Momentum transport in full-f gyrokinetic simulations

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- Background and motivation
- Gyrokinetic Toroidal 5D full-f Eulerian code GT5D
- Accuracy of momentum transport in GT5D
  - Collisionless equilibrium given by P_φ
  - Neoclassical force balance relation
  - Accuracy of toroidal momentum conservation
  - Influences of higher order drifts
- Roles of momentum transport in ITG turbulence
- Summary

Study momentum transport using gyrokinetic model

- Turbulent momentum transport, which may drive intrinsic rotation, is one of critical issues in predicting performances of ITER, where external momentum input is expected to be small
- Gyrokinetic simulations have been widely used in studying turbulent momentum transport
  - Quasilinear simulation of momentum pinch and residual stress [Peeters,PRL07, Camenen,PRL09,NF11]
  - Nonlinear δf simulation of momentum pinch and residual stress [Peeters,PPCF06, Waltz,POP07,POP11, Holod,POP09,PPCF10, Casson,POP09, Wang,PRL09]
  - Nonlinear full-f simulation
    - Formation of intrinsic rotation [Idomura,NF09]
    - Identification of residual stress [Ku,IAEA10,Jolliet,NF11]
    - Accuracy of toroidal momentum balance [Sarazin,IAEA10]
- However, significant concern has been raised about the accuracy of momentum transport in gyrokinetic model

Controversial arguments on GK momentum transport

- Assertion raised in [Parra,Catto,POP10 and earlier works]
  - Fokker-Planck equation yields

$$\frac{\partial}{\partial t}\left\langle Zen_i - en_e\right\rangle_f + \frac{\partial}{\partial V}V'\left\langle c\frac{\partial\phi}{\partial\varphi}\left(Zen_i - en_e\right)\right\rangle_f$$
$$= -c\frac{\partial}{\partial V}V'\left(\frac{\partial}{\partial t}\left\langle Rn_i m_i U_\varphi\right\rangle_f + \frac{\partial}{\partial V}\left\langle R^2\nabla\varphi\cdot\pi\cdot\nabla V\right\rangle_f\right)$$

  - Low flow ordering $U_\varphi/v_{ti}\sim\mathrm{O}(\varepsilon)$ and gyro-Bohm diffusion gives $\mathrm{O}(\varepsilon^3)$ flux
  - Momentum balance does not hold unless f is solved up to $\mathrm{O}(\varepsilon^3)$

$\rightarrow$Conventional $\mathrm{O}(\varepsilon)$ gyrokinetics and QN eq. can not determine U_φ and E_r

- Avoidance of this ordering issue by large flow ordering [Sugama,PPCF11]
- Demonstration of toroidal momentum conservation [Scott,POP10]
  - Modern gyrokinetic theory assures toroidal momentum conservation at any order, provided that energetic consistency is satisfied

$\rightarrow$Is there erroneous momentum flux satisfying momentum balance?

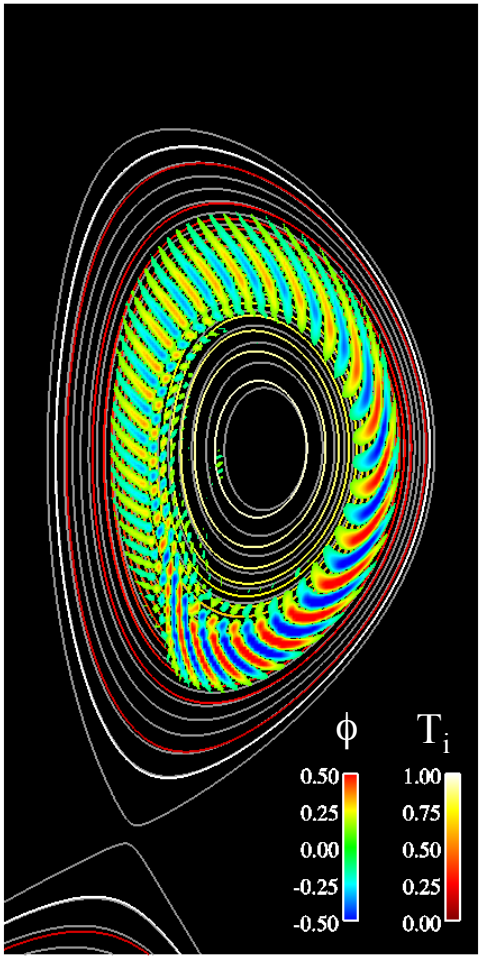
- In this work, we discuss
  - Accuracy of toroidal momentum balance in GT5D
  - Influences of higher order drifts on turbulent momentum flux

Gyrokinetic Toroidal 5D full-f Eulerian code GT5D

[Idomura, Comput.Phys.Commun. (2008); Nucl. Fusion (2009)]

- GT5D code
  - Global full-f gyrokinetic simulations of turbulent transport in ITG-TEM turbulence
  - 5D Eulerian code based on non-dissipative conservative FD scheme [Idomura,JCP07]
- Verification [Idomura,CPC08,Satake,CPC10,Camenen,NF10]
  - ITG-TEM benchmark (GT3D,GKW,etc…)
  - Neoclassical benchmark (FORTEC-3D)
- Validation [Idomura,NF09,IAEA10,Jolliet,IAEA10]
  - Avalanche-like non-local ion heat transport
  - Stiffness of ion temperature profile
  - Formation of intrinsic rotation
  - Scaling studies on ρ^*, safety factor, rotation

ITG mode in JT-60SA with ITER like shape



First principle models used in GT5D

- Hamiltonian in the gyro-centre coordinates $\mathbf{Z}_{\mathrm{GY}}=(t;\mathbf{R},v_{//},\mu,\alpha)$

$$H=\frac{1}{2}mv_{//}^2+\mu B+e\langle\phi\rangle_\alpha$$

- Gyrokinetic equations based on modern GK theory [Brizard,RMP07]

$$\frac{\partial f}{\partial t}+\{f,H\}=\frac{\partial f}{\partial t}+\dot{\mathbf{R}}\cdot\nabla f+\dot{v}_{//}\frac{\partial f}{\partial v_{//}}=C(f)+S_{src}$$

$$-\nabla_\perp\cdot\frac{\rho_{ti}^2}{\lambda_{Di}^2}\nabla_\perp\phi+\frac{1}{\lambda_{De}^2}\left[\phi-\langle\phi\rangle_f\right]=4\pi e\left[\int f\delta\left(\left[\mathbf{R}+\rho\right]-\mathbf{x}\right)d^6Z-n_{0e}\right]$$

  - Minimum model (1st order particle Lagrangian + 2nd order field Lagrangian) satisfying energetic consistency in GK field theory [Scott,POP10]
    - Energy conservation
    - Toroidal momentum conservation
  - Linear Fokker-Planck collision operator [Xu,PFB91]
    - Field particle operator with exact particle, momentum, and energy conservation [Satake,PFR08]

Conservative form of gyrokinetic equation

- Conservative gyrokinetic equation

$$\frac{Dm^2B_{//}^*f}{Dt}=\frac{\partial m^2B_{//}^*f}{\partial t}+\nabla\cdot\left(m^2B_{//}^*\dot{\mathbf{R}}f\right)+\frac{\partial m^2B_{//}^*\dot{v}_{//}f}{\partial v_{//}}=0$$

- Phase space conservation (incompressible Hamiltonian flows)

$$\nabla\cdot\left(m^2B_{//}^*\dot{\mathbf{R}}\right)+\partial_{v//}\left(m^2B_{//}^*\dot{v}_{//}\right)=0$$

$$m^2B_{//}^*\dot{\mathbf{R}}=m\mathbf{B}^*\frac{\partial H}{\partial v_{//}}+\frac{m^2c}{e}\mathbf{b}\times\nabla H\ ,\quad m^2B_{//}^*\dot{v}_{//}=-m\mathbf{B}^*\cdot\nabla H$$

- Centered FD operator for phase space conservation [Idomura,CPC08]

$$\frac{\delta_2}{\delta_2\mathbf{R}}.\left[m^2B_{//}^*R\dot{\mathbf{R}}\right]+\frac{\delta_2}{\delta_2v_{//}}\left[m^2B_{//}^*R\dot{v}_{//}\right]=0$$

$$\left[m^2B_{//}^*R\dot{\mathbf{R}}\right]\equiv m\left(\frac{\delta_2}{\delta_2\mathbf{R}}\times\left[\mathbf{A}+\frac{cm}{e}v_{//}\mathbf{b}\right]\right)\frac{\delta_2H}{\delta_2v_{//}}+\frac{m^2c}{e}\left(H\frac{\delta_2}{\delta_2\mathbf{R}}\times\mathbf{b}-\frac{\delta_2}{\delta_2\mathbf{R}}\times\left[H\mathbf{b}\right]\right)$$

$$\left[m^2B_{//}^*R\dot{v}_{//}\right]\equiv-m\frac{\delta_2}{\delta_2\mathbf{R}}\times\mathbf{A}\cdot\frac{\delta_2H}{\delta_2\mathbf{R}}-\frac{m^2c}{e}v_{//}\frac{\delta_2}{\delta_2\mathbf{R}}.\left(H\frac{\delta_2}{\delta_2\mathbf{R}}\times\mathbf{b}\right)$$

Non-dissipative conservative FD scheme

[Morinishi, J. Comput. Phys. (1998); Idomura, J. Comput. Phys. (2007)]

- Continuity equation for f transported by incompressible flows

$$\frac{DJf}{Dt} \equiv \frac{\partial Jf}{\partial t} + \frac{\partial Jv_j f}{\partial x_j} = \frac{\partial Jf}{\partial t} + (Conv.) = 0 \quad \text{with} \quad \frac{\partial Jv_j}{\partial x_j} = 0$$

$$v_j \equiv \mathbf{v} \cdot \nabla x_j, \quad J : \text{Jacobian}$$

- Conservation of f and f^2 assures numerical stability

$$[Conv.] \equiv \frac{1}{2}\frac{\delta_2 Jv_j f}{\delta_2 x_j} + \frac{1}{2} Jv_j \frac{\delta_2 f}{\delta_2 x_j} = \frac{\delta_1 \overline{Jv_j}^{1xj} \overline{f}^{1xj}}{\delta_1 x_j} - \frac{1}{2} f \frac{\delta_2 Jv_j}{\delta_2 x_j}$$

$$f[Conv.] = \frac{\delta_1 \overline{Jv_j}^{1xj} \langle f, f \rangle^{1xj} / 2}{\delta_1 x_j}$$

conserve f and f^2 if $\dfrac{\delta_2 Jv_j}{\delta_2 x_j} = 0$

Definitions of discrete operators with grid spacing h_j

$$\frac{\delta_n A}{\delta_n x_j} \equiv \left[A\left(x_j + nh_j/2\right) - A\left(x_j - nh_j/2\right) \right] / \left(nh_j\right)$$

$$\overline{A}^{nj} \equiv \left[A\left(x_j + nh_j/2\right) + A\left(x_j - nh_j/2\right) \right] / 2$$

$$\langle A, B \rangle^{nj} \equiv \left[A\left(x_j + nh_j/2\right) B\left(x_j - nh_j/2\right) + A\left(x_j - nh_j/2\right) B\left(x_j + nh_j/2\right) \right] / 2$$

Advantages of non-dissipative conservative FD scheme

- Centered FD approach in φ keeps toroidal symmetry numerically
- Drifts implemented by FD of H can be easily extended to higher order
- Local conservation of f leads to balance relations of $v_{//}$, P_φ moments

$$\frac{\partial f}{\partial t} + \frac{1}{\mathcal{J}}\frac{\partial}{\partial \mathbf{Z}} \cdot \left(\mathcal{J}\dot{\mathbf{Z}} f\right) = 0$$

Particle balance

$$\left\langle \frac{\partial f}{\partial t} \right\rangle_{gf} + \left\langle \frac{1}{\mathcal{J}}\frac{\partial}{\partial \mathbf{Z}} \cdot \left(\mathcal{J}\dot{\mathbf{Z}} f\right) \right\rangle_{gf} = 0$$

Parallel momentum balance

$$\left\langle \frac{\partial m v_{\|} f}{\partial t} \right\rangle_{gf} + \left\langle m v_{\|} \frac{1}{\mathcal{J}}\frac{\partial}{\partial \mathbf{Z}} \cdot \left(\mathcal{J}\dot{\mathbf{Z}} f\right) \right\rangle_{gf} = 0$$

Toroidal angular momentum balance

$$\left\langle \frac{\partial P_\varphi f}{\partial t} \right\rangle_{gf} + \left\langle P_\varphi \frac{1}{\mathcal{J}}\frac{\partial}{\partial \mathbf{Z}} \cdot \left(\mathcal{J}\dot{\mathbf{Z}} f\right) \right\rangle_{gf} = 0$$

❖ gyro/flux-surface average moments $\langle A \rangle_{gf}(\psi) = \left\langle \int A(\mathbf{Z})\delta(\mathbf{R} + \rho - \mathbf{x}) d\mathbf{Z} \right\rangle_f$

Summary of numerical models in GT5D

- Gyrokinetic solver in $(R,\zeta,Z,v_{//})$
  - 4th or 6th order NDCFD for 4D advection in $(R,\zeta,Z,v_{//})$

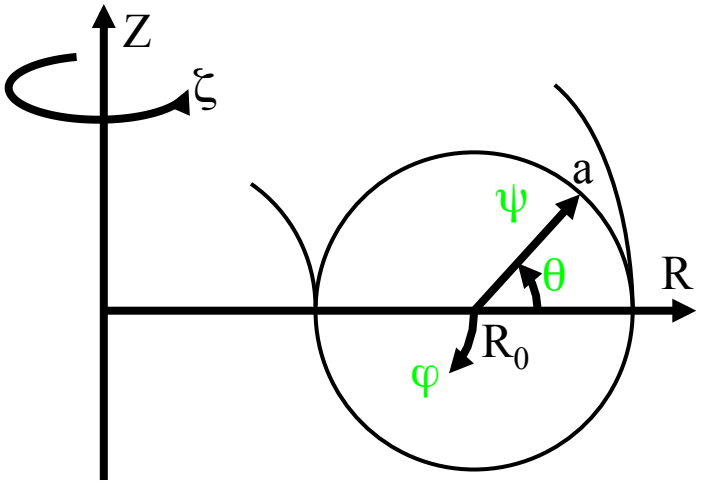
    $\rightarrow$ parallelized in (R,Z,μ) : boundary data commun. in (R,Z)
  - Implicit treatment of stiff parallel advection using 2nd order additive semi-implicit Runge-Kutta method [Zhong,JCP98]
- Collision operator in $(v_{//},\mu)$
  - 6th order centered FD for 2D advection-diffusion in $(v_{//},\mu)$

    $\rightarrow$ parallelized in (R,Z) : data transpose $(R,Z,\mu) \leftrightarrow (R,Z)$
- Field solver in (ψ,θ,φ)
  - Fourier mode expansion in φ
  - 2D FEM solver in (ψ,θ)

    with field-aligned filter [Jolliet,JCP10]

    $\rightarrow$ parallelized in (φ, μ) :

    data transpose $(R,Z,\mu) \leftrightarrow (\varphi, \mu)$

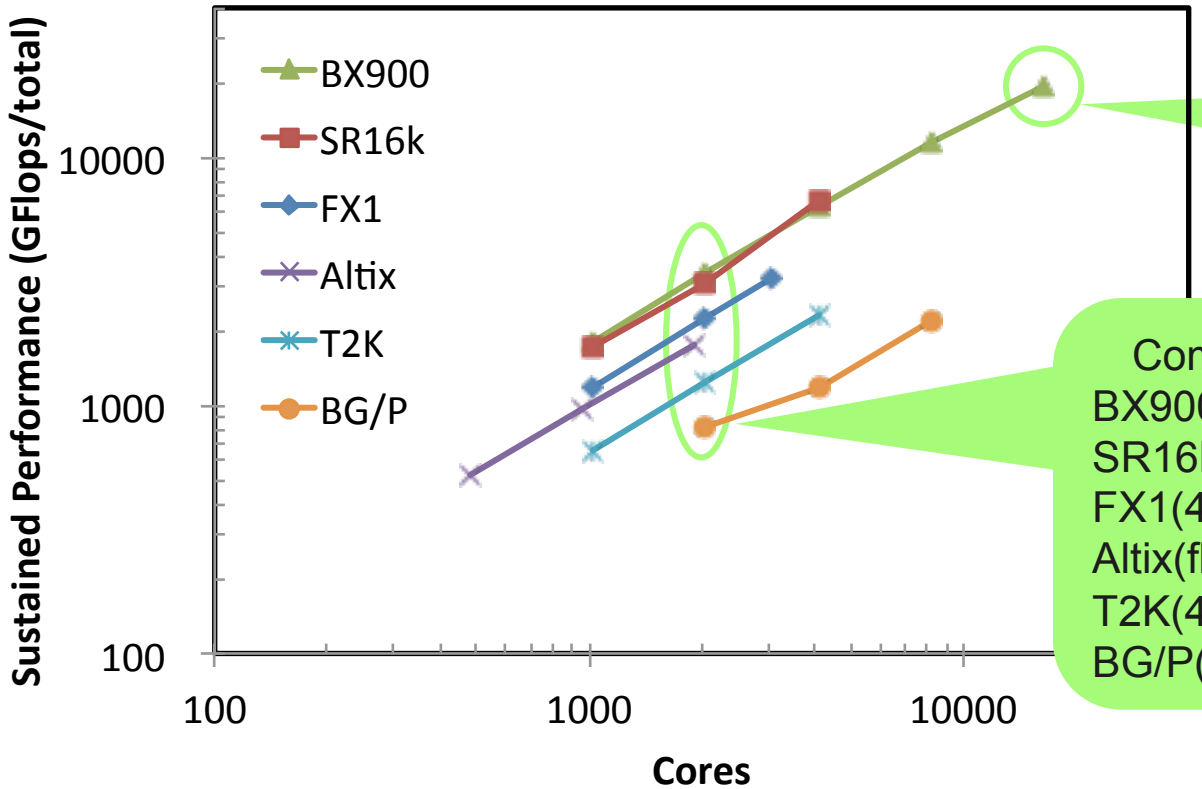


Strong scaling of GT5D on multi-core platforms

[Idomura, Jolliet, accepted for SC'11 conference]

BX900,FX1,SR16000,BG/P:$(N_R,N_\xi,N_Z,N_{v//},N_\mu)=(240,64,240,128,32)$

Altix3700,HA8000:$(N_R,N_\xi,N_Z,N_{v//},N_\mu)=(240,64,240,100,32)$



BX900/16384 core
Sustained~19.4TF(10.1%)

Comparisons at ~2000 cores
BX900(4SMP): ~3.55TF(14.8%)
SR16k(4SMP): ~3.12TF(8.1%)
FX1(4SMP): ~2.26TF(11.0%)
Altix(flatMPI): ~1.75TF(14.3%)
T2K(4SMP): ~1.23TF(6.6%)
BG/P(flatMPI): ~0.81TF(11.7%)

- Multi-layer hybrid parallelization based on symmetry of operators
- Scale beyond 10^4 cores with keeping sustained performance of >10%
- Porting on K-computer is ongoing

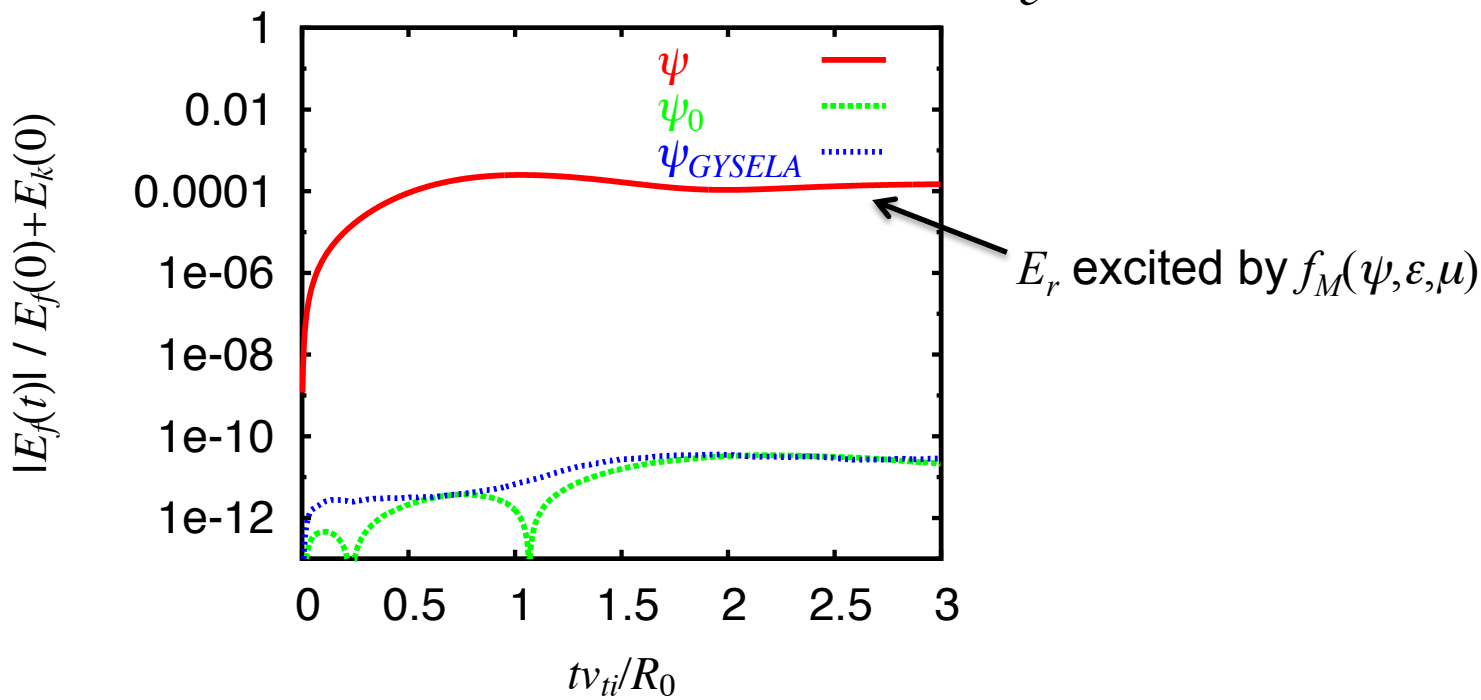
Collisionless equilibrium distribution

[Idomura et al., Comput.Phys.Commun. (2008)]

- Collisionless equilibrium $f_0(\psi_0,\varepsilon,\mu)$ tested in the axisymmetric limit

$$\psi_0 = -\frac{c}{e}P_\varphi, \quad P_\varphi = -\frac{e}{c}\psi + mRv_{//}b_\varphi, \quad \varepsilon = \frac{1}{2}mv_{//}^2 + \mu B$$

❖ modified label to cancel parallel flows $\psi_{GYSELA} = \psi - \frac{c}{e}m\left(Rv_{//} - R_0\bar{v}_{//}\right)b_\varphi$



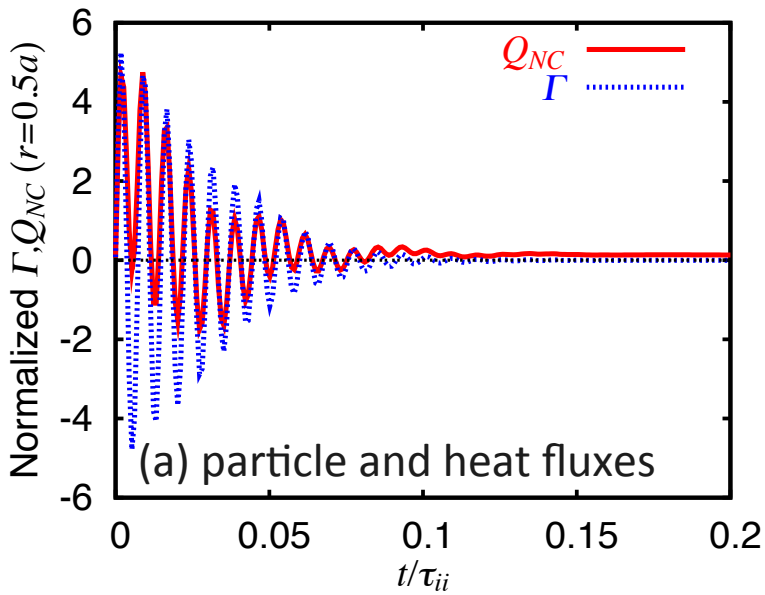
- GT5D satisfies $\{f_0,H_0\}=0$ or $dP_\varphi/dt=0$ with good accuracy
  - Present version solve only $\{\delta f,H_0\}$ and $\{f,\delta H\}$ based on this property

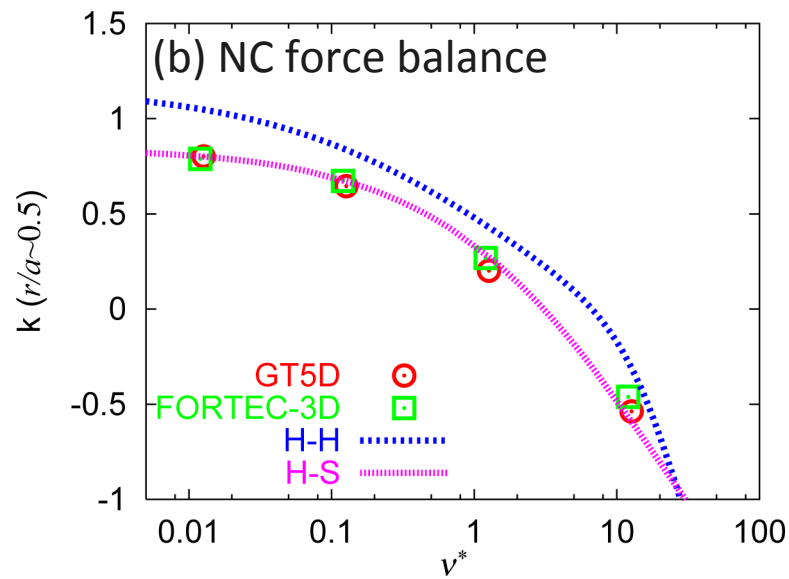
Neoclassical benchmark against FORTEC-3D

[Satake,Idomura,Sugama,Watanabe, Comput.Phys.Commun. (2010)]

- Neoclassical benchmark tests against FORTEC-3D [Satake,NF05]
  - Ambipolar condition in axisymmetric tokamak
  - C-H formula $\chi_{CH}=K_{CH}(\nu^*)\varepsilon^{1/2}\rho_{i\theta}^2/\tau_{ii}$ [Chang-Hinton,PF82]
  - NC force balance [Hinton-Hazeltine,RMP76, Hirshman-Sigmar,NF81]

$$\langle V_{//}\rangle_f = \frac{T_i I}{m_i \Omega_i}\left(\frac{\partial \psi}{\partial r}\right)^{-1}\left[-\frac{\partial \ln n_i}{\partial r}-\frac{\partial \ln T_i}{\partial r}+\frac{e}{T_i}E_r + k\frac{\partial \ln T_i}{\partial r}\right]$$





- QN condition can determine E_r satisfying NC force balance

Conservation of toroidal momentum

- Toroidal momentum transport equation [Scott, POP2010]

$$\frac{\partial P_\varphi f}{\partial t} + \frac{1}{\mathcal{J}}\frac{\partial}{\partial \mathbf{Z}}\cdot\left(\mathcal{J}\dot{\mathbf{Z}}P_\varphi f\right) = -f\frac{\partial H}{\partial \varphi}$$

$$\rightarrow \frac{\partial}{\partial t}\left\langle \rho_M R V_{E\varphi} + m R v_\parallel b_\varphi f\right\rangle_f + \frac{\partial}{\partial V}\left\langle \nabla V\cdot\left(m R v_\parallel b_\varphi f\dot{\mathbf{R}} - \rho_M\frac{c^2}{B^2}\frac{\partial\phi}{\partial\varphi}\nabla\phi\right)\right\rangle_f = 0$$

- Toroidal momentum balance equation checked in GT5D

$$\frac{\partial P_\varphi f}{\partial t} + P_\varphi\frac{1}{\mathcal{J}}\frac{\partial}{\partial \mathbf{Z}}\cdot\left(\mathcal{J}\dot{\mathbf{Z}}f\right) = P_\varphi C + P_\varphi S$$

❖ recover the above equation by adding $f\dot{P}_\varphi = -f\partial_\varphi H$

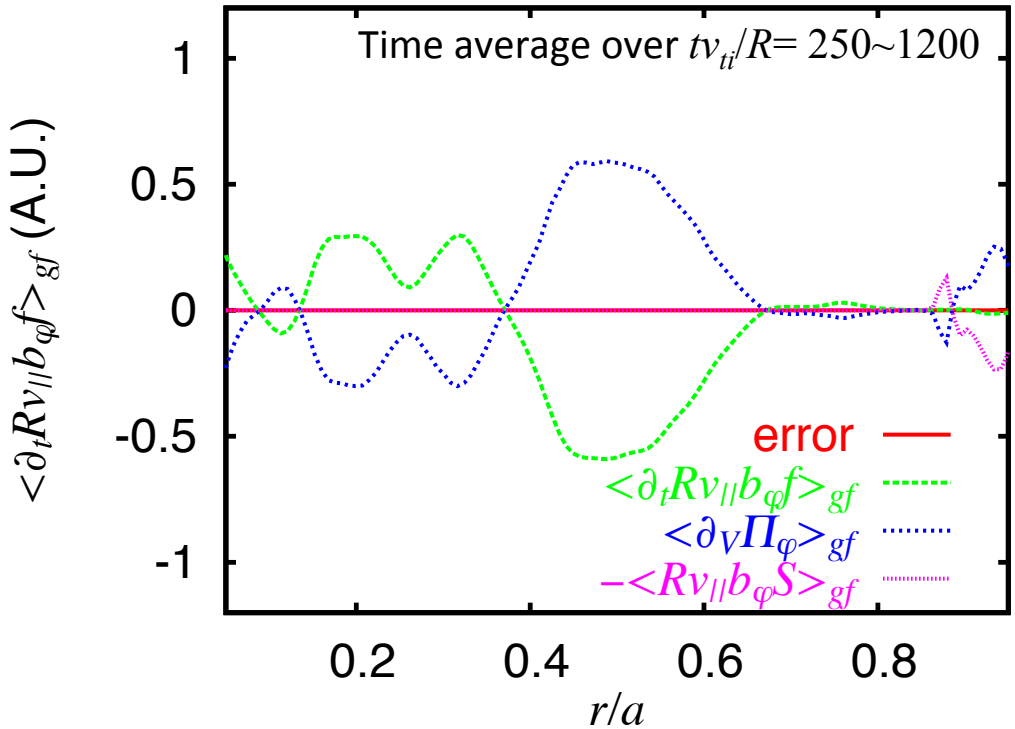
$$\rightarrow \left\langle\frac{\partial m R v_\parallel b_\varphi f}{\partial t}\right\rangle_{gf} + \left\langle\frac{1}{\mathcal{J}}\frac{\partial}{\partial \mathbf{R}}\cdot\left(\mathcal{J}\dot{\mathbf{R}} m R v_\parallel b_\varphi f\right)\right\rangle_{gf} = \left\langle m R v_\parallel b_\varphi S\right\rangle_{gf}$$

- A_φ terms are canceled by exact particle conservation
- C term disappear due to exact particle and momentum conservation

Accuracy of toroidal momentum conservation

- Toroidal momentum balance condition in flux-driven ITG turbulence

Cyclone case with $1/\rho^*\sim150$, fixed heat source without particle and momentum input



- Momentum conservation satisfied with good accuracy
  - Bipolar flow generation determined mainly by global E_r shear structure
  - Co-current momentum injection from no-slip plasma boundary

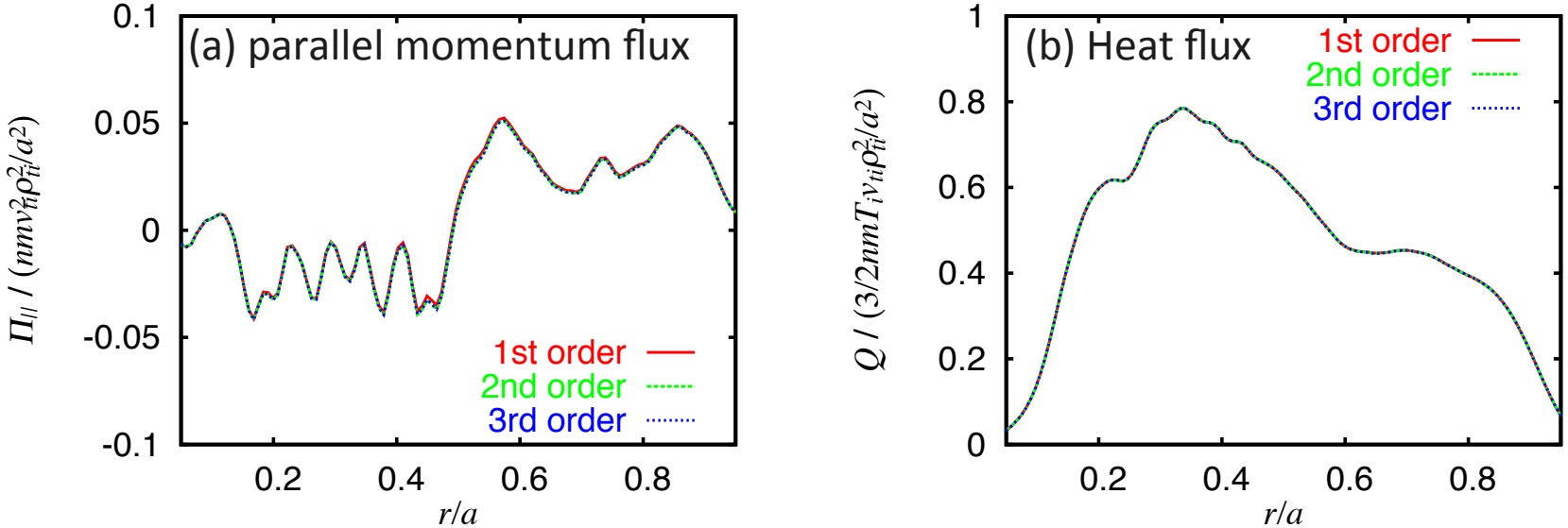
Influences of higher order drifts on turbulent fluxes

- Higher order gyro-center Hamiltonian [Mishchenko,POP2010]

$$H = \frac{1}{2}mv_{\parallel}^2 + \mu B + e\langle\phi\rangle_g - \frac{mc^2}{2B^2}\left(\nabla_\perp\phi\right)^2 + \frac{e}{4B^2\Omega_c^2}\left(\nabla_\perp\phi\cdot\nabla_\perp\right)\left[\left(\nabla_\perp\phi\right)^2\right]$$

- Convergence of turbulent fluxes in flux-driven ITG turbulence

Cyclone case with $1/\rho^*\sim150$, time average over $tv_{ti}/R= 250\sim1200$



- Influences of higher order drifts are negligible

c.f. Intrinsic statistical error bar of gyrokinetic simulation is ~15%

[McMillan,POP08, Villard,PPCF10, Jolliet,JCP10]

Flux driven ITG turbulence simulations

- Calculation parameters (Cyclone like)

  R_0/a=2.8, B_0=1.9T, q=0.85+2.18$(r/a)^2$, n_e~5×10^{19}m^{-3}, T_i~2keV

  $1/\rho^*$=100, 150, 225, ν^*=0.025~0.1

  1/6 wedge torus (n=0,6,12,…)

  $(N_R,N_\xi,N_Z,N_{v//},N_\mu)$=(110,24,110,80,20) ~ (230,48,230,80,20)

- Fixed heat source (r/a<0.4)

  $S_{src}=A_{src}(\psi)\,\tau_{src}^{-1}(f_{M1}-f_{M2})$

  $P_{in}=\int(m_i v^2/2)S_{src}d^6Z$ = 1.3~3MW

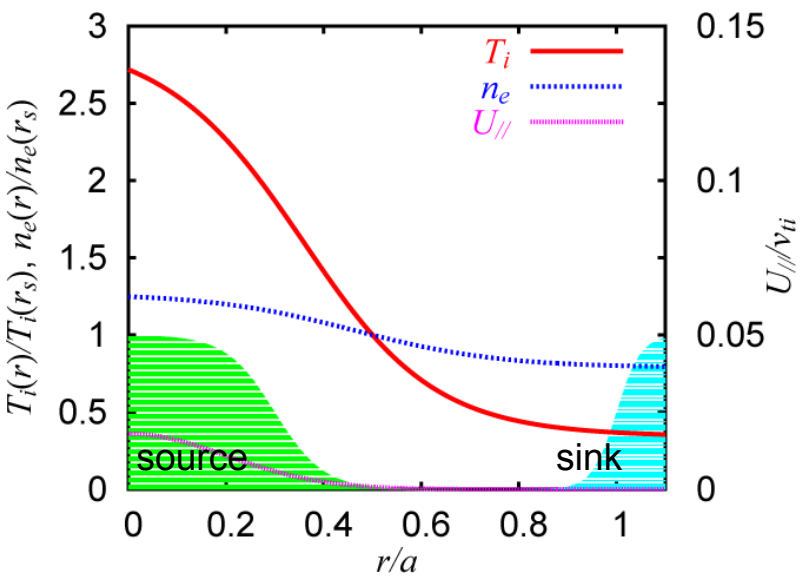
  with no particle/momentum input

- Sink (r/a>0.9)

  $S_{snk}=A_{snk}(\psi)\tau_{snk}^{-1}[f_0-f]$

  No slip boundary with fixed edge T_i

Initial profiles and source/sink



- Adaptive momentum source

  $S_{ad}=\tau_{ad}^{-1}\,[f_M(\langle n\rangle_f,\, V_{//ad},\, T_{ad})-f_M(\langle n\rangle_f,\, \langle V_{//}\rangle_f,\, \langle T\rangle_f)]$

  Adaptive momentum input without particle/power input

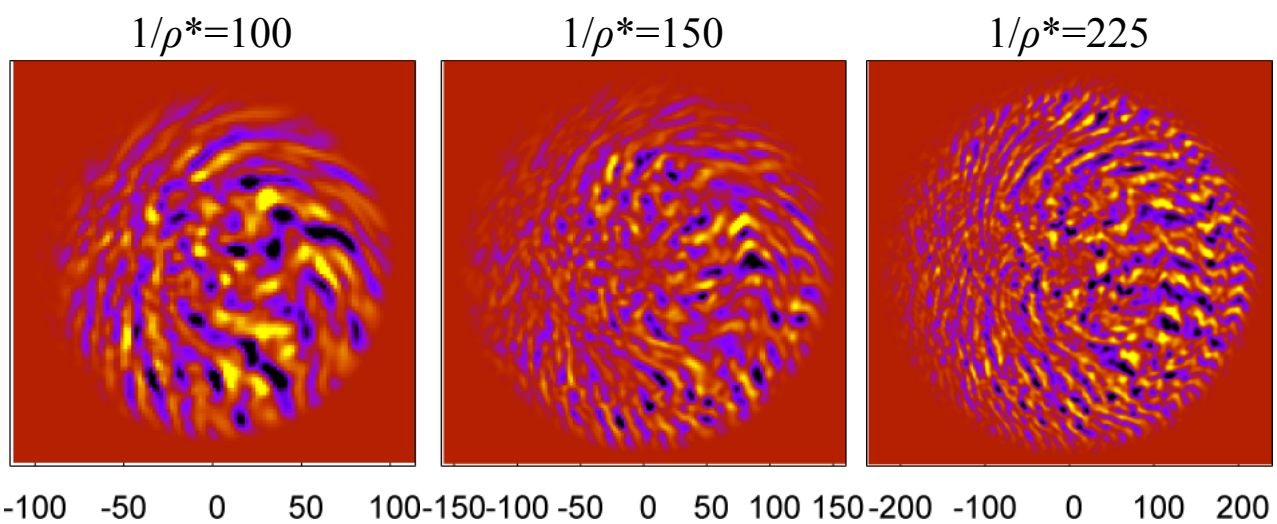
Plasma size scaling of ITG turbulence

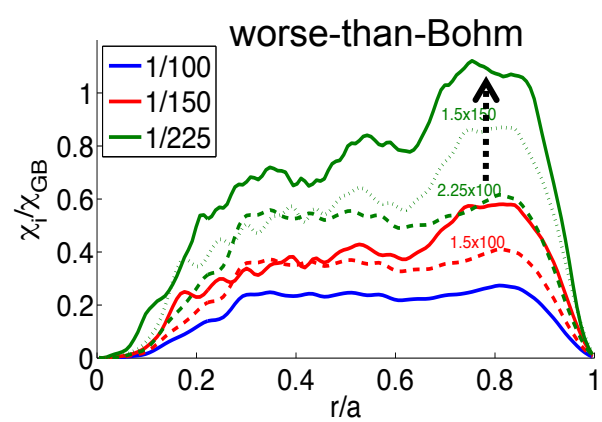
[Jolliet,Idomura, IAEA2010, submitted to Nucl. Fusion]

- First size scaling study of ITG turbulence near critical L_{ti}
  - worse-than-Bohm scaling with gyro-Bohm like turbulent correlations

    c.f. Size scaling on DIIID L-mode plasmas [Petty,PRL95,McKee,NF01]
- ρ^* effects and non-local transport mechanisms
  - avalanche-like heat flux due to radial propagation of blobs
  - non-Gaussian features in PDF of turbulent heat flux
  - ρ^* dependence of global E_r structure

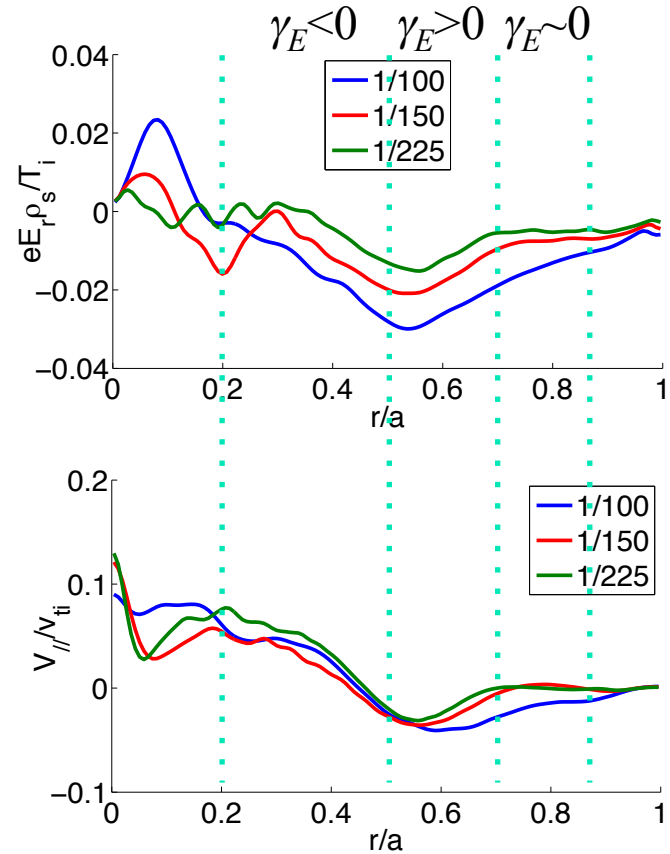
Flux-driven ITG turbulence, Cyclone like parameters with $1/\rho^*$=100,150,225





ρ^* dependence of global E_r structure

- Mean E_r profiles
  - negative / positive / flat E_r shear regions appear at smaller ρ^*
  - correlated with parallel flow profiles through force balance relation



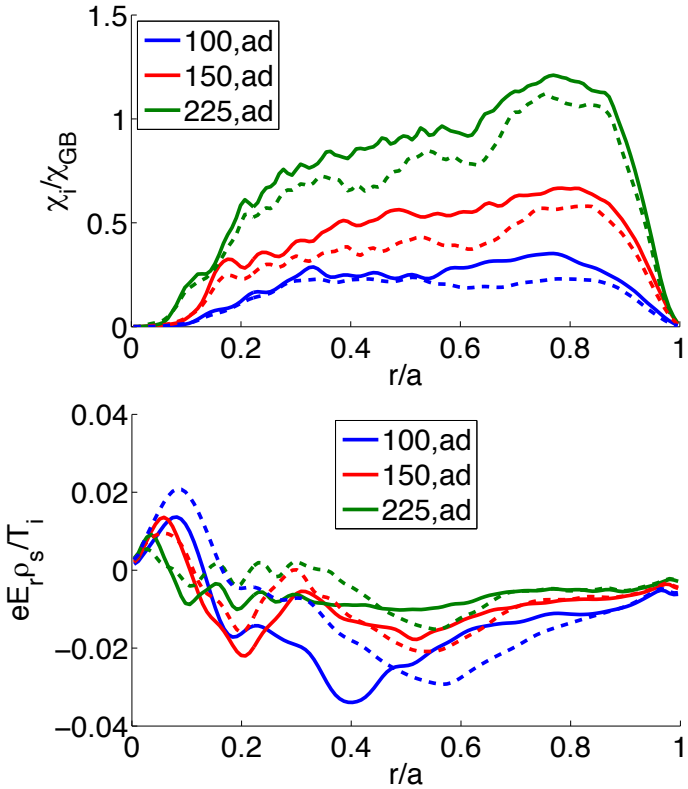
- E_r shearing rates γ_E (c_s/a units)

$1/\rho^*$	γ_L	γ_E <0	γ_E>0	γ_E~0
100	0.073	-0.084	0.067	0.048
150	0.073	-0.074	0.070	0.018
225	0.074	-0.080	0.065	0.010

- Force balance relation with $V_{//}$~0 suggests $\gamma_E \propto \rho^*$
- In γ_E <0 and γ_E >0 regions, ρ^* dependence of γ_E is weak, $\gamma_E \sim \gamma_L \sim$ const.
- In γ_E ~0 region, ρ^* dependence of γ_E is enhanced by formation of flat $V_{//}$ profiles at smaller ρ^*

Decoupling momentum transport using adaptive source

- ρ^* scan with adaptive momentum source
  - $V_{//}$ profiles canceled by adaptive source
    c.f. [Solomon,POP10,Ida,NF10,Ku,IAEA10]
  - higher transport levels than original cases
    →suppression of turbulent heat transport by turbulent momentum transport



❖ dashed lines: original case

- E_r shearing rates γ_E (c_s/a units)

$1/\rho^*$	γ_L	original		ad. source	
		$\gamma_E>0$	$\gamma_E\sim0$	$\gamma_E>0$	$\gamma_E\sim0$
100	0.073	0.067	0.048	0.072	0.018
150	0.073	0.070	0.018	0.048	0.011
225	0.074	0.065	0.010	0.025	0.009

  - without parallel flows, E_r shear follows ρ^* scaling, $\gamma_E \propto \rho^*$
    →Overall reduction of E_r shear enhances transport levels
    →Worse-than-Bohm scaling becomes weaker

Summary

- Accuracy of momentum transport in GT5D is tested
  - Collisionless equilibrium given by P_φ
  - Neoclassical force balance relation
  - Accuracy of toroidal momentum conservation
  - Influences of higher order drifts on turbulent fluxes

  →Test results suggest correctness of momentum transport in GT5D

  →Influences of higher order polarization terms are yet to be examined

- Roles of momentum transport in ITG turbulence
  - Global E_r structure has significant impact on turbulent transport
  - Global E_r profiles are connected with intrinsic $V_{//}$ profiles, which seem to be ρ^* independent effect in force balance relation
  - Simulations with adaptive momentum source suggest

  →suppression of heat transport by turbulent momentum transport