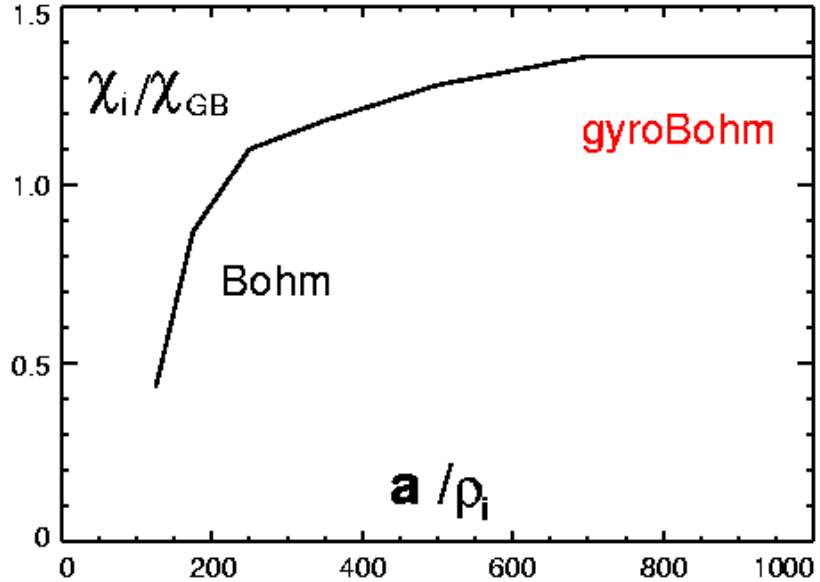
- Simulation solves gyrokinetic-Poisson equations in 5D phase space: field data on 3D fixed grids; Particles moving in 5D.
- I. 1D MPI domain-decomposition for particle-field interactions
- II. Particle-decomposition with series/parallel field solvers
- III. Loop level parallelism using OpenMP
- Vectorization: work-vector for scatter operation
- Optimization for GPU & MIC



Application: Transition from Bohm to Gyro-Bohm

- Gradual transition from Bohm to gyro-Bohm *[Lin et al, PRL2002]*
- Transport driven by local intensity
- Intensity driven nonlocally
- Turbulence spreading introduces nonlocality: breaking of Gyro-Bohm
- Time scales: key to understanding saturation vs. transport





Kinetic & Fluid Time Scales in ETG Turbulence

- Transport driven by local intensity: diffusive?
- Wave-particle decorrelation of parallel resonance $\delta(\omega - k_{\|} v_{\|})$ dominates
- Quasilinear calculation of χ_e agrees well with simulation
- Saturation: wave-wave coupling determines fluctuation intensity
- Transport: wave-particle decorrelation determines transport level
- Streamers do not determine directly transport level

[Lin et al, PRL 2007]

τ_{wp}	$\tau_{\|}$	$\tau_{\perp} = \dfrac{3}{4 s^2 \bar{\theta}^2 \bar{k}_{\theta}^2 \chi_e}$	τ_{rb}	τ_{eddy}	τ_{auto}	τ_s	$1/\gamma$
4.2	5.3	8.0	437	42	346	∞	33

Time Scales in CTEM Turbulence

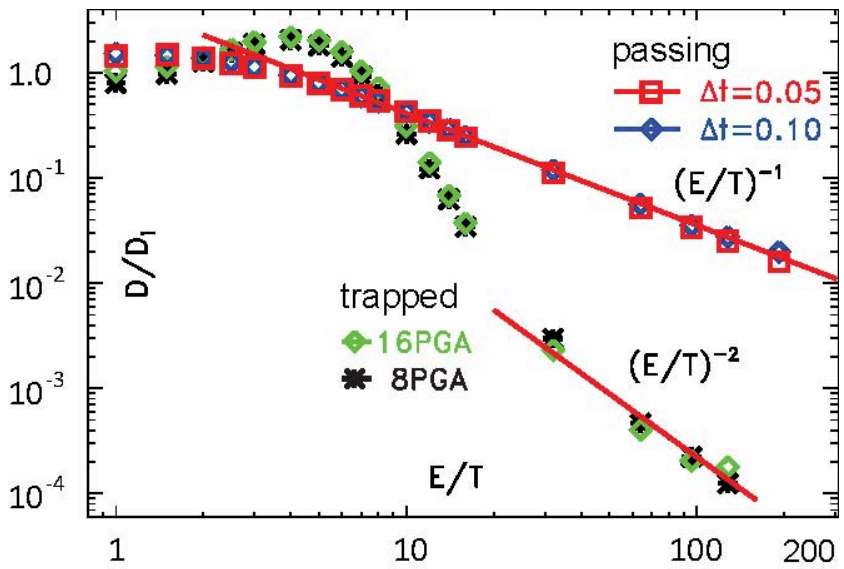
- CTEM instability drive is kinetic: toroidal precessional resonance of trapped electrons
- CTEM electron transport is from fluid eddy mixing, which regulated by zonal flows
- Leading to non-diffusive component of electron transport
- Ion transport is diffusive due to parallel decorrelation: ion transport follows local intensity of turbulence

[Xiao and Lin, PRL 2009]

$[L_{ne}/v_i]$	τ_{wp}	$\tau_{\parallel}$	$\tau_{\perp}$	τ_{rb}	τ_{eddy}	τ_{au}	τ_s	$\frac{1}{\gamma_{\max}}$
$CTEM\ e$	0.61	∞	∞	5.1	1.6	11	0.66	4.0
$ITG\ i$	1.7	1.8	2.0	21	4.9	7.2	1.4	9.1

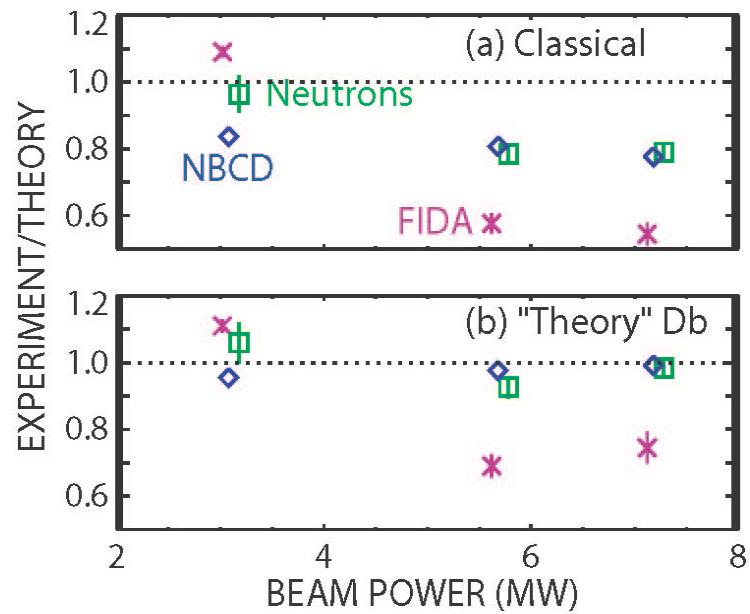
Energetic Particle Turbulent Transport: Energy Scaling

- GTC simulations find ITG diffusivity decreases drastically for high energy particles due to gyro- and orbit-averaging and wave-particle decorrelation
- GTC results are used to successfully to explain the transport of NBI fast ion transport in DIII-D tokamak



GTC diffusivity D as a function of particle energy for passing & trapped particles.

[W. Zhang, Z. Lin , L. Chen, PRL2008; PoP2010; PRL2011; PoP2013]



Measured neutron rate, beam-driven current, FIDA radiance from fast ions divided by (a) classical prediction & (b) simulation-based prediction vs. beam power in DIII-D

[W. Heidbrink et al, PRL2009]

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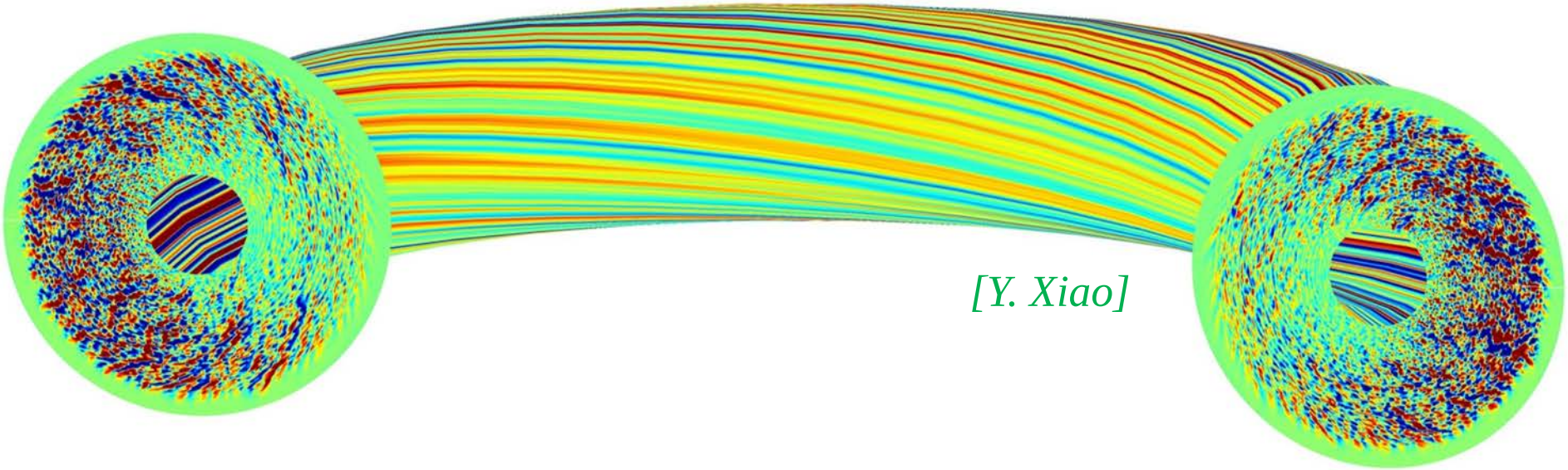


Multi-scale Gyrokinetic Simulation of Kinetic-MHD

- Macroscopic MHD modes limit burning plasma performance and threaten fusion device integrity
- Kinetic effects at microscopic scales and coupling of multiple processes play a crucial role in excitation and evolution MHD modes
- Neoclassical tearing modes (NTM): set principal performance limit in both ITER baseline and hybrid scenarios
  - Predictive NTM simulation needs to incorporate kinetic physics at multiple spatial and temporal scales: microturbulence, neoclassical bootstrap current, magnetic island dynamics
- Fully self-consistent simulation of Alfven eigenmode excited by energetic particle (EP) must incorporate three new physics elements
  - Linear and nonlinear kinetic effects of thermal particles
  - Nonlinear interaction of meso-scale shear Alfven waves with micro-scale kinetic effects and wave-particle resonance
  - Cross-scale couplings of meso-micro turbulence

http://phoenix.ps.uci.edu/GSEP

Kinetic-MHD via Gyrokinetic Particle Simulation

- Nonlinear gyrokinetic equation, Poisson equation, Ampere's law

$$\frac{\partial F}{\partial t} + (v_{\parallel}\mathbf{b} + \mathbf{v}_d)\cdot\frac{\partial F}{\partial \mathbf{R}} + \dot{v}_{\parallel}\frac{\partial F}{\partial v_{\parallel}} = 0$$

$$\phi - \tilde{\phi} = -\sum_s 4\pi e Z_s \bar{n}_s$$

$$\nabla^2 A_{\parallel} = -\sum_s \frac{4\pi e}{c} Z_s \bar{n}_s u_s$$

- In fluid limit, gyrokinetic system recover MHD modes including Alfven wave, interchange mode, kink mode, KBM

KBM

SAW

$$\frac{\omega(\omega-\omega_{*P})}{v_A^2}\nabla_\perp^2\delta\phi - i\boldsymbol{B}_0\cdot\nabla\left\{\frac{\boldsymbol{b}_0\cdot\nabla\times[\nabla\times(k_\parallel\delta\phi\boldsymbol{b}_0)]}{B_0}\right\}$$

$$-\frac{i\omega}{c}\delta\boldsymbol{B}\cdot\nabla\left(\frac{\boldsymbol{b}_0\cdot\nabla\times\boldsymbol{B}_0}{B_0}\right)$$

kink drive

$$-i\omega\frac{4\pi}{c}\left[\nabla\times\boldsymbol{b}_0\cdot\nabla\left(\frac{\delta P_\parallel}{B_0}\right) + \boldsymbol{b}_0\times\nabla B_0\cdot\nabla\left(\frac{\delta P_\perp}{B_0^2}\right) + \frac{\nabla\times\boldsymbol{b}_0\cdot\nabla B_0}{B_0^2}\delta P_\perp\right]$$

$=0$

interchange drive

*[W. Deng, Z. Lin, and I. Holod, Nuclear Fusion **52**, 023005 (2012)]*

Electron Models

- For low frequency mode $\omega/k_{||} << v_{||}$, electron response mostly adiabatic

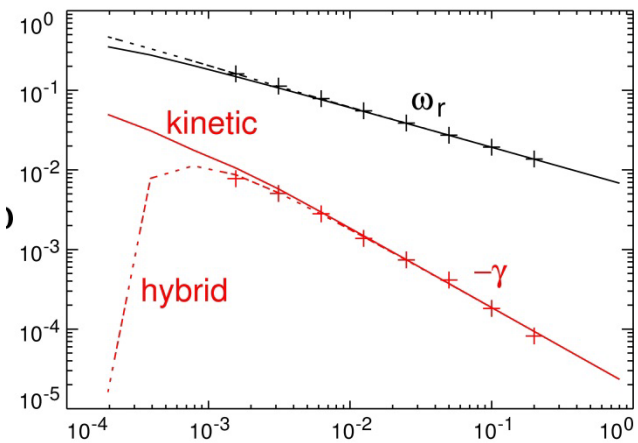
$$\delta f_e = \frac{e\delta\phi}{T_e} f_M (1 + \frac{\omega}{k_{||}v_{||} - \omega})$$

- Dynamically evolve non-adiabatic part

$$\delta f_e = f_M e^{e\delta\phi/T_e} + \delta g$$

- Perturbed potential $\phi = \delta\phi + \Phi(k_{||}=0)$

$$L\delta g = e^{e\phi/T_e} f_M [\kappa \cdot \mathbf{v}_{\delta\phi} + \frac{e}{T_e}\frac{\partial\delta\phi}{\partial t} - \frac{e}{T_e}(\mathbf{v}_{\delta\phi} + \mathbf{v}_d) \cdot \nabla\Phi]$$

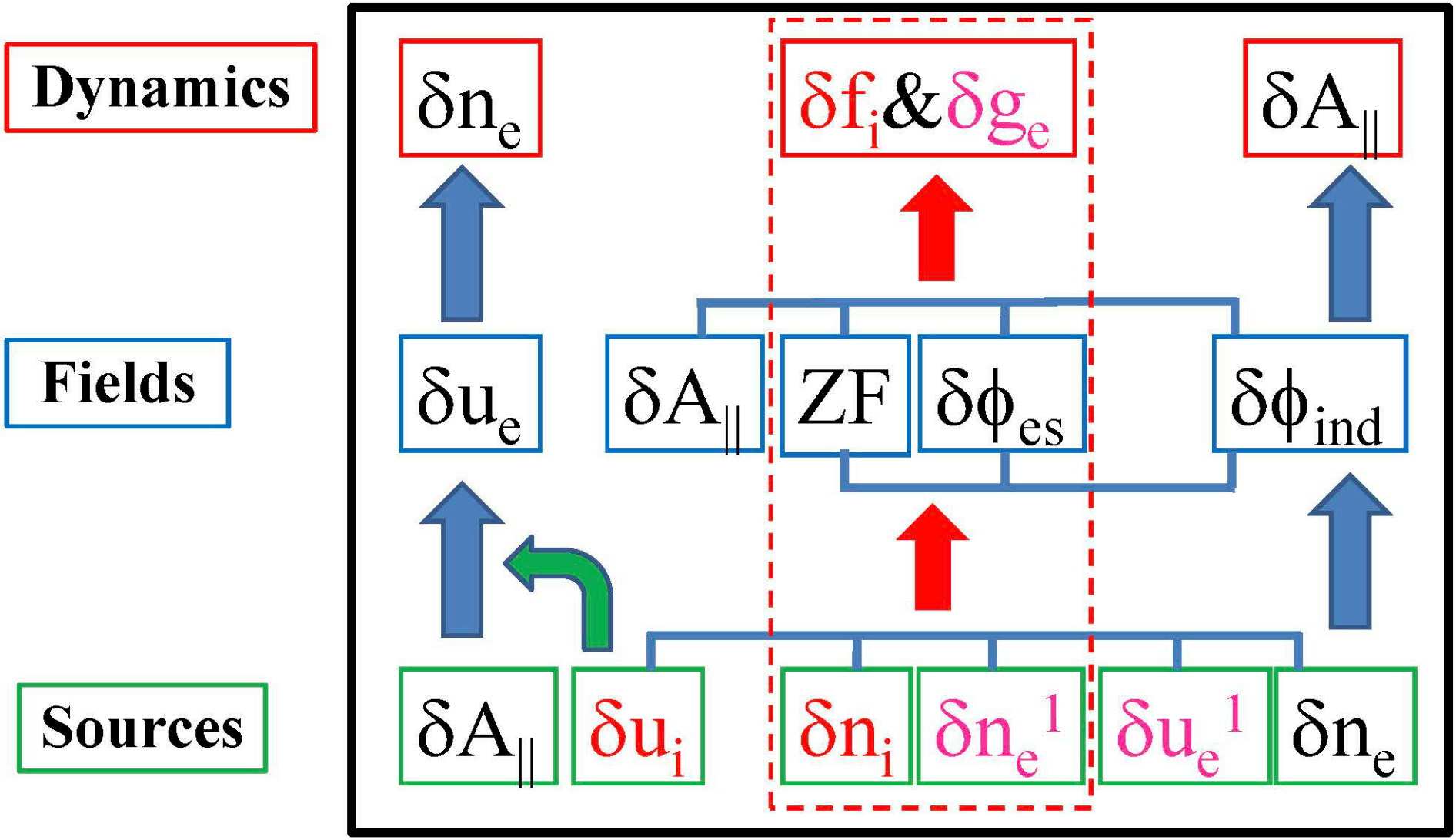


- Split-weigh scheme *[Mamuilskiy & Lee, PoP2000; J. Lewandowski; Y. Chen]*

  Fluid-kinetic hybrid *model* *[Lin & Chen, PoP2001]*
  - Lowest order: fluid, adiabatic response & non-resonance current
  - Higher order: kinetic, resonant contribution
  - Requires $\omega_t > \omega$; neglects $E_{||}(k_{||}=0)$ inductive electric field

- Resistive tearing mode demonstrated; collisionless tearing mode pursued

Gyrokinetic Toroidal Code (GTC)

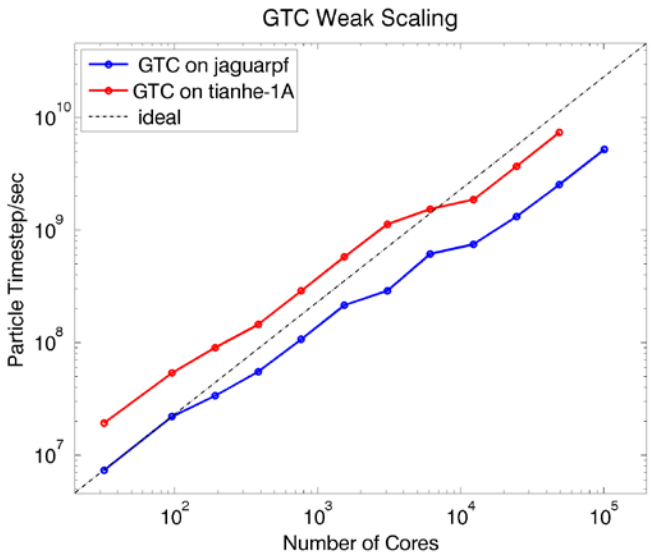


[Lin, Hahm, Lee, Tang, White, Science 281, 1835 (1998)]

http://phoenix.ps.uci.edu/GTC/

Gyrokinetic Toroidal Code (GTC)

- GTC physics goal: first-principles, integrated simulations of microturbulence, energetic particle (EP), magnetohydrodynamic (MHD), neoclassical, radio-frequency (RF) heating/current drive
- Current capability for kinetic MHD simulation: microturbulence + EP + MHD + neoclassical
  - General geometry & experimental profiles
  - Kinetic electrons & electromagnetic fluctuations
  - Gyrokinetic or fully kinetic ions
  - Equilibrium current
  - Neoclassical effects
- Next step: collisionless tearing mode
- Ported to GPU (titan) & MIC (tianhe-2)
- Developed by GTC team in US & China in support of ITER



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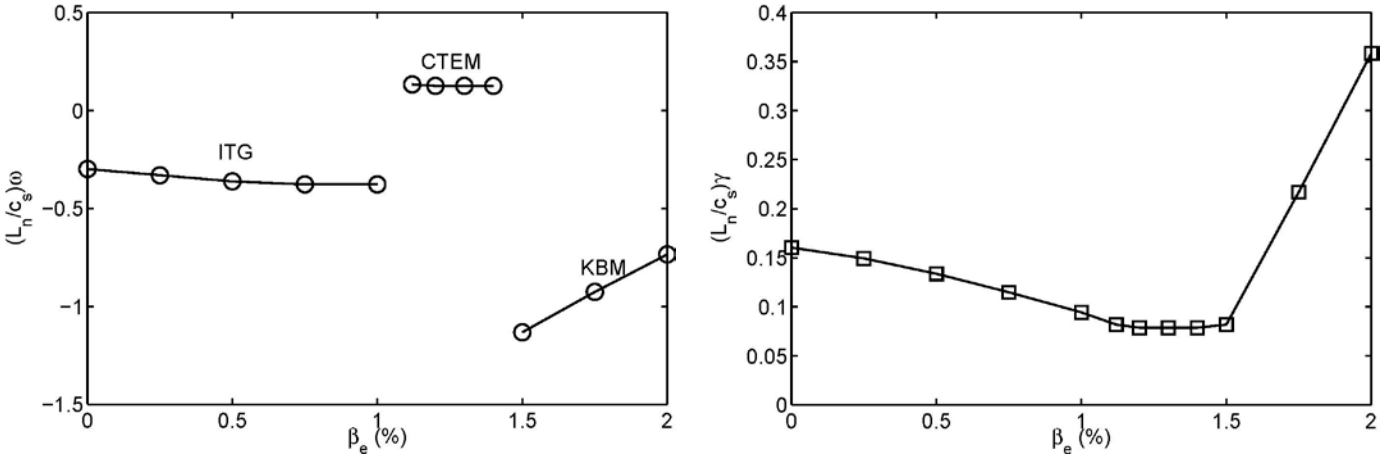
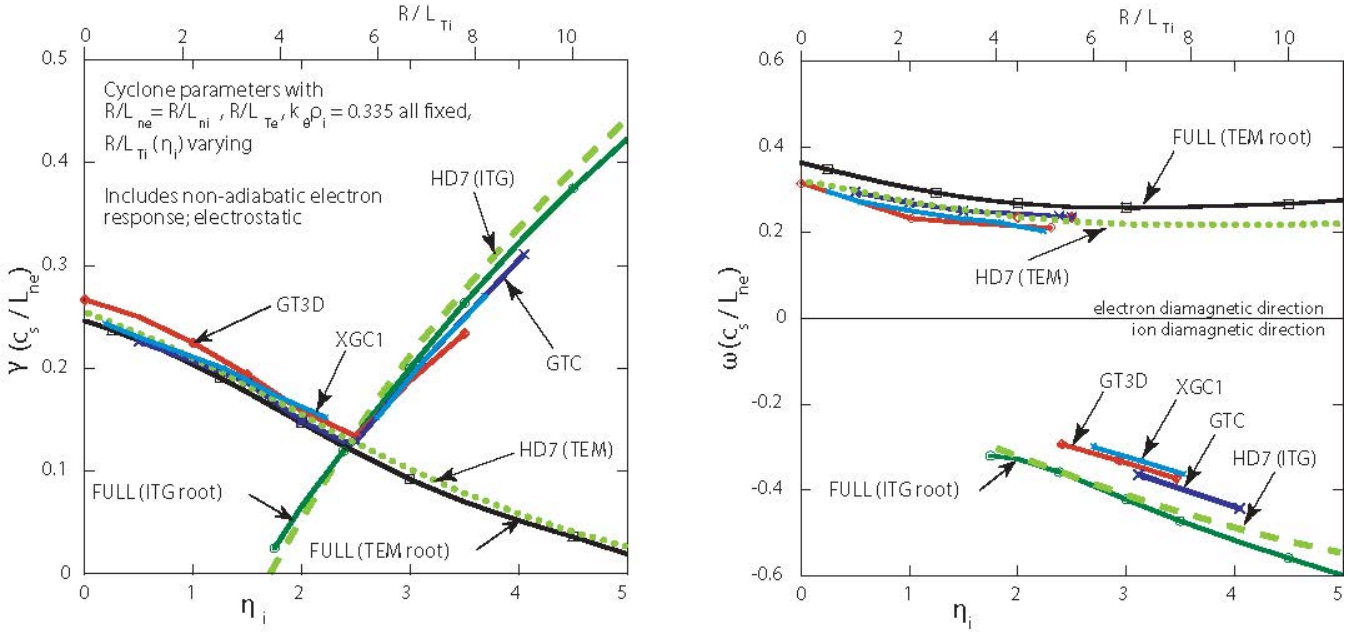
Verification of finite-β Simulation

- Finite-β stabilization of ITG and excitation of KBM

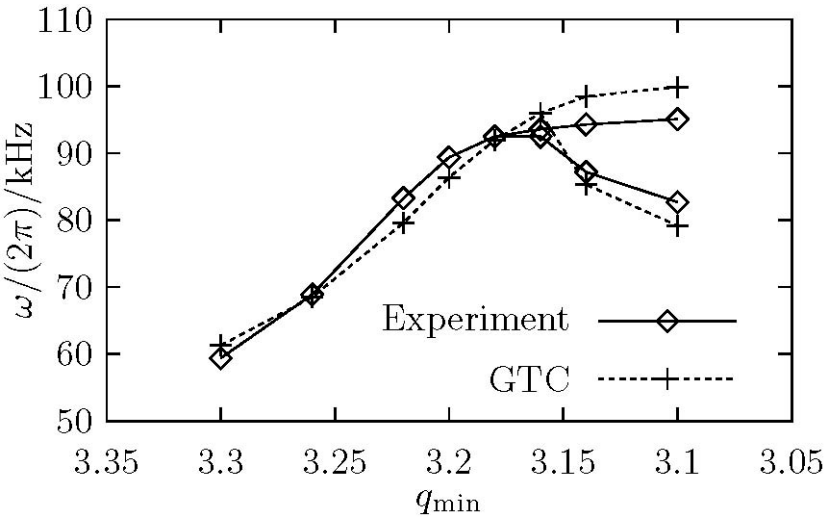
[Holod & Lin, PoP2013]





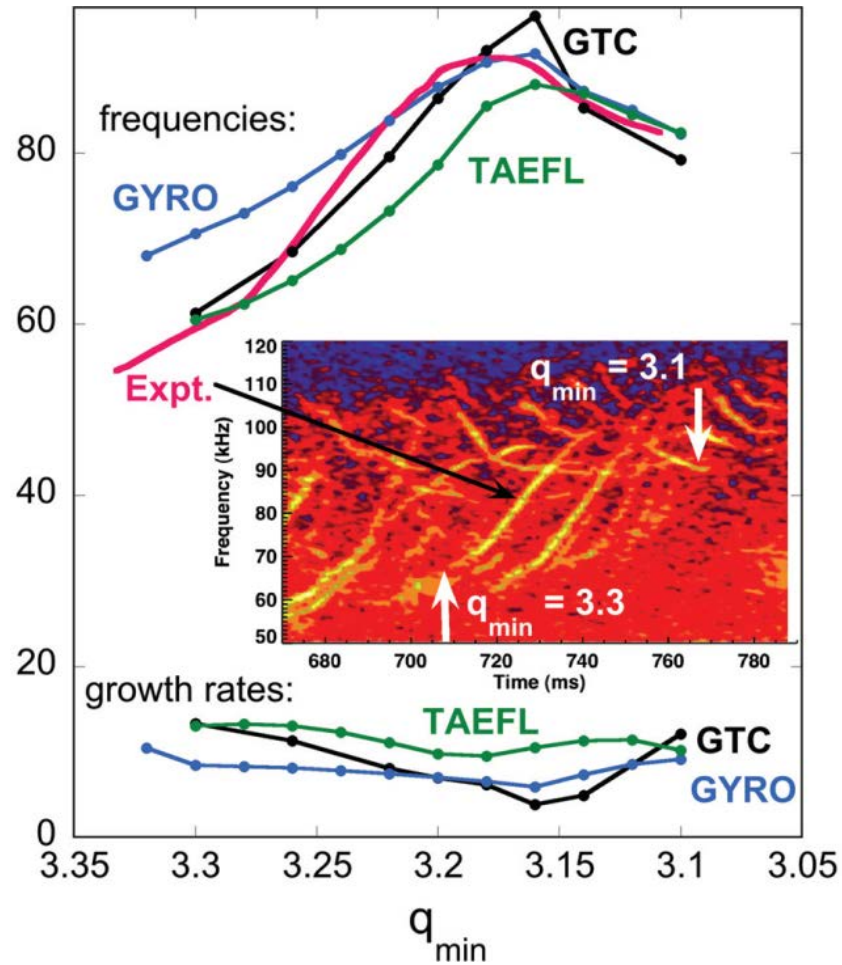
Linear Simulations of Alfven Eigenmodes Validated

- GTC, GYRO, and TAEFL simulations of RSAE frequency up-sweeping, and mode structures in good agreement with DIII-D experiments (shot # 142111)
- Verification of GTC simulation of other modes:
  - BAE *[H. Zhang et al, PoP2010]*
  - TAE *[W. Zhang et al, PoP2012]*
  - EPM *[C. Zhang et al, PoP2013]*
  - KBM *[Holod & Lin, PoP2013]*



GTC simulation of RSAE to TAE transition with real geometry & kinetic electrons

*[Deng et al, NF**52**, 043006 (2012);PoP2010]*

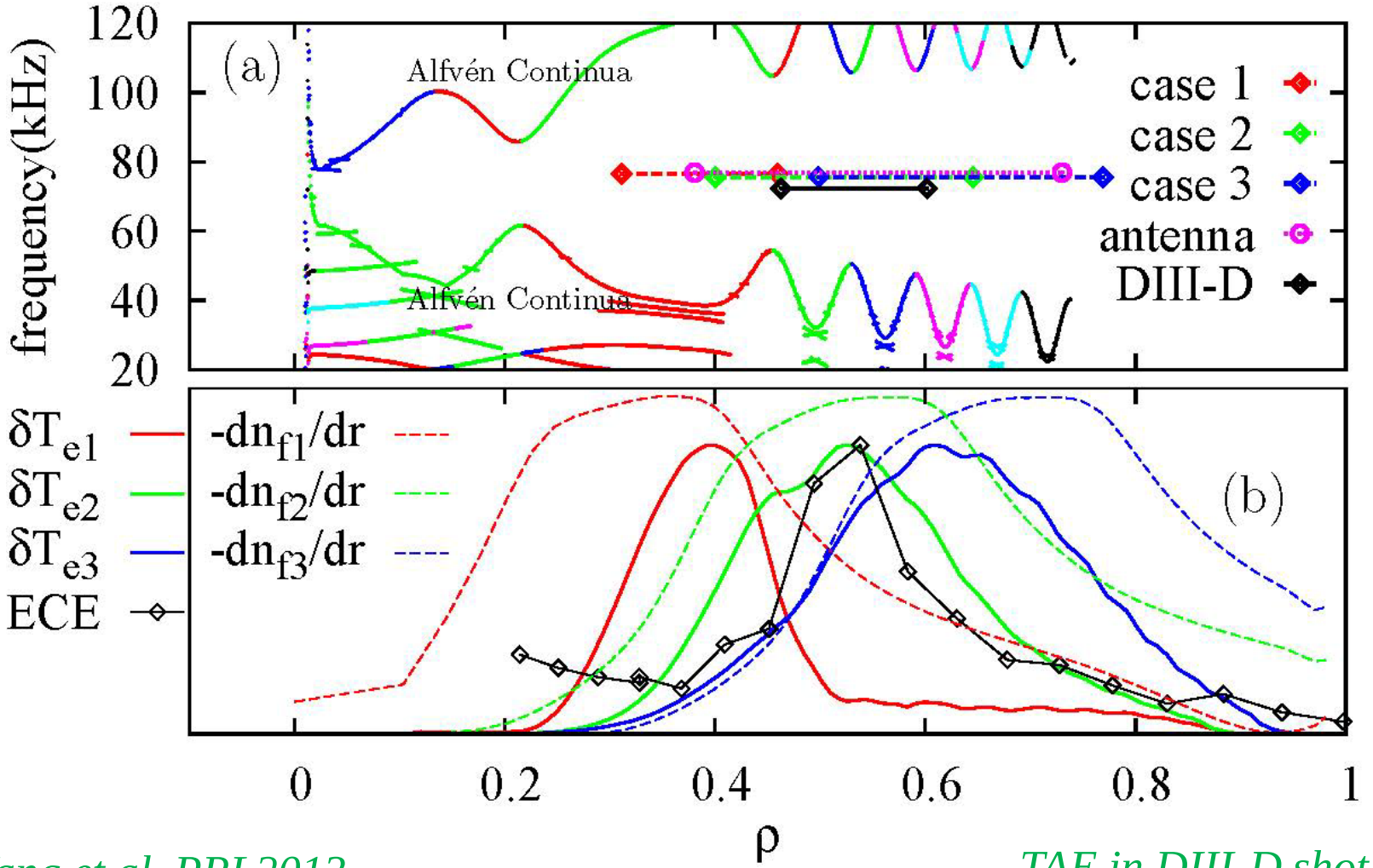


RSAE in DIII-D shot # 142111 at 725ms

[D. Spong et al, PoP2012]

GTC Simulation Finds TAE Radial Localization in DIII-D

- TAE radial structure peaks at and moves with EP density gradient
- EP non-perturbative contribution to MHD mode

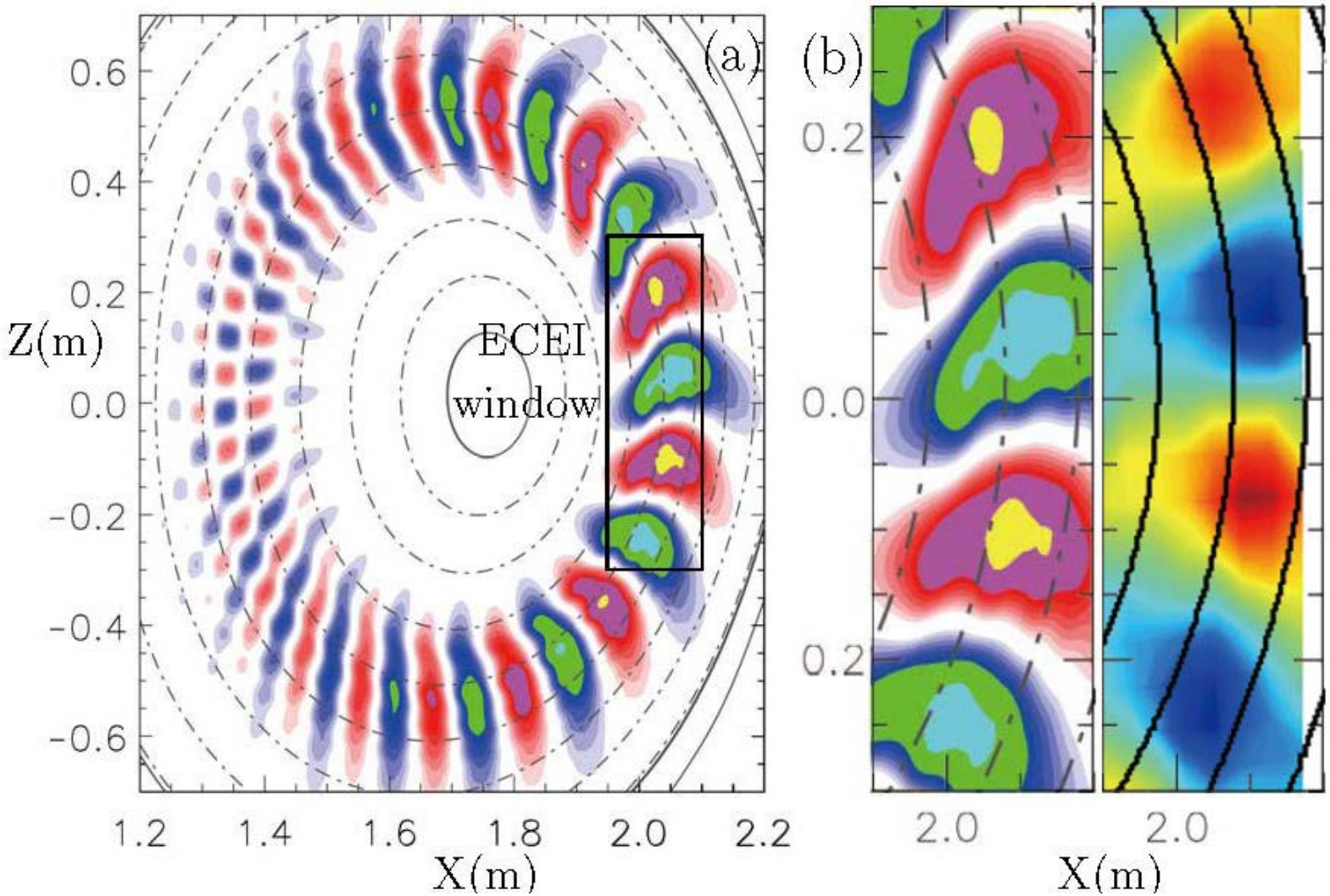


Z. X. Wang et al, PRL2013

TAE in DIII-D shot # 142111 at 525ms

Comparison of TAE Mode Structures between Simulation & Experiment

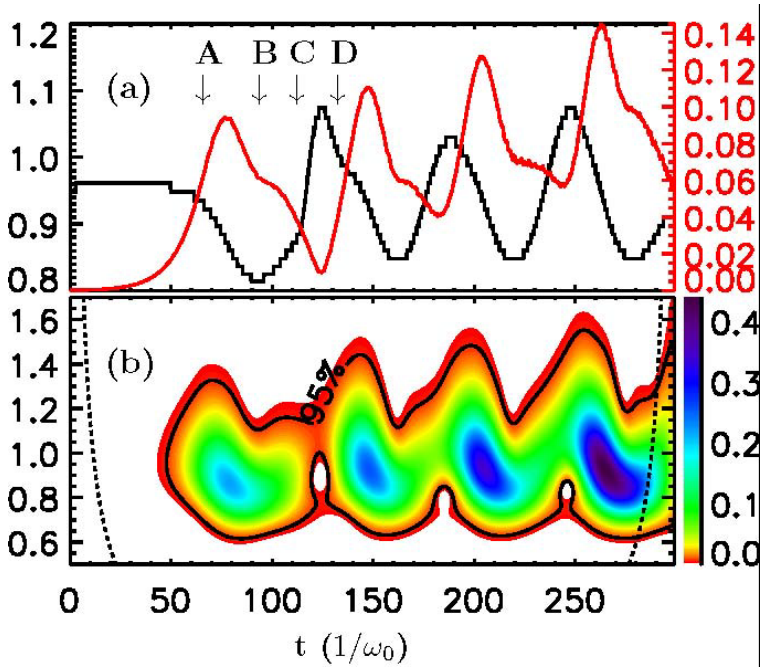
- EP non-perturbative contribution breaks radial symmetry



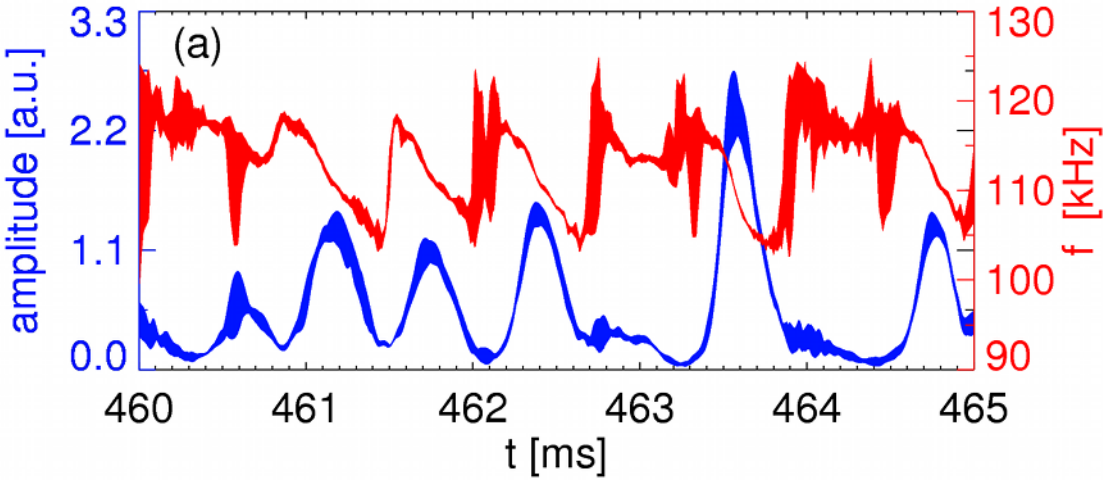
TAE in DIII-D shot # 142111 at 525ms

GTC Nonlinear Simulations of BAE Find Fast Chirping

- Fast, repetitive, mostly downward chirping, sub-millisecond period
- 90° phase shift between intensity oscillation and frequency chirping
- Simulation features observed in recent NSTX TAE, ASDEX BAE
- Chirping induced by nonlinear dynamics of phase space coherent structures



[H. S. Zhang, Z. Lin, I. Holod, PRL2012]



[M. Podesta et al, NF2011; NF2012]

Backup Slides

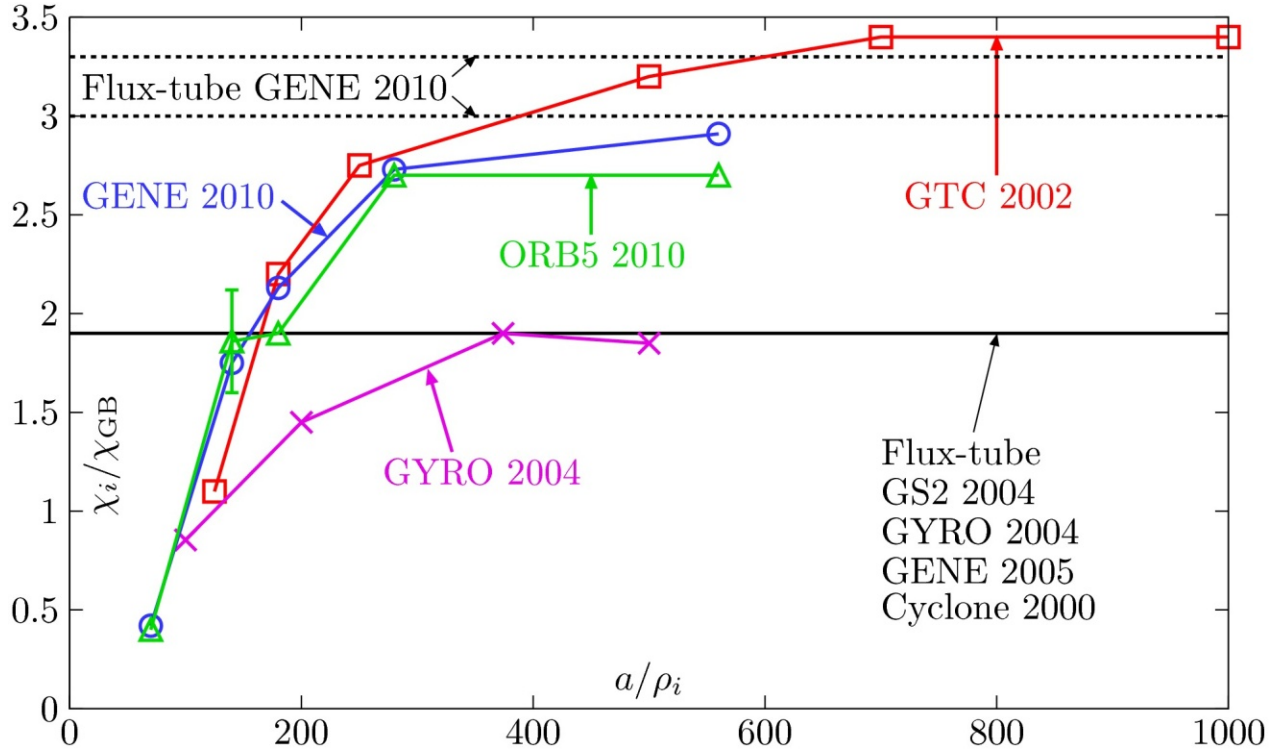
Relevant Time Scales in ETG Turbulence

$\tau_{wp} = \frac{4\chi_e}{3\delta v_r^2}$	Effective wave-particle decorrelation time
$\tau_{\parallel} = \frac{1}{\Delta k_{\parallel} v_e}$	Parallel decorrelation time (Electron streaming across wave fields; independence of amplitude)
$\tau_{\perp} = \frac{3}{4s^2\bar{\theta}^2\bar{k}_\theta^2\chi_e}$	Radial turbulence scattering time (Diffusion across radial width of *m*-harmonics)
$\tau_{rb} = \frac{4L_r^2}{3\chi_e}$	Resonant broadening time (Diffusion across radial streamer length)
$\tau_{eddy} = \frac{L_r}{\delta v_r}$	Eddy turnover time (Streamer rotation)
τ_{auto}	Auto-correlation time (eddy life time)
$\tau_s = [\frac{L_r}{L_\theta}\frac{\partial}{\partial r}(\frac{qV_{EXB}}{r})]^{-1}$	Zonal flow shearing time
$1/\gamma$	Linear growth time

Microturbulence: Nonlinear Verification

- GTC results of device size scaling of ITG transport in 2002 verified after 8 years by global particle code ORB5 and continuum code GENE
  - [Lin, Hahm, Ethier, Tang, PRL2002]: GTC device size scaling: Bohm to gyroBohm transition
  - 2004: GYRO agrees with GTC qualitatively: Bohm to gyroBohm transition
  - [Lin & Hahm, PoP2004]: quantitative difference due to s-α model in continuum codes
  - 2010: [McMillian, PRL2010] ORB5 & GENE agree with GTC qualitatively & quantitatively: Bohm to gyroBohm transition; quantitative difference due to s-α model in continuum codes

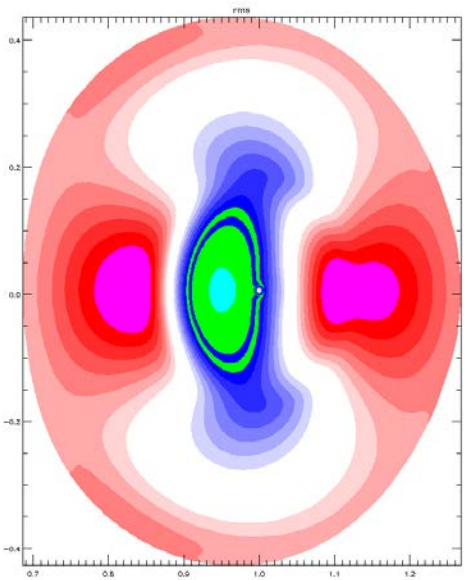
Data: [Lin PRL2002] (GTC 2002), [Candy PoP2004] (GYRO 2004, Flux-tube GS2 2004, GYRO 2004), [Jenko PPCF2005] (Flux-tube GENE 2005), [Dimits PoP2000] (Cyclone 2000), [McMillan PRL2010] (ORB5 2010, GENE 2010, Flux-tube GENE 2010).



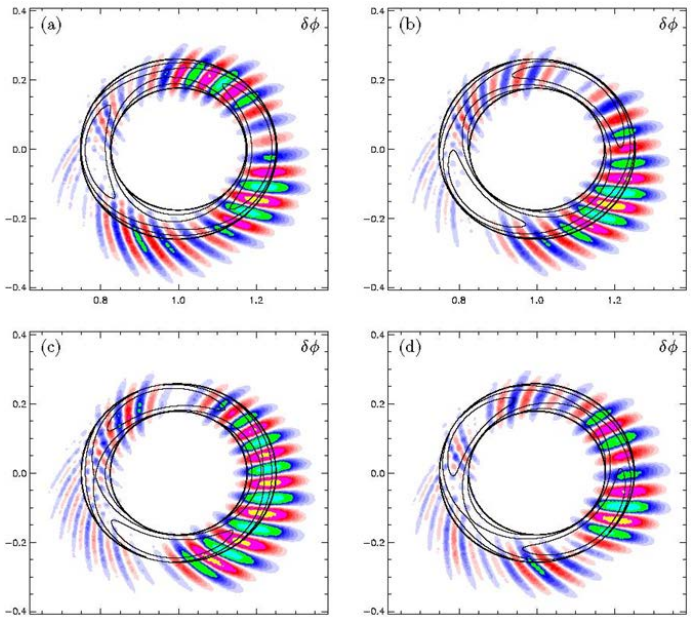
[Z. H. Lin, S. Ethier, T. S. Hahm, and W. M. Tang, PST2012]

Toward First-Principles Simulation of NTM

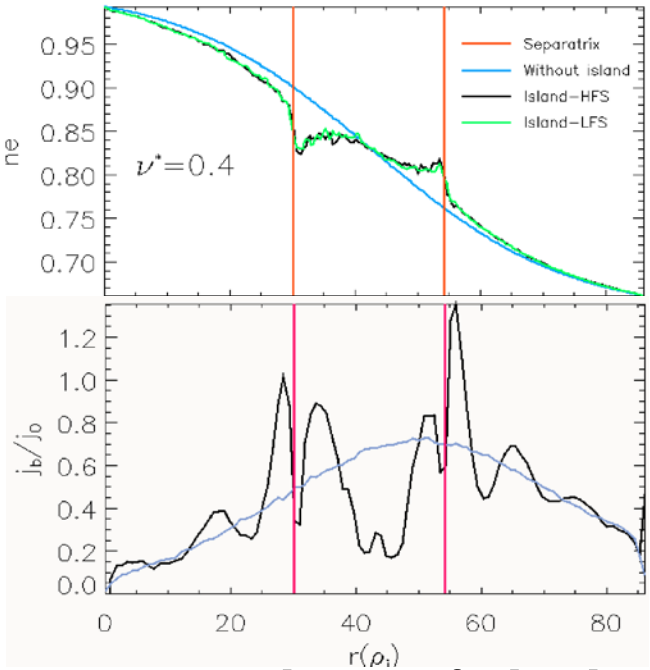
- GTC simulation of kink mode in DIII-D finds instability driven by both equilibrium current and pressure gradient
- GTC simulation finds depression of bootstrap current and suppression of ITG due to flattening of pressure profile in the island center



GTC simulation of kink in DIII-D #150363 [*J. McClanehan, 2013*]



GTC simulation of island effects on ITG [*P. Jiang, 2013*]

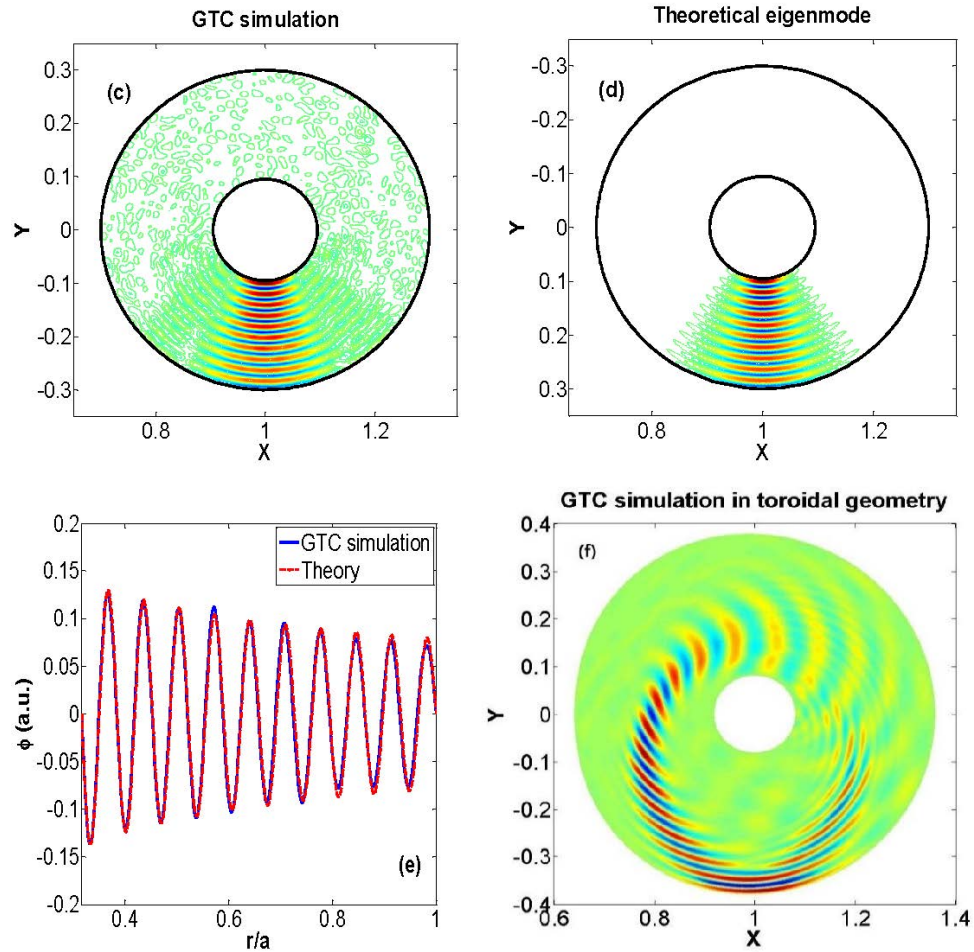


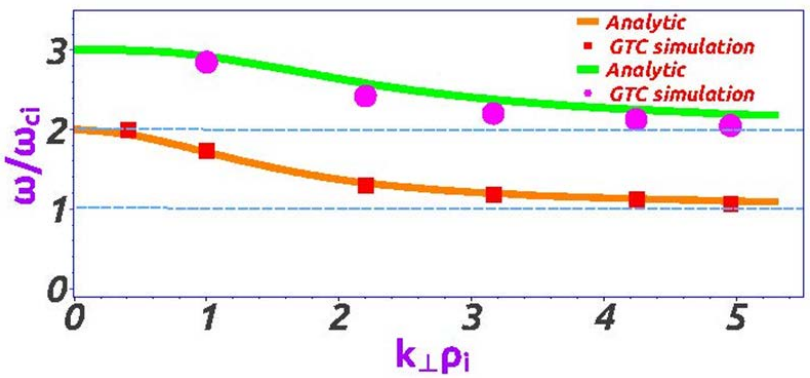
GTC simulation of island effects on bootstrap current [*G. Dong, 2013*]

GTC Simulation of RF Waves in Tokamak

- GTC recovers IBW dispersion relation
- GTC simulation of LHW propagation in cylindrical geometry agrees well with theoretical results
- Poloidal asymmetry in LHW propagation in tokamak

GTC simulation of LHW in cylinder & tokamak
[*J. Bao, 2013*]





GTC simulation of IBW
[*A. Kuley et al, 2013, PoP2013*]