Kinetic Simulations of Turbulent Fusion Plasmas

Y.Idomura, T.H.Watanabe, H.Sugama, Comptes Rendus Physique 7, 650 (2006)

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Acknowledgements to **H. Sugama and T.H. Watanabe**

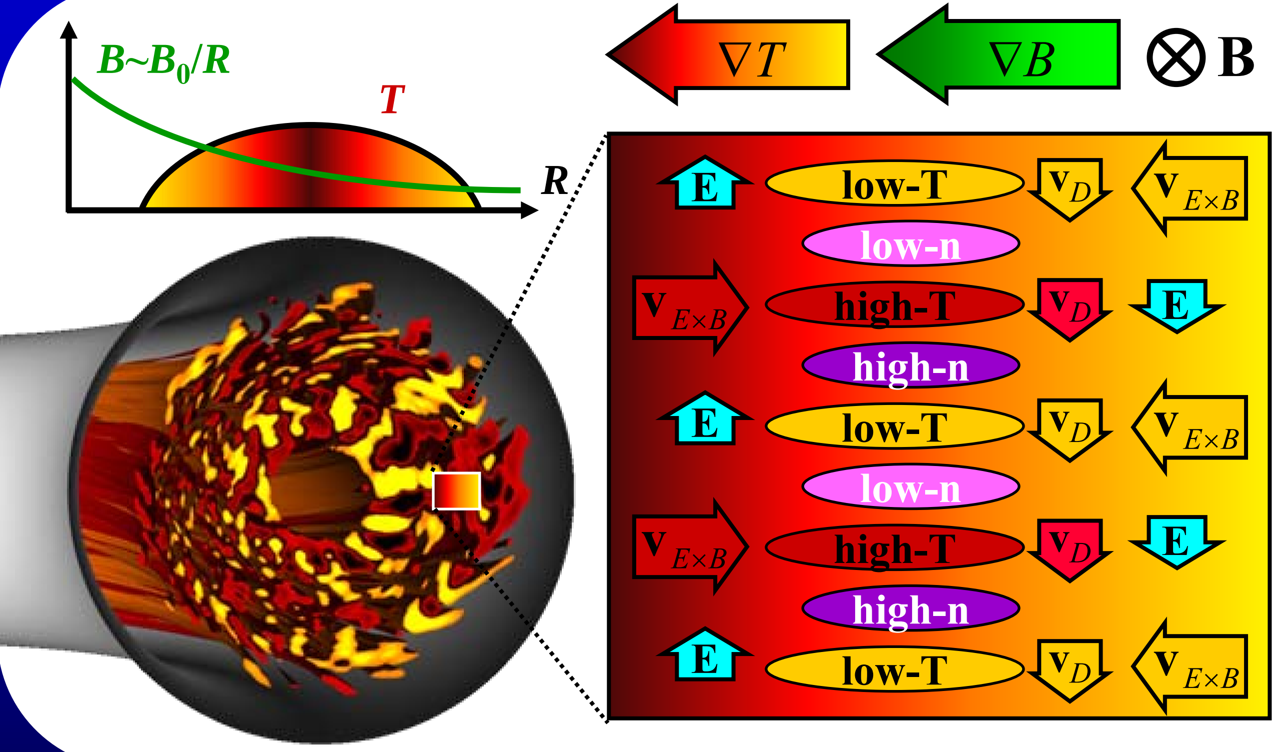
1st ITER Summer School, Aix-en-Province, France, July 16-20, 2007

- Outline

1. Introduction
2. Gyrokinetic model
3. Various approaches in gyrokinetic simulations
4. Particle/Lagrangian approach
5. Mesh/Eulerian approach
6. Collisionless gyrokinetic simulation

1. Introduction

Micro-instabilities in tokamak plasmas



Magnetic drift

$$\mathbf{v}_D = \frac{v_{//}^2/2 + v_\perp^2}{\Omega}\mathbf{b}\times\nabla \ln B$$

ExB drift

$$\mathbf{v}_{E\times B} = \frac{c}{B^2}\mathbf{E}\times\mathbf{B}$$

Unstable side given by

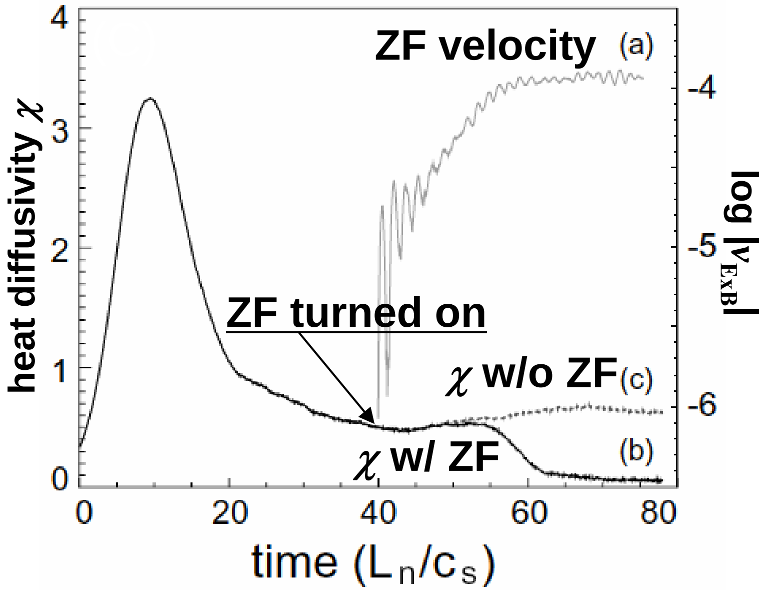
$$\nabla T\cdot\nabla B > 0$$

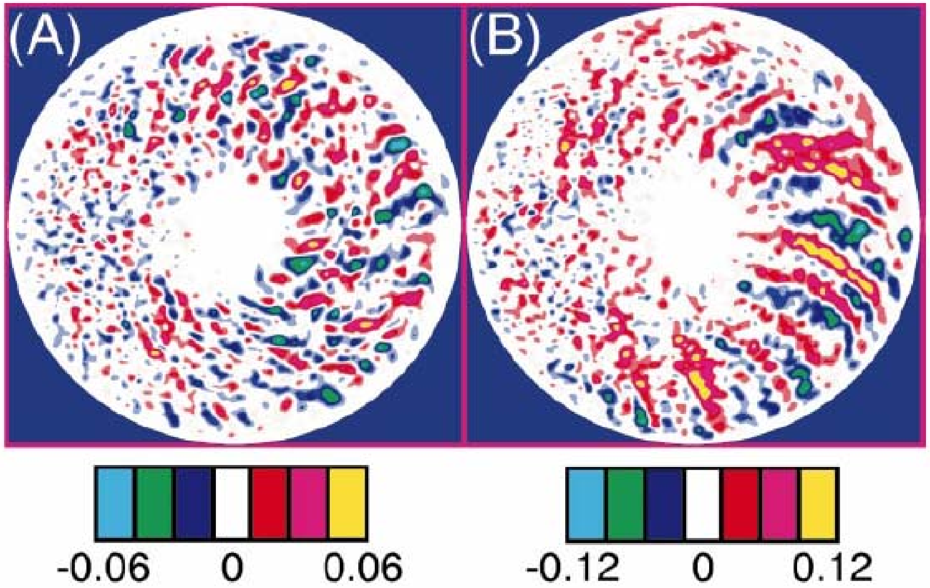
- Temperature gradient driven modes in tokamaks
  - Ion temperature gradient driven (ITG) modes $k_\perp^{-1} \sim \rho_i$
  - Electron temperature gradient driven (ETG) modes $k_\perp^{-1} \sim \rho_e, \lambda_{De}$
- Trapped particle modes, Electromagnetic modes, etc…

ITG turbulence suppression by zonal flows

Toroidal ITG turbulence simulation with and without zonal flows

(Lin,Science98, Diamond,NF01)

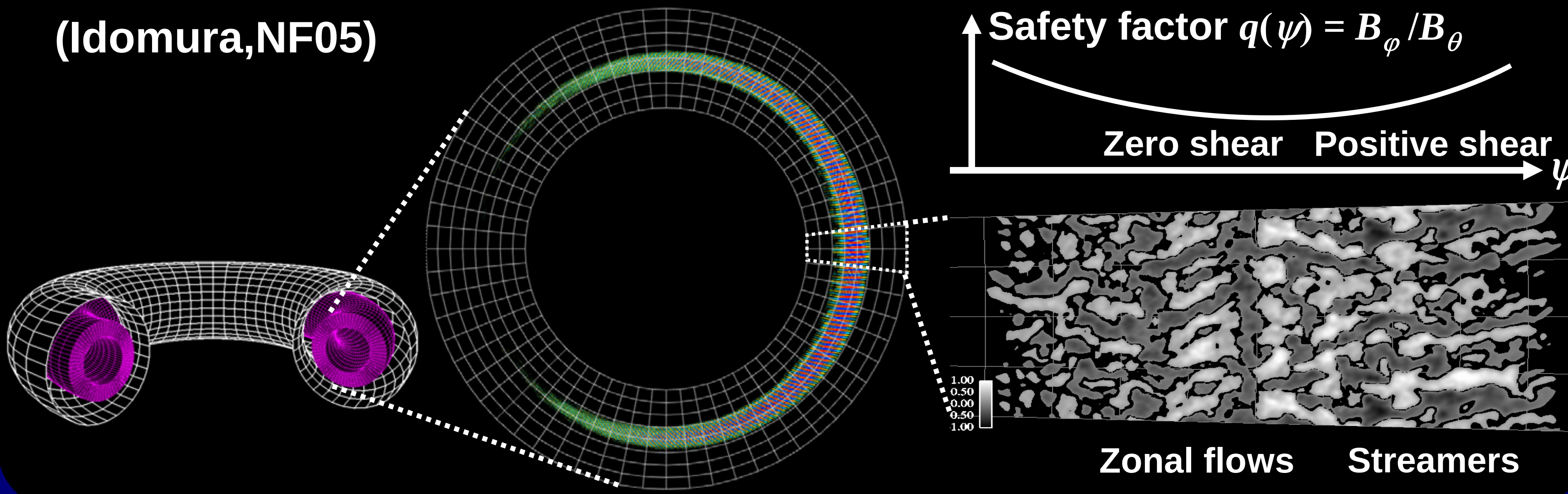




- Various zonal flow instabilities
  (Diamond,IAEA98, Chen,POP00, Rogers,PRL00)
- Nonlinear upshift of effective critical ITG by zonal flows
  (Dimits,POP00)
- Linear damping mechanism of zonal flows
  (Rosenbluth-Hinton,PRL98)

Structure formations in microscopic ETG turbulence

Toroidal ETG turbulence simulation in reversed shear tokamak (Idomura,NF05)

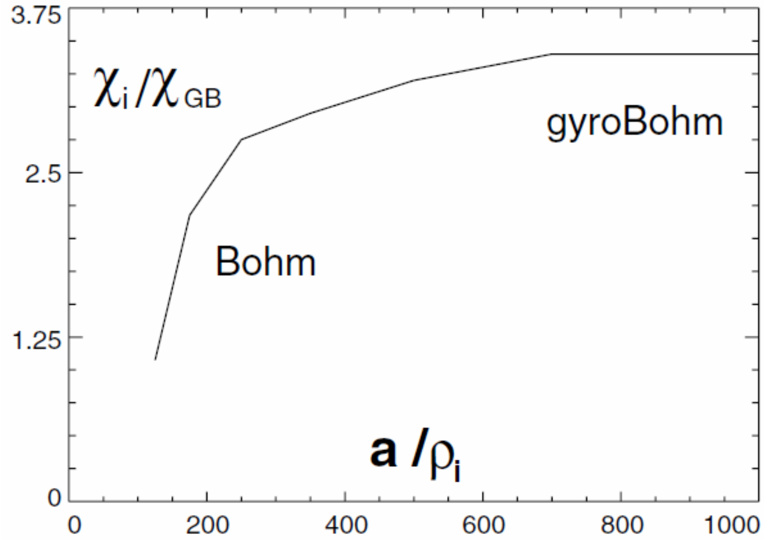


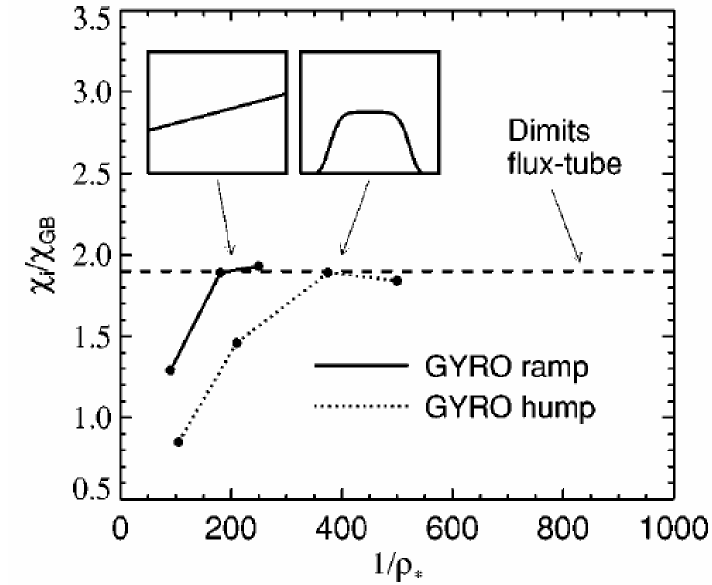
- Enhanced transport by streamers in positive magnetic shear
  (Jenko,POP00, Dorland,PRL00)
- Transport reduction by zonal flows in reversed magnetic shear
  (Idomura,NF05,POP06)
- Various secondary/tertiary instabilities for streamers/zonal flows
  (Idomura,POP00, Jenko,PRL02, Holland,POP02, Li,POP02)

Plasma size scaling of ITG turbulence

Transition of plasma size scaling from Bohm to gyro-Bohm

(Lin,PRL02, Candy,POP04)

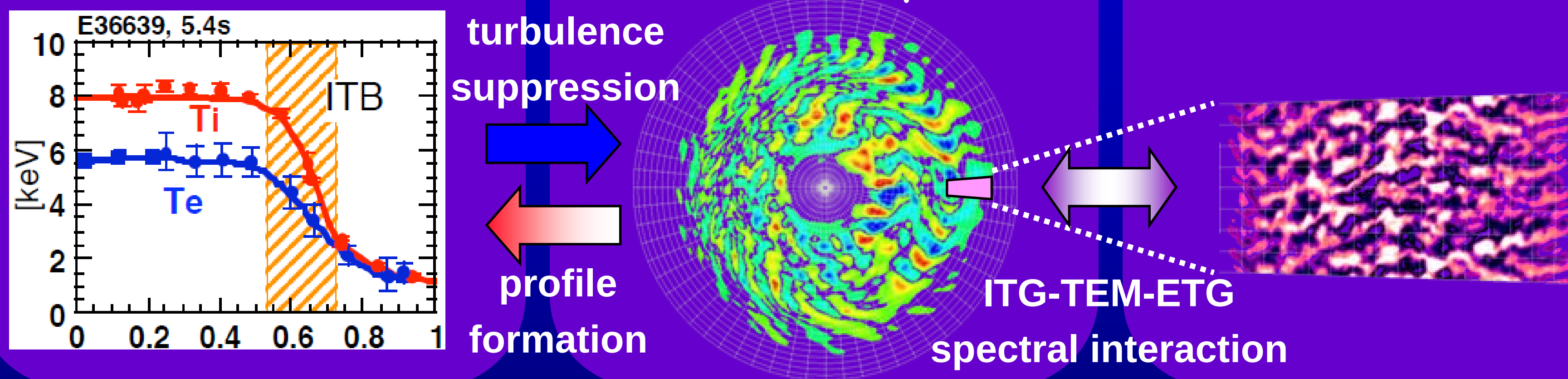




- Linear ballooning theory with equilibrium profile shear effects
  (Connor,PRL93, Romanelli,PFB93, Kim,PRL94)
- Shearing effects of equilibrium *E*x*B* flows on size scaling
  (Garbet,POP96, Waltz,POP02)
- Turbulence spreading into less unstable or stable regions
  (Lin,POP04, Hahm,PPCF04, Waltz,POP05)

Simulation for multi-scale tokamak micro-turbulence

- **Profile formation** **~10cm,~10ms**
- **Ion scale turbulence** **~5mm,~1μs**
- **Electron turbulence** **~0.1mm,~10ns**



- Future issues addressed using first principle simulations
  - Formation of transport barriers
  - ITG-TEM-ETG, electromagnetic turbulence
  - Edge/SOL turbulence

  Advanced multi-scale gyrokinetic simulations are needed
- Purpose of this lecture
  - To explain physical and numerical models of GK simulations

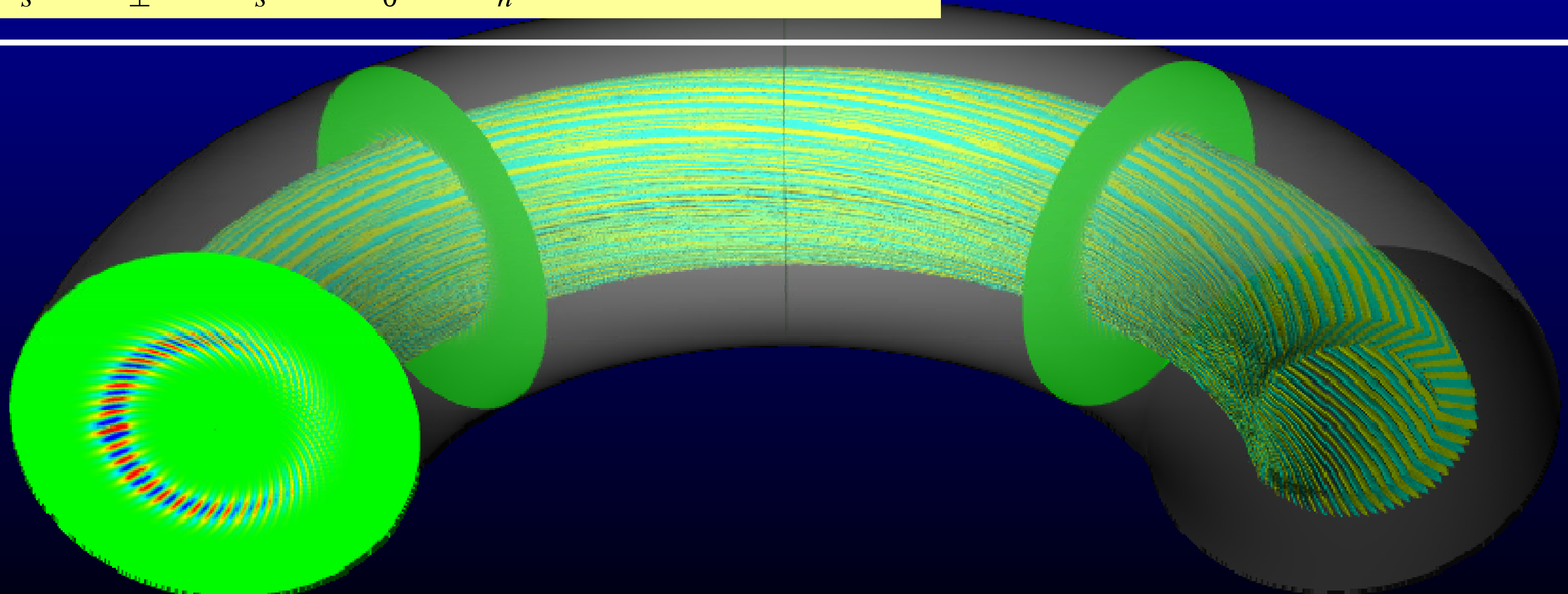
2. Gyrokinetic model

Physical properties of turbulent fusion plasmas

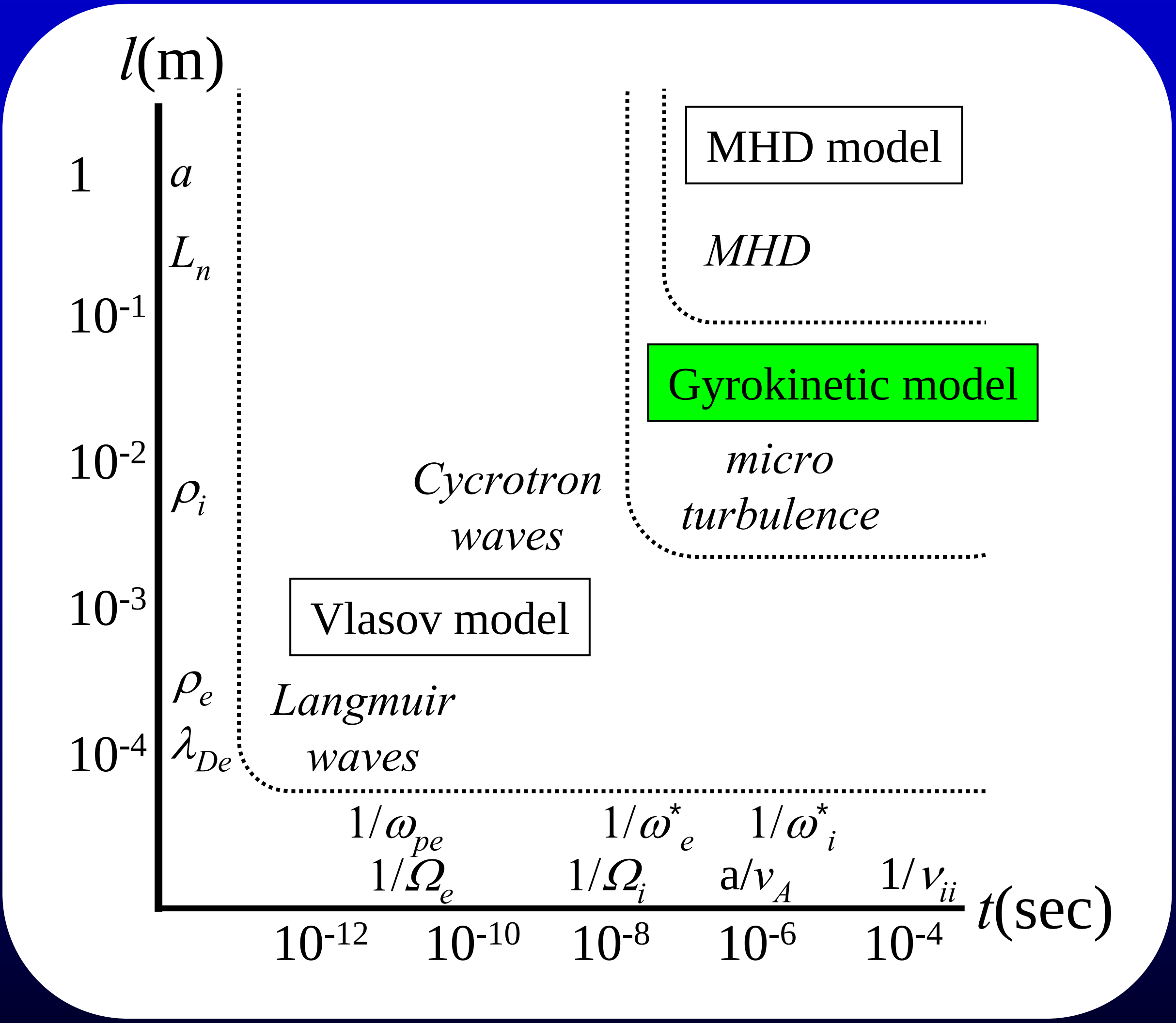
- **Fusion plasma ($n\sim10^{19}\mathrm{m}^{-3}$, $T\sim10\mathrm{keV}$) is weakly coupled plasma**
  - **Low collisionality $\sim1\mathrm{kHz}$, mean free path $\sim10\mathrm{km}$**
  - **Orbit effects and wave-particle resonance are important**

  5D kinetic model is needed instead of 3D fluid model
- **Turbulent fluctuations are considered to follow the ordering**

$$\frac{\omega}{\Omega_s} \approx \frac{k_{//}}{k_\perp} \approx \frac{e_s\phi}{T_s} \approx \frac{B_1}{B_0} \approx \frac{\rho_s}{L_n} \approx O(\varepsilon_g), \quad k_\perp\rho_s \le 1$$



Spatio-temporal scales in fusion plasmas



What is a physical model appropriate for studying micro-turbulence?

Primitive kinetic model of weakly coupled plasma

- Vlasov-Poisson system in canonical coordinates $\mathbf{Z}_{CC}=(t;\mathbf{q},\mathbf{p})$

$$\frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} + \{f_{CC}, H_{CC}\} = \frac{\partial f}{\partial t} + \frac{\partial H_{CC}}{\partial \mathbf{p}} \cdot \frac{\partial f}{\partial \mathbf{q}} - \frac{\partial H_{CC}}{\partial \mathbf{q}} \cdot \frac{\partial f}{\partial \mathbf{p}} = 0 \quad \text{Vlasov Eq.}$$

$$\{F, G\} = \frac{\partial F}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial G}{\partial q_i} \quad \text{Poisson bracket}$$

$$H_{CC}(\mathbf{q},\mathbf{p}) = \frac{1}{2m}\left|\mathbf{p} - \frac{e}{c}\mathbf{A}\right|^2 + e\phi(\mathbf{q}) \quad \text{Hamiltonian}$$

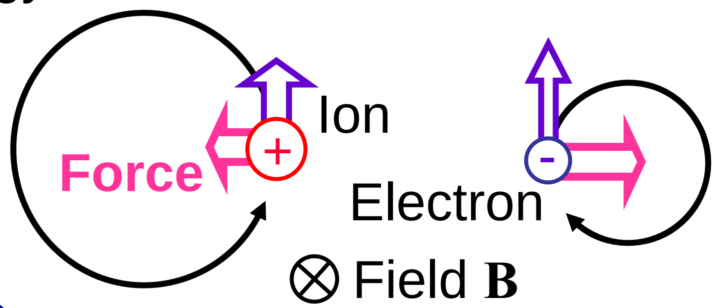
$$-\nabla^2\phi = 4\pi\sum_s e_s n_s, \quad n_s = n_{0s}\int f_s d\mathbf{p} \quad \text{Poisson Eq.}$$

  - Continuity equation of f transported by Hamiltonian flows in 6D phase space
  - Spatio-temporal scales are given by $\sim\lambda_{De}$ and $\sim\omega_{pe}$

Very expensive model for studying tokamak micro-turbulence

Gyrokinetic model for tokamak micro-turbulence

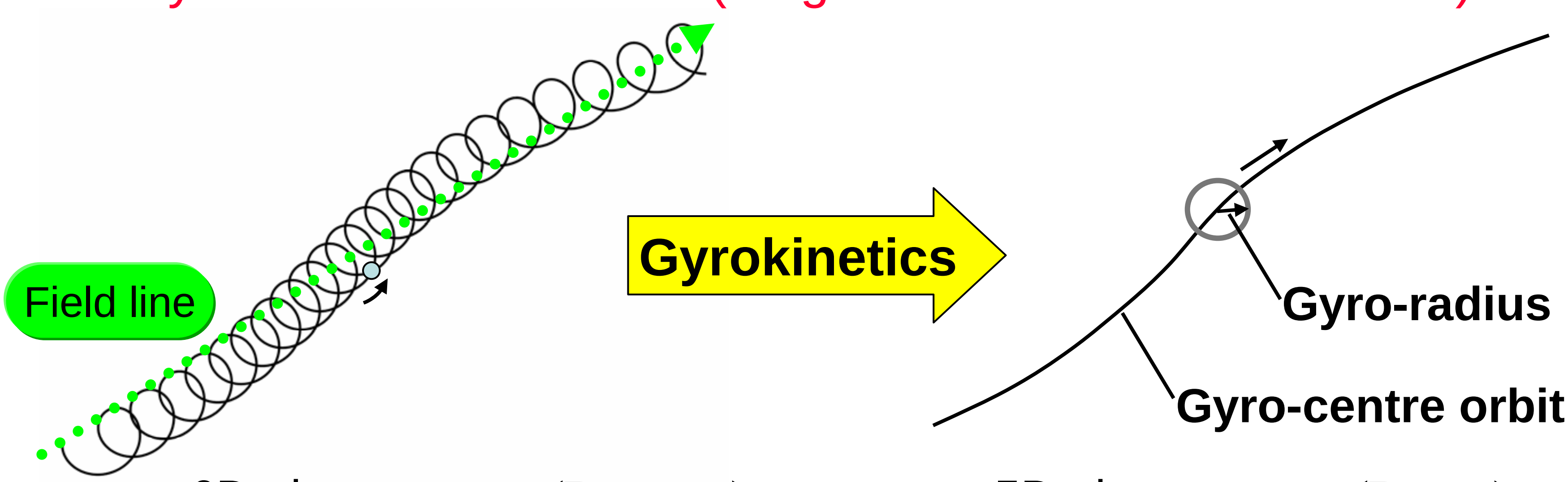
gyro-motion due to Lorenz force



- **Minimum scale of turbulence**
  Ion ~5mm, Electron ~0.1mm
- **Fast gyro-motion is adiabatic**
  Gyrokinetics in 5D phase space

Fast gyro-motion ~1GHz + slow drift-motion ~100kHz

Gyro-motion is adiabatic (magnetic moment is conserved)



6D phase space $(\mathbf{R}, v_{//}, \mu, \alpha)$ 5D phase space $(\mathbf{R}, v_{//}, \mu)$

Particle motion in guiding-centre coordinates

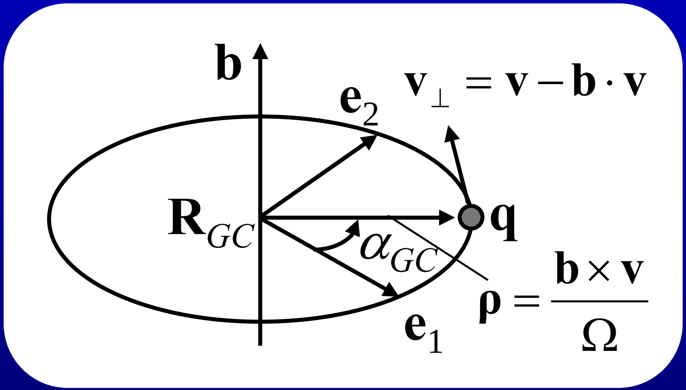
- Lagrangian in canonical coordinates $\mathbf{Z}_{CC}=(t;\mathbf{q},\mathbf{p})$

$$\gamma_{CC}=\mathbf{p}\cdot d\mathbf{q}-H_{CC}dt,\quad H_{CC}=\frac{1}{2m}\left|\mathbf{p}-\frac{e}{c}\mathbf{A}\right|^2+e\phi(\mathbf{q})$$

- Guiding-centre coordinates $\mathbf{Z}_{GY}$

$$\mathbf{R}_{GC}=\mathbf{q}-\boldsymbol{\rho},\quad v_{//GC}=\mathbf{b}\cdot\mathbf{v}$$

$$\mu_{GC}=\frac{m|\mathbf{v}_\perp|^2}{2B},\quad \alpha_{GC}=\tan^{-1}\left(\frac{\mathbf{v}\cdot\mathbf{e}_1}{\mathbf{v}\cdot\mathbf{e}_2}\right)$$



- Lagrangian in $\mathbf{Z}_{GC}=(t;\mathbf{R}_{GC},v_{//GC},\mu_{GC},\alpha_{GC})$

(Littlejohn, J. Math. Phys.79, PF81, J. Plasma Phys.83)

$$\gamma_{GC}=\left(\frac{e}{c}\mathbf{A}+v_{//GC}\mathbf{b}\right)\cdot d\mathbf{R}_{GC}+\frac{mc}{e}\mu_{GC}d\alpha_{GC}-H_{GC}dt$$

$$H_{GC}(\mathbf{R}_{GC},v_{//GC},\mu_{GC},\alpha_{GC})=\frac{1}{2}mv_{//GC}^2+\mu_{GC}B+e\phi(\mathbf{R}_{GC},\mu_{GC},\alpha_{GC})$$

  – Fast α-dependence in H_{GC} (μ_{GC} is approximate invariant)

Reduction of problem to 5D phase space

- Find gyro-centre coordinates $\mathbf{Z}_{GY}$ using near identity transformations
  (Cary-Littlejohn,Ann. Phys.83, Brizard-Hahm,Rev. Mod. Phys.06)

$$\mathbf{Z}_{GY} \equiv T_\varepsilon \mathbf{Z}_{GC} = \mathbf{Z}_{GC} + \varepsilon_g \mathbf{G}_1 + \cdots \qquad \mathbf{G}_1 : \text{generating vector}$$

$$f_{GY}(\mathbf{Z}_{GY}) = f_{GC}(\mathbf{Z}_{GC}) = f_{GC}(T_\varepsilon^{-1}\mathbf{Z}_{GY}) = T_\varepsilon^{-1} f_{GC}(\mathbf{Z}_{GY}) \qquad \text{push-forward transform}$$

$$\gamma_{GY} = T_\varepsilon^{-1}\gamma_{GC} + dS \qquad S : \text{gauge scalar}$$

- Lagrangian in gyro-centre coordinates $\mathbf{Z}_{GY}=(t;\mathbf{R}_{GY},v_{//GY},\mu_{GY},\alpha_{GY})$
  (Dubin,PF83, Hahm,PF88, Brizard,POP95, Sugama,POP00, Wang,PRE01)

$$\mathbf{Z}_{GY} \equiv T_\varepsilon \mathbf{Z}_{GC} = \mathbf{Z}_{GC} + \{S, \mathbf{Z}_{GC}\}, \quad S = \frac{e}{\Omega}\int^{\alpha}\left[\phi - \langle\phi\rangle_\alpha\right] d\alpha', \quad \langle\phi\rangle_\alpha \equiv \frac{1}{2\pi}\oint \phi\, d\alpha$$

$$\gamma_{GY} = \left(\frac{e}{c}\mathbf{A} + v_{//GY}\mathbf{b}\right)\cdot d\mathbf{R}_{GY} + \frac{mc}{e}\mu_{GY}\, d\alpha_{GY} - H_{GY}\, dt$$

$$H_{GY}(\mathbf{R}_{GY}, v_{//GY}, \mu_{GY}) = \frac{1}{2} m v_{//GY}^2 + \mu_{GY} B + e\langle\phi\rangle_\alpha(\mathbf{R}_{GY}, \mu_{GY})$$

  - H_{GY} becomes α-independent (μ_{GY} is exact invariant)
  - γ_{GY} keeps form invariance (canonical transform)

Gyro-centre Hamilton's equation

- Poisson bracket in $\mathbf{Z}_{GC}$ and $\mathbf{Z}_{GY}$

$$\{F,G\} \equiv \frac{\Omega}{B}\left(\frac{\partial F}{\partial \alpha}\frac{\partial G}{\partial \mu} - \frac{\partial F}{\partial \mu}\frac{\partial G}{\partial \alpha}\right) + \frac{\mathbf{B}^*}{mB_{//}^*}\cdot\left(\nabla F \frac{\partial G}{\partial v_{//}} - \frac{\partial F}{\partial v_{//}}\nabla G\right) - \frac{c}{eB_{//}^*}\mathbf{b}\cdot\nabla F\times\nabla G$$

$$\mathbf{B} = \nabla\times\mathbf{A}, \quad B = |\mathbf{B}|, \quad \mathbf{b} = \mathbf{B}/B, \quad \mathbf{B}^* = \mathbf{B} + \frac{cm}{e}\nabla\times\mathbf{b}v_{//}, \quad B_{//}^* = \mathbf{b}\cdot\mathbf{B}^*, \quad \Omega = \frac{eB}{mc}$$

- Gyro-centre Hamilton's equation

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

$$\dot{\mathbf{Z}} \equiv \{\mathbf{Z}, H\}$$

$$\dot{\mathbf{R}} = \frac{\mathbf{B}^*}{B_{//}^*}\frac{\partial H}{\partial v_{//}} + \frac{mc}{eB_{//}^*}\mathbf{b}\times\nabla H = v_{//}\mathbf{b} + \frac{c}{eB_{//}^*}\mathbf{b}\times\left(e\nabla\langle\phi\rangle_\alpha + mv_{//}^2\mathbf{b}\cdot\nabla\mathbf{b} + \mu\nabla B\right)$$

$E\times B$ — curvature — ∇B

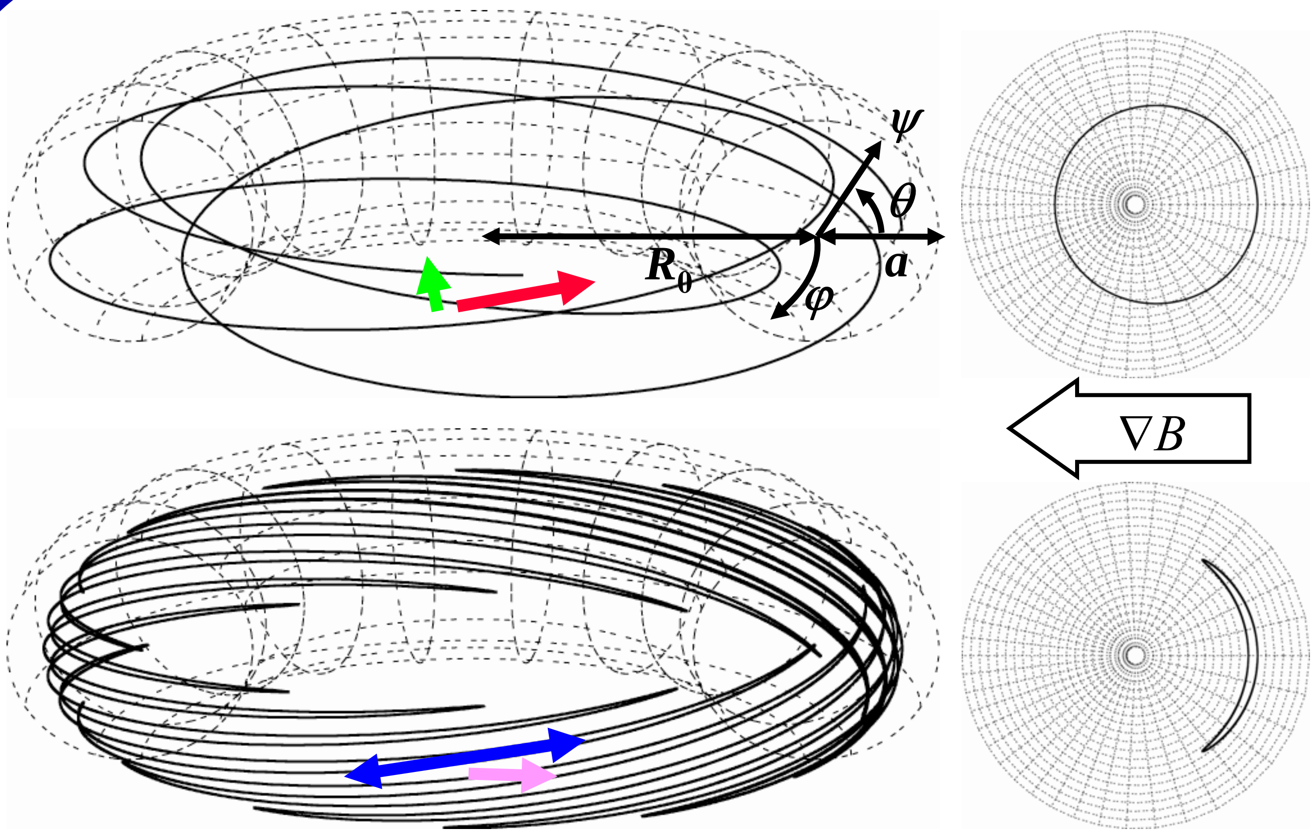
$$\dot{v}_{//} = -\frac{\mathbf{B}^*}{B_{//}^*}\cdot\nabla H = -\frac{\mathbf{B}^*}{mB_{//}^*}\cdot\left(e\nabla\langle\phi\rangle_\alpha + \mu\nabla B\right)$$

$E_{//}$ — mirror

$$\dot{\mu} = 0$$

Unperturbed particle orbits in tokamak configuration

- **Wave particle resonant interaction excites micro-turbulence**
  Slab, toroidal, and trapped particle modes are excited by passing motion, magnetic drift, and toroidal precession



Passing particles for large $v_{//}/v_{\perp}$
passing motion +
magnetic drift

Trapped particles for small $v_{//}/v_{\perp}$
bounce motion +
toroidal precession

Gyrokinetic equation

- Gyrokinetic equation

$$\frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} + \left\{ f, H \right\} = \frac{\partial f}{\partial t} + \dot{\mathbf{R}} \cdot \nabla f + \dot{v}_{//} \frac{\partial f}{\partial v_{//}} = 0$$

- Conservative form of gyrokinetic equation

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

- Phase space conservation

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

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

$m^2 B_{//}^*$: Jacobian of gyro-centre coordinates $\mathbf{Z}_{GY}$

Continuity equation of f transported by incompressible Hamiltonian flows in 5D phase space (4D:$\mathbf{R}, v_{//}$ + 1D parameter:μ)

GK Poisson equation for self-consistent fields

- f_{GC} obtained by pull-back transform

$$f_{GC}(\mathbf{Z}_{GC}) \equiv T_\varepsilon f_{GY}(\mathbf{Z}_{GC}) = f_{GY}(\mathbf{Z}_{GC}) + \{S, f_{GY}\} \cong f_{GY}(\mathbf{Z}_{GC}) + \frac{\Omega}{B}\frac{\partial S}{\partial \alpha_{GC}}\frac{\partial f_{GY}}{\partial \mu_{GC}}$$

- Poisson equation in $\mathbf{Z}_{CC}$

$$-\nabla^2\phi = 4\pi\sum_s e_s n_s(\mathbf{q})$$

$$n_s(\mathbf{q}) = n_{0s}\int f_{GCs}(\mathbf{Z}_{GC})\delta[(\mathbf{R}_{GC}+\boldsymbol{\rho})-\mathbf{q}]m_s^2 B_{//}^* d\mathbf{Z}_{GC}$$

$$\cong n_{0s}\int f_{GYs}(\mathbf{Z}_{GC})\delta[(\mathbf{R}_{GC}+\boldsymbol{\rho})-\mathbf{q}]m_s^2 B_{//}^* d\mathbf{Z}_{GC} - \frac{e n_{0s}}{T_s}\left(\phi - \langle\bar{\phi}\rangle_\alpha\right)$$

$$\langle\bar{\phi}\rangle_\alpha \equiv \int \langle\phi\rangle_\alpha f_{0s}\delta[(\mathbf{R}_{GC}+\boldsymbol{\rho})-\mathbf{q}]m_s^2 B_{//}^* d\mathbf{Z}_{GC}$$

  - 2nd term shows polarization density due to FLR effect

- Gyrokinetic Poisson equation

$$-\nabla^2\phi + \sum_s \frac{1}{\lambda_{Ds}^2}\left(\phi - \langle\bar{\phi}\rangle_\alpha\right) = 4\pi\sum_s e_s n_{0s}\int f_{GYs}(\mathbf{Z}_{GC})\delta[(\mathbf{R}_{GC}+\boldsymbol{\rho})-\mathbf{q}]m_s^2 B_{//}^* d\mathbf{Z}_{GC}$$

First principles in gyrokinetic equations

- Conservation of phase space volume

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

- Conservation of Casimir invariants $C(f)$ in Liouville equation

$$\frac{DC(f)}{Dt}\equiv\frac{\partial C(f)}{\partial t}+\left\{C(f),H\right\}=0$$

  - particle number f, kinetic entropy $f\log(f)$, f^2, etc…

- Energy conservation

$$\sum_s\int H n_s\frac{\partial f_s}{\partial t}m_s^2 B_{//}^{*}d\mathbf{Z}=\frac{dE_k}{dt}+\frac{dE_f}{dt}=0$$

$$E_k=\sum_s\int\left(\frac{1}{2}m_s v_{//}^2+\mu B\right)n_s f_s m_s^2 B_{//}^{*}d\mathbf{Z}$$

$$E_f=\frac{1}{8\pi}\int\left|\nabla\phi\right|^2 d\mathbf{x}+\frac{1}{8\pi}\sum_s\sum_{\mathbf{k}}\frac{1}{\lambda_{Ds}^2}\left[1-I_0\left(k_\perp^2\rho_{ts}^2\right)\exp\left(-k_\perp^2\rho_{ts}^2\right)\right]\left|\phi_{\mathbf{k}}\right|^2$$

Summary of modern gyrokinetic theory

- Gyrokinetic Vlasov-Poisson system

$$\frac{\partial f_s}{\partial t}+\{f_s,H_s\}=0$$

$$-\nabla^2\phi+\sum_s\frac{1}{\lambda_{Ds}^2}\left(\phi-\langle\bar{\phi}\rangle_\alpha\right)=4\pi\sum_s e_s n_{0s}\int f_s\delta[(\mathbf{R}+\boldsymbol{\rho})-\mathbf{q}]m_s^2B_{//}^*d\mathbf{Z}$$

  - Spatio-temporal scales are given as $\sim\rho_i$ and $\omega << \Omega_i$
  - Problem is reduced to 5D (4D hyperbolic PDE + 1D parameter)
  - Keeps important kinetic effects (FLR, Landau resonance, etc…)
  - Keeps all the first principles which the original system has
    - Phase space conservation
    - Conservation of particle number, kinetic entropy, etc…
    - Total energy conservation

Important for avoiding spurious phenomena

Useful for checking the quality of numerical simulations

3. Various approaches in gyrokinetic simulations

Coordinate system in tokamak configuration

- Tokamak configuration written using poloidal flux function ψ

$$\mathbf{B} = \nabla\psi \times \nabla(q\theta - \varphi), \quad q(\psi) = \mathbf{B}\cdot\nabla\varphi / \mathbf{B}\cdot\nabla\theta, \quad \theta : \text{straight field line angle}$$

- Field aligned flute perturbation with $k_{//}$~0 (gyrokinetic ordering)

$$\phi(\psi,\theta,\varphi) = \sum_{m,n} \phi_{mn}(\psi)\exp(im\theta - in\varphi)$$

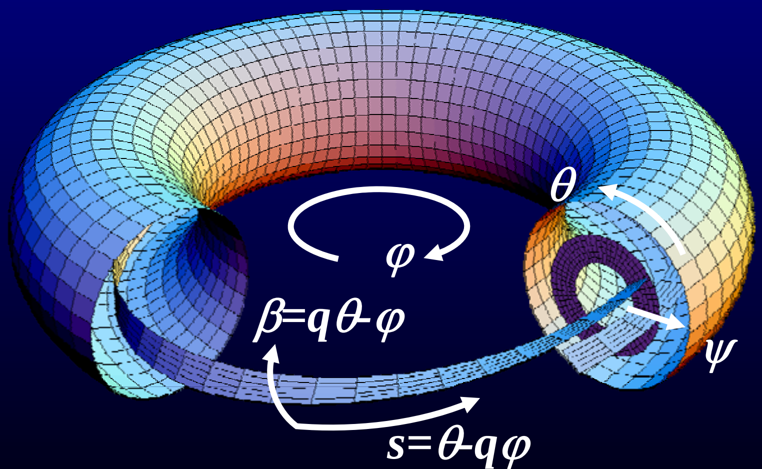
$$\mathbf{B}\cdot\nabla\phi = \mathbf{B}\cdot\nabla\theta \sum_{m,n} i(m - nq)\phi_{mn}(\psi)\exp(im\theta - in\varphi) \approx 0$$

  – Components far from m~nq suffer from Landau damping

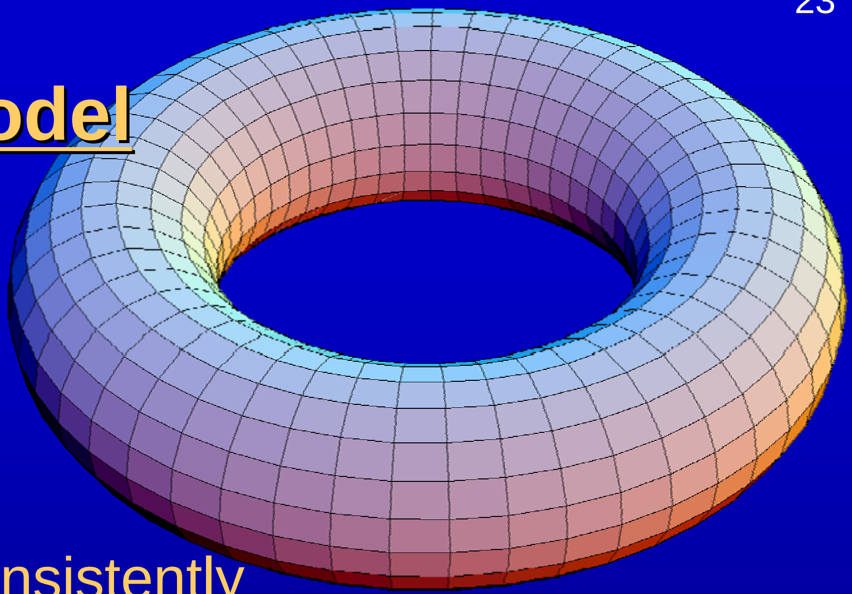
- Quasi 2D representation of flute perturbation

$$\phi(\psi,\theta,\varphi) = \sum_{n} \tilde{\phi}_n(\psi,\theta)\exp(in[q\theta - \varphi])$$

  – Field-line-following coordinates (ψ,β,s)
  – GK equation can be further reduced to quasi-3D+1D



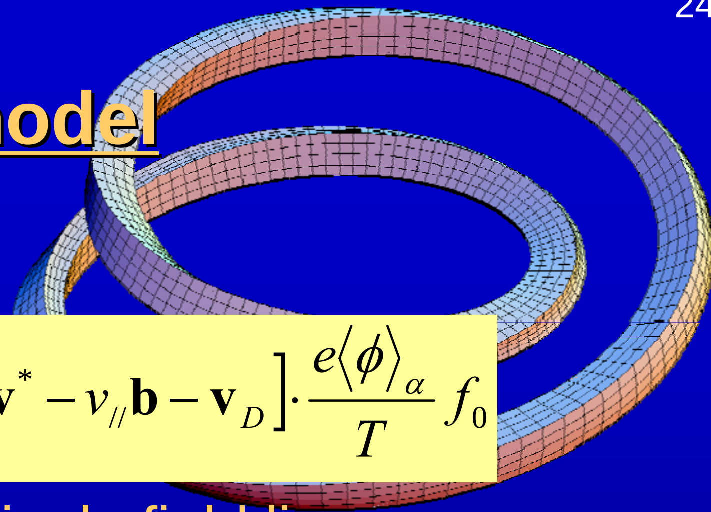
Global model



- Global gyrokinetic simulation

$$\frac{\partial f}{\partial t} + \{f, H\} = 0$$

  - Keep all the first principles
  - Both f_0 and δf are solved self-consistently
  - Full (annular) torus calculation with fixed B.C.
  - Benchmark is difficult because of ambiguities in B.C. (edge, axis), heat source model, additional ordering, etc…
- Physics application
  - Global effects (ω^*-shearing, turbulence spreading, avalanches)
  - Plasma size scaling (Bohm like features in experiments)
  - Advanced tokamak configuration with reversed q profile
  - Expensive for electron turbulence, electromagnetic turbulence



Local flux tube model

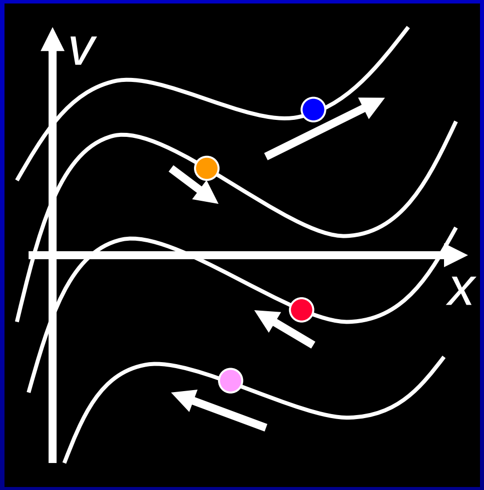
- Local flux tube gyrokinetic simulation

$$\frac{\partial \delta f}{\partial t}+\left[v_{//}\mathbf{b}+\mathbf{v}_{E\times B}+\mathbf{v}_D\right]\cdot\nabla\delta f-\frac{\mu}{m}\mathbf{b}\cdot\nabla B\frac{\partial \delta f}{\partial v_{//}}=\left[\mathbf{v}^*-v_{//}\mathbf{b}-\mathbf{v}_D\right]\cdot\frac{e\langle\phi\rangle_\alpha}{T}f_0$$

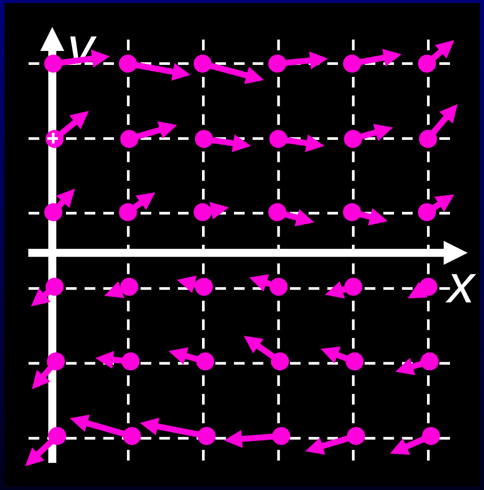
  - Narrow calculation domain along a single field line
  - Complete scale separation by neglecting $O(\rho_i/a)$ effects
    $T, T', q, q' \rightarrow const.$, radial periodic B.C.
  - Only δf is solved with fixed gradient parameters
  - First principles are lost
  - Benchmark results are well converged among several codes
- Physics application
  - Advanced issues (electron turbulence, multi-scale turbulence)
  - Widely used in experimental data analysis
  - Difficulty with meso-scale turbulent structures (streamers, etc...)

Numerical approaches in solving GK equations

- Particle/Lagrangian approach (PIC)
  - Particle-In-Cell (PIC) method
    (Birdsal-Langdon,Hockney-Eastwood,Tajima)
  - Nonlinear δf method
    (Parker,PFB93,Aydemir,POP94)
  - Relatively small memory usage

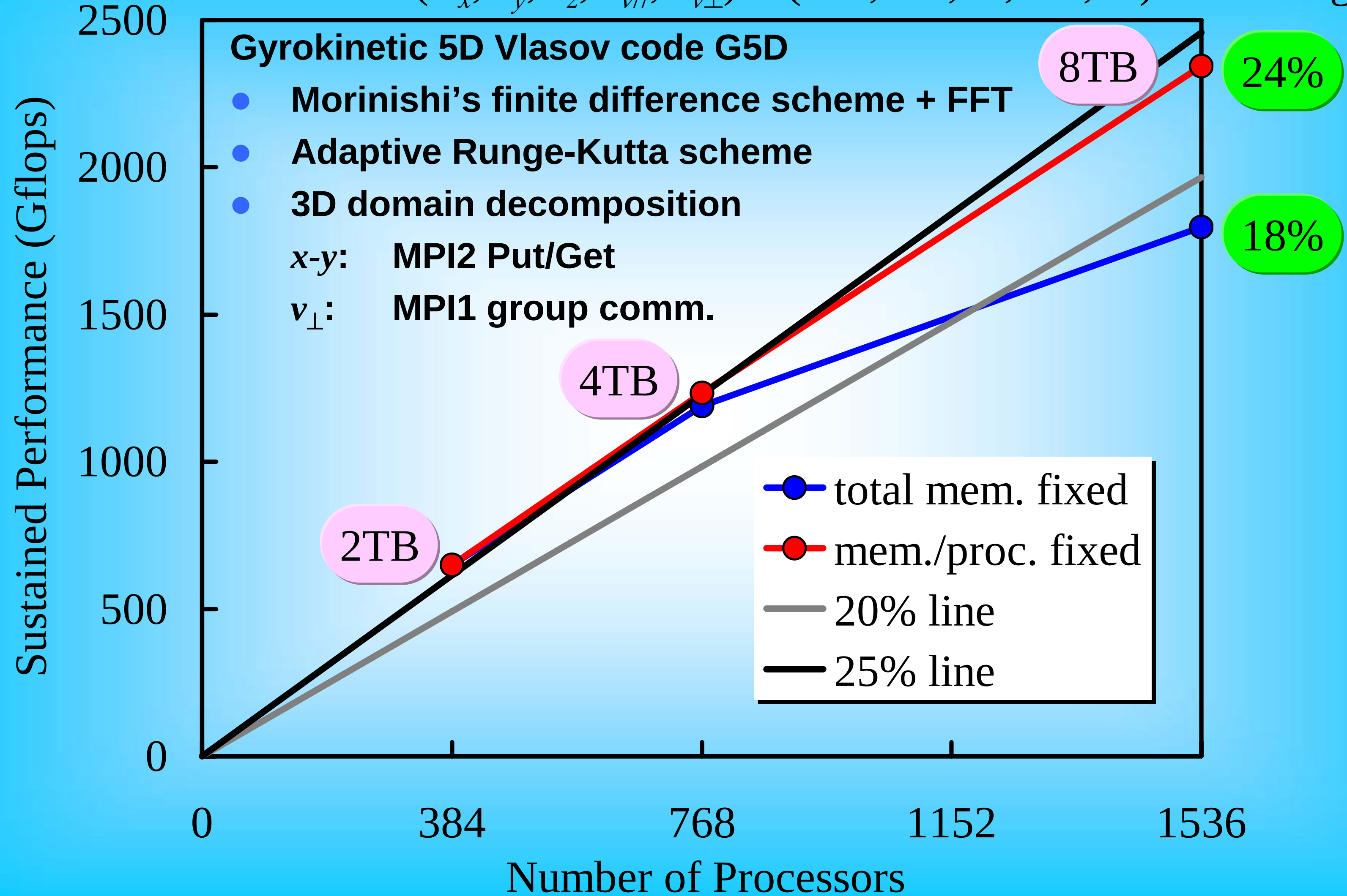


- Mesh/Eulerian approach (Vlasov)
  - CFD scheme in 5D phase space
    - Semi-Lagrangian method
    - Finite difference method
    - Spectral method
  - Huge memory usage



Parallel performance of mesh code on Altix3700Bx2

Problem size with 8TB: $(N_x, N_y, N_z, N_{v//}, N_{v\perp}) = (512,512,64,100,98) \sim 0.164$Tgrids



JAEA Altix3700Bx2: 2048 Itanium2 (1.6GHz,6.4Gflops), 13TB memory

4. Particle/Lagrangian approach

Physical model of many body system

- Newton-Poisson system for electrostatic one component plasma

$$\dot{x}_j = v_j(t), \quad \dot{v}_j = -\frac{e}{m}\frac{\partial}{\partial x}\phi(x_j, t) \qquad \text{Eqs. of motion}$$

$$K(x,v,t) = \sum_{j=1}^{N} \delta(x - x_j(t))\delta(v - v_j(t)) \qquad \text{Klimontovich distribution}$$

$$-\frac{\partial^2 \phi}{\partial x^2} = 4\pi e \int K(x,v,t)dv \quad \rightarrow \quad \phi(x,t) = e\int \frac{K(x',v',t)}{|x-x'|}dx'dv' \qquad \text{Poisson Eq.}$$

- Klimontovich equation

$$\frac{DK}{Dt} \equiv \frac{\partial K}{\partial t} + v\frac{\partial K}{\partial x} - \frac{e}{m}\frac{\partial \phi}{\partial x}\frac{\partial K}{\partial v}$$

$$= \frac{\partial K}{\partial t} + v\frac{\partial K}{\partial x} - \frac{e^2}{m}\frac{\partial}{\partial x}\int \frac{K(x',v',t)}{|x-x'|}dx'dv'\frac{\partial K}{\partial v} = 0$$

  - Involve all the dynamics (collisions, multiple body correlation)
  - Prohibitive for macro-scale simulation with $n_0 \sim 10^{19} \mathrm{m}^{-3}$

From Klimontovich Eq. to Vlasov Eq.

- Introduce statistical average $< >$ for Klimontovich distribution

$$\langle K(x,v,t)\rangle = n_0 f_1(x,v,t)$$

$$\langle K(x,v,t)K(x',v',t)\rangle = n_0^2 f_2(x,v,x',v',t) - \delta(x-x')\delta(v-v')n_0 f_1(x,v,t)$$

$$\vdots$$

- Statistical average of Klimontovich equation

$$\frac{\partial f_1}{\partial t} + v\frac{\partial f_1}{\partial x} - \frac{e^2}{mn_0}\left\langle \int \frac{\partial}{\partial x}\frac{K(x',v',t)}{|x-x'|}\frac{\partial K(x,v,t)}{\partial v}dx'dv' \right\rangle = 0$$

- Lowest order equation in BBGKY hierarchy

$$\frac{\partial f_1}{\partial t} + v\frac{\partial f_1}{\partial x} - \frac{e}{m}\frac{\partial \phi_1}{\partial x}\frac{\partial f_1}{\partial v} = \frac{n_0 e^2}{m}\int \frac{\partial}{\partial x}\frac{1}{|x-x'|}\frac{\partial g_2(x,v,x',v',t)}{\partial v}dx'dv'$$

$$\phi_1(x,t) = en_0\int \frac{f_1(x',v',t)}{|x-x'|}dx'dv'$$

$$f_2(x,v,x',v',t) = f_1(x,v,t)f_1(x',v',t) + g_2(x,v,x',v',t)$$

  – g_2 is $\sim O(\varepsilon_d)$ effect in discreteness parameter $\varepsilon_d = 1/(n_0\lambda_D^3) << 1$

Vlasov limit and super particles

- Lowest order equation in BBGKY hierarchy

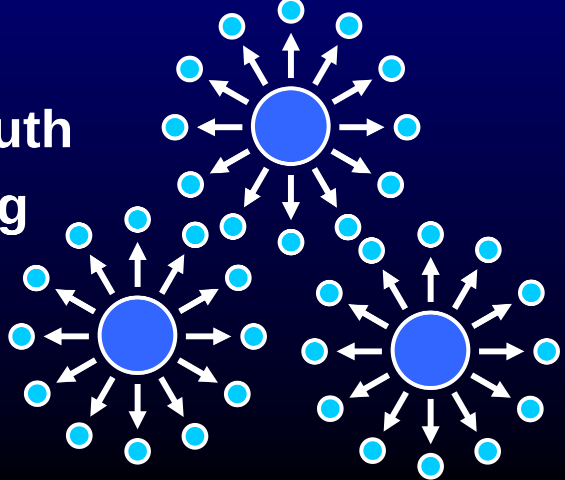
$$\frac{\partial f_1}{\partial t}+v\frac{\partial f_1}{\partial x}-\frac{e^2 n_0}{m}\int\frac{\partial}{\partial x}\frac{f_1(x',v',t)}{|x-x'|}dx'dv'\frac{\partial f_1}{\partial v}=\varepsilon_d C(g_2)$$

- Rosenbluth chopping with $e_{SP}=\mathcal{M}e$, $m_{SP}=\mathcal{M}m$, and $n_{SP0}=n_0/\mathcal{M}$

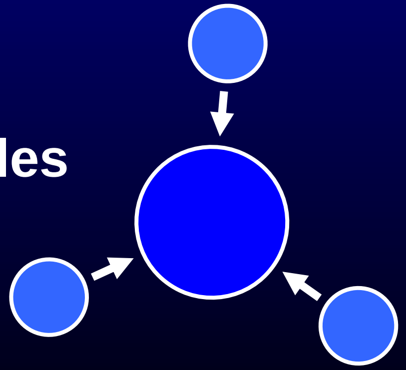
$$\frac{\partial f_1}{\partial t}+v\frac{\partial f_1}{\partial x}-\frac{e^2 n_0}{m}\int\frac{\partial}{\partial x}\frac{f_1(x',v',t)}{|x-x'|}dx'dv'\frac{\partial f_1}{\partial v}=\mathcal{M}\varepsilon_d C(g_2)$$

  - Collective motion in l.h.s. is not affected by $\mathcal{M}$
  - Rosenbluth chopping ($\mathcal{M}<<1$) naturally lead to Vlasov limit
  - Super particles ($\mathcal{M}>>1$) enhance collisions by $\mathcal{M}$ times

Rosenbluth Chopping



Super Particles



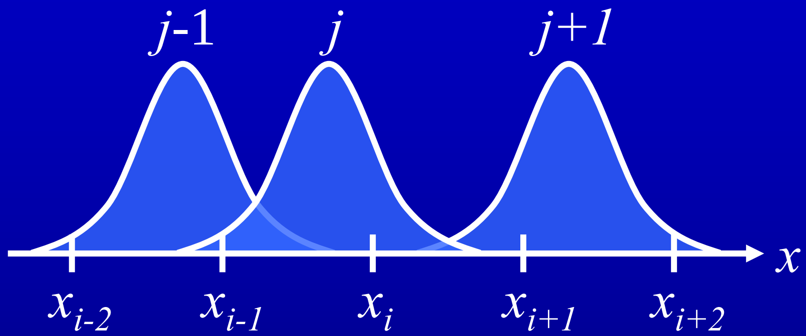
Reduce enhanced collisions with finite size particles

- Newton-Poisson system for PIC simulation

$$\dot{x}_j = v_j, \quad \dot{v}_j = -\frac{e}{m}\frac{\partial}{\partial x}\phi\left(x_j, t\right)$$

$$K_{SP}\left(x, v, t\right) = \sum_{j=1}^{N_{SP}} S_{SP}\left(x - x_j(t)\right)\delta\left(v - v_j(t)\right)$$

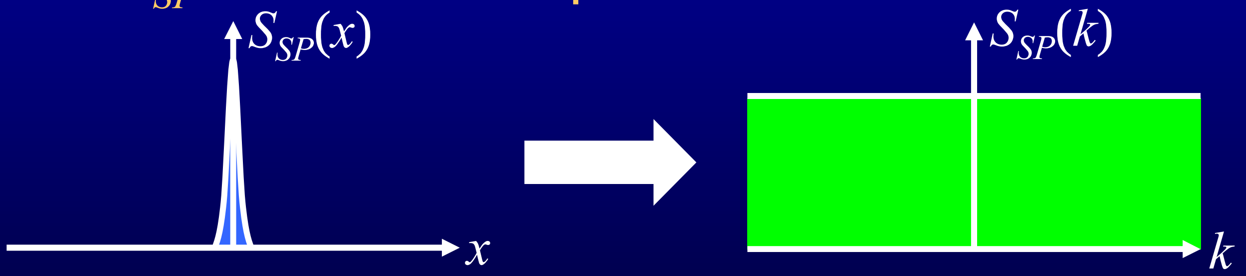
$$-\frac{\partial^2 \phi}{\partial x^2} = 4\pi e \mathcal{M} \int K_{SP}\left(x, v, t\right) dv$$



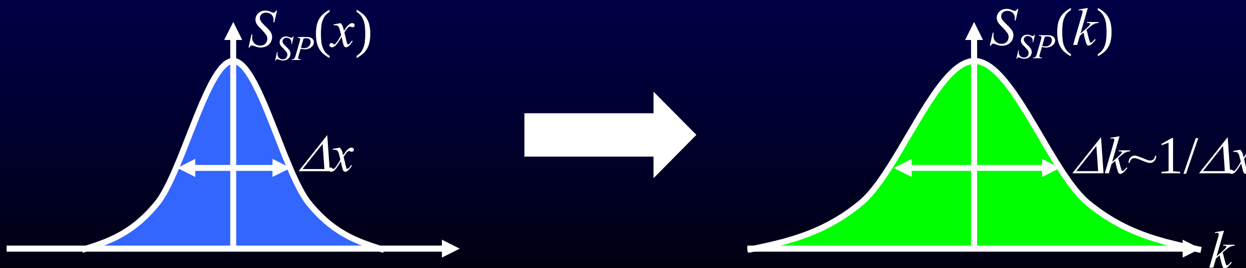
  – Shape factor S_{SP} works as low-pass Fourier filter

Point charge

$S_{SP}(x)=\delta(x)$



Finite size particle



Reduce particle weight with δf PIC method

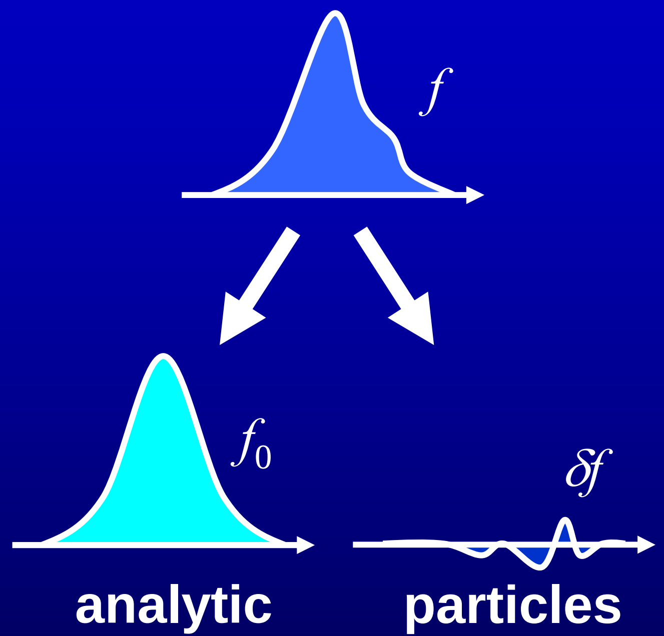
- Equation system of δf PIC simulation
  (Parker-Lee,PFB93, Aydemir,POP94, Allfrey,CPC03)

$$\dot{x}_j = v_j, \quad \dot{v}_j = -\frac{e}{m}\frac{\partial}{\partial x}\phi(x_j,t)$$

$$\dot{w}_j = \Delta V_j\left[-v\frac{\partial f_0}{\partial x} + \frac{e}{m}\frac{\partial \phi}{\partial x}\frac{\partial f_0}{\partial v}\right]_{x=x_j, v=v_j}$$

$$\delta\hat{f}(x,v,t) \equiv \sum_{j=1}^{N_{SP}} w_j(t) S_{SP}(x - x_j(t))\delta(v - v_j(t))$$

$$-\frac{\partial^2 \phi}{\partial x^2} = 4\pi e n_0 \int \left[f_0(x,v) + \delta\hat{f}(x,v,t)\right] dv$$

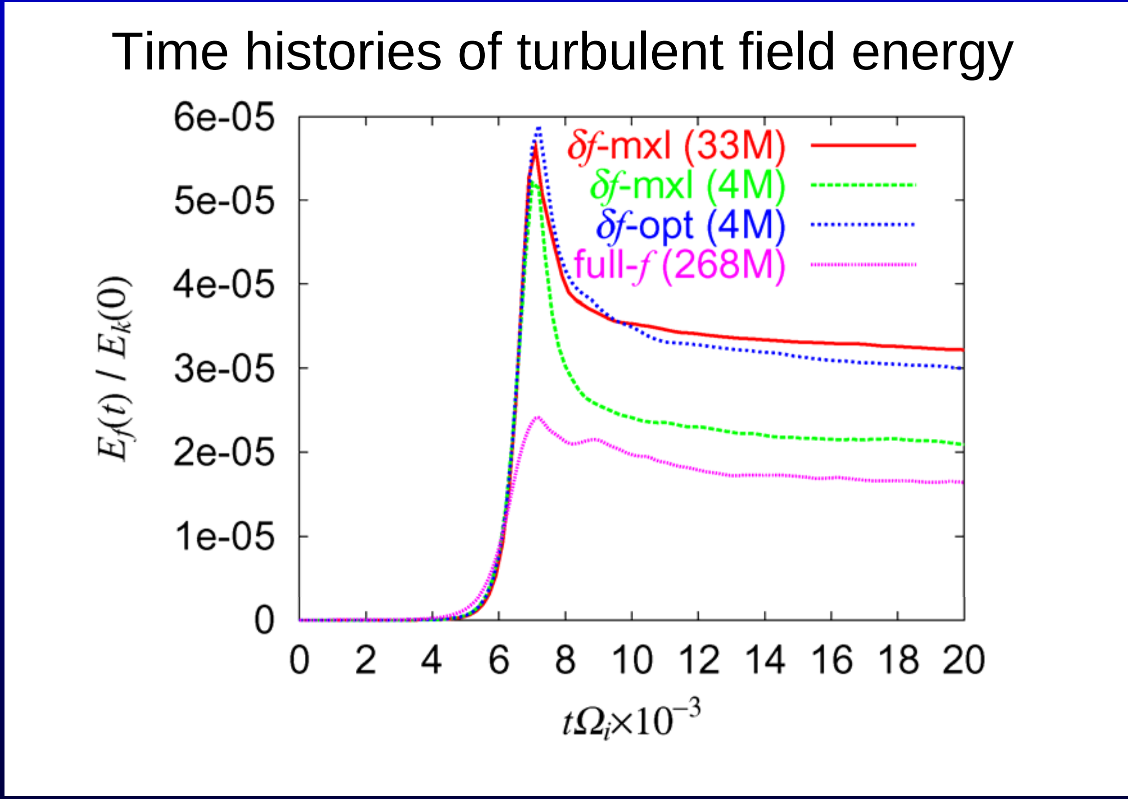


  - Particle weight can be reduced by $\delta f / f_0 \sim 0.01$
  - $Df/Dt=0$ is assumed in weight evolution equation
  - Monte-Carlo sampling of δf (sampling points can be optimized) (Hatzky,POP02)

Comparisons of PIC and δf PIC simulations

- Gyrokinetic simulations of ion temperature gradient driven turbulence

  G3D code (Idomura,POP00), $L_x=L_y=16\rho_{ti}$, $L_z=8000\rho_{ti}$, $L_x/L_n=0$, $L_x/L_{ti}=0.42$



- δf-mxl(33M)

  δf-PIC, Maxwellian K_{SP}

  ~9.9×10^3 particles/cell-mode
- δf-mxl(4M)

  δf-PIC, Maxwellian K_{SP}

  ~1.2×10^3 particles/cell-mode
- δf-opt(4M)

  δf-PIC, Optimised K_{SP}

  ~1.2×10^3 particles/cell-mode
- full-f(268M)

  PIC, Maxwellian K_{SP}

  ~8×10^4 particles/cell-mode

– δf PIC converges significantly faster than conventional PIC

– Optimization of sampling points accelerates convergence

Summary of Particle/Lagrangian approach

- PIC simulation model
  - Many body system with heavier particles enhance collisions
  - Enhanced collisions are reduced by finite size particle model
- δf PIC simulation model
  - Monte-Carlo sampling of δf using marker particles
  - Particle weight and collisions reduced by $\delta f/f_0$~0.01
  - Significantly faster convergence than conventional PIC
- Issues in δf PIC simulations
  - δf and particle weight increase monotonically in time
    Limited for short time scale before $Df/Dt=0$ breaks down
  - $Df/Dt=0$ is severe constraint of δf PIC simulations
    Difficult to implement relevant sources and collisions
    (Brunner,POP99, Wang,PPCF99, Hu,POP94, Lin,POP04)

5. Mesh/Eulerian approach

Vlasov simulation based on mesh approaches

- Vlasov-Poisson system for electrostatic one component plasma

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \frac{e}{m}\frac{\partial \phi}{\partial x}\frac{\partial f}{\partial v} = 0 \qquad \text{Vlasov Eq.}$$

$$-\frac{\partial^2 \phi}{\partial x^2} = 4\pi e n_0 \int f(x,v,t)\,dv \qquad \text{Poisson Eq.}$$

  - All the dynamics determined by f_1 and ϕ_1
- Semi-Lagrangian approach: mapping of f using $Df/Dt=0$

$$f(x,v,t) = f(x-\Delta t\dot{x}, v-\Delta t\dot{v}, t-\Delta t)$$

  - Splitting method, Semi-Lagrangian method, CIP method, etc (Cheng,JCP76, Sonnendrucker,JCP99, Nakamura,JCP99)
- Eularien approach: discretize PDE on phase space grids (x_i,v_j)

$$\left[\frac{\partial f}{\partial t}\right]_{i,j} = -v_j\left[\frac{\partial f}{\partial x}\right]_{i,j} + \frac{e}{m}\left[\frac{\partial \phi}{\partial x}\right]_i\left[\frac{\partial f}{\partial v}\right]_{i,j}$$

  - Spectral method, Non-dissipative/Dissipative finite difference

Splitting scheme (Cheng-Knorr,JCP76)

- Vlasov equation is given by separable Hamiltonian

$$H(x,v) = \frac{1}{2}mv^2 + e\phi(x) = T(v) + V(x)$$

$$\dot{x} = \frac{\partial H}{\partial v} = \frac{\partial T(v)}{\partial v}, \quad \dot{v} = -\frac{\partial H}{\partial x} = \frac{\partial V(x)}{\partial x}$$

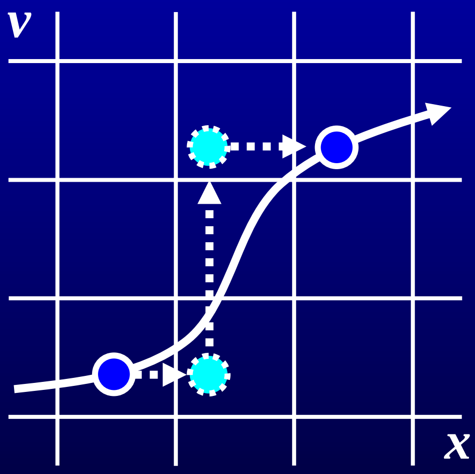
  – Hamilton's Eq. consists of free motions in x and v

- Mapping is splitted into three free motions

$$f^*(x,v) = f^n(x - \dot{x}\Delta t/2, v)$$

$$f^{**}(x,v) = f^*(x, v - \dot{v}\Delta t)$$

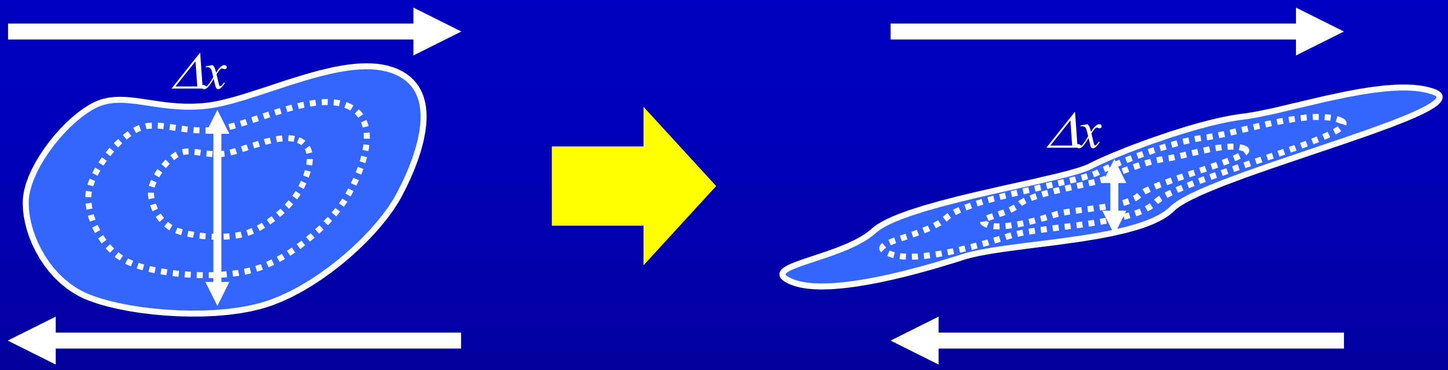
$$f^{n+1}(x,v) = f^{**}(x - \dot{x}\Delta t/2, v)$$



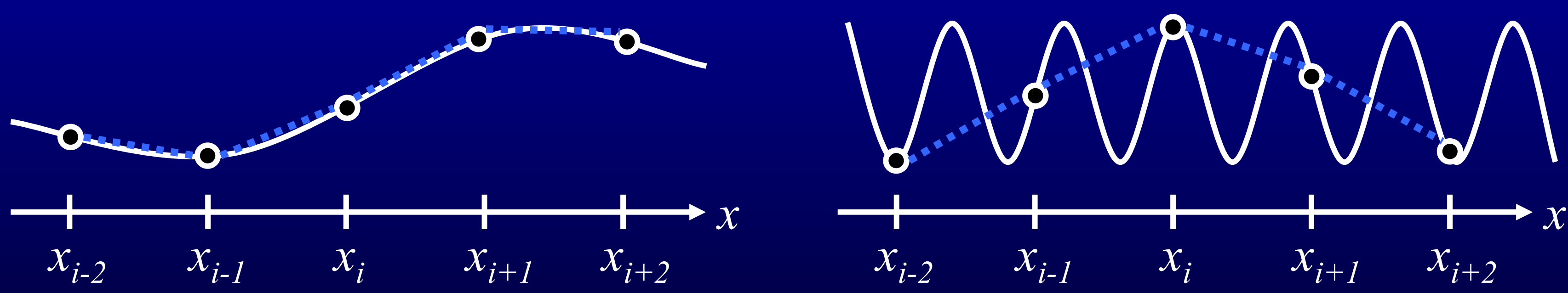
  – Each free motions are canonical transform
  – 2nd order symplectic integrator
  – Semi-Lagrangian method for non-separable Hamiltonian (Brunetti,CPC04, Grandgirard,JCP06)

Aliasing errors

- Phase mixing leading to fine scale structures in turbulent flows



- Aliasing errors in resolving fine scales with finite grid widths



  – Aliasing errors are inevitable in finite difference approach
  – Spurious sub-grid oscillations cause numerical instability

Dissipative finite difference operator

- Finite difference approximation for 1D advection problem

$$\frac{\partial f}{\partial t}+c\frac{\partial f}{\partial x}=0,\quad c>0$$

$$c\left[\frac{\partial f}{\partial x}\right]_{i,center}=\frac{cf_{i+1}-cf_{i-1}}{2h}=cf_i'+\frac{h^2}{6}cf_i'''+cO\left(h^4\right)\qquad \text{Centred finite difference}$$

$$c\left[\frac{\partial f}{\partial x}\right]_{i,upwind}=\frac{cf_i-cf_{i-1}}{h}=cf_i'+\frac{h}{4}cf''+cO\left(h^3\right)\qquad \text{Upwind finite difference}$$

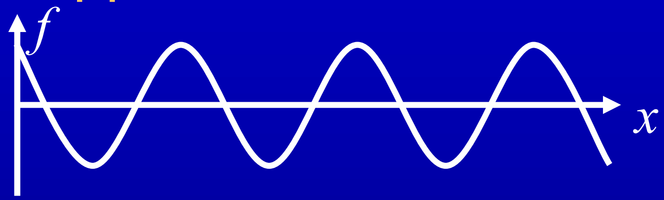
$$f_{i\pm1}=f_i\pm hf_i'+\frac{h^2}{2}f_i''\pm\frac{h^3}{6}f_i'''+\cdots$$

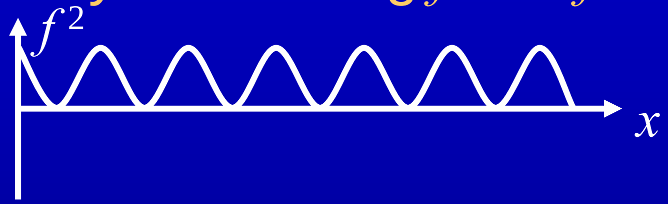
- Centered finite difference is non-dissipative, but its dispersive errors do not suppress numerical oscillations
- Dissipative error in upwind finite difference smear out not only numerical oscillations but also solution itself
- Various less dissipative higher order schemes are available

(Candy,JCP03, Watanabe,NF06, Xu,IAEA06)

Non-dissipative finite difference operator

- Finite difference method for Poisson bracket operator (Arakawa,JCP66, Morinishi,JCP97)
  - Suppress numerical oscillations by conserving f and f^2





- Finite difference operators proposed by Arakawa and Morinishi

$$\frac{\partial f}{\partial t}+\{f,H\}=\frac{\partial f}{\partial t}+\frac{\partial V_\mu f}{\partial X_\mu}=0,\quad \frac{\partial V_\mu}{\partial X_\mu}=0$$

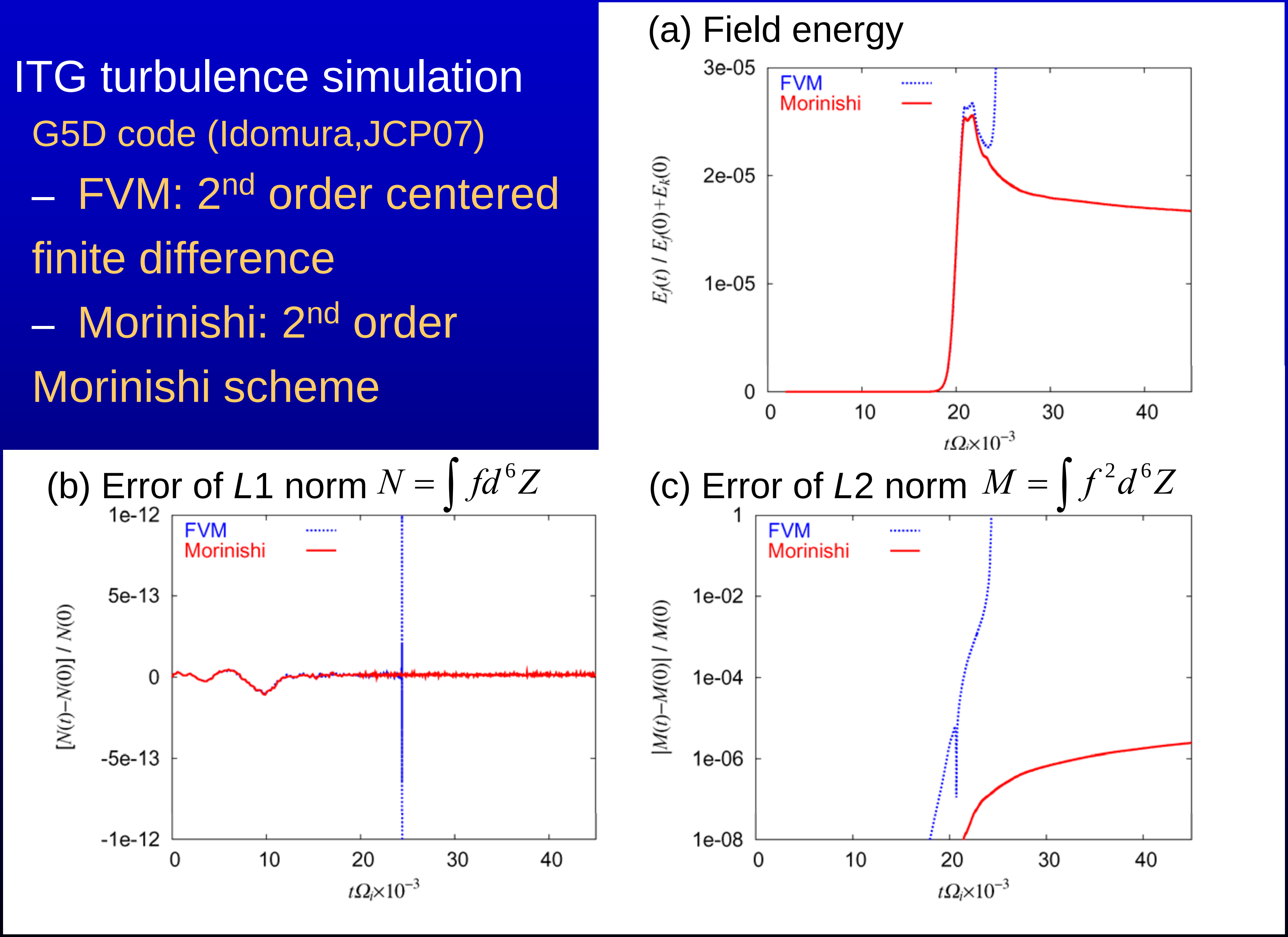
$$[\{f,H\}]=c_1 J_{i,j}^{++}(f,H)+c_2 J_{i,j}^{+\times}(f,H)+c_3 J_{i,j}^{\times+}(f,H) \qquad \text{2D Arakawa scheme}$$

$$\left[\frac{\partial V_\mu f}{\partial X_\mu}\right]=\frac{1}{2}\left[\frac{\partial V_\mu f}{\partial X_\mu}\right]_{center}+\frac{1}{2}V_\mu\left[\frac{\partial f}{\partial X_\mu}\right]_{center} \qquad \text{Morinishi scheme}$$

  - Both operators are conservative for $\{f,H\}$ and $f\{f,H\}$
  - Morinishi scheme can be extended to higher dimension (Idomura,JCP07)

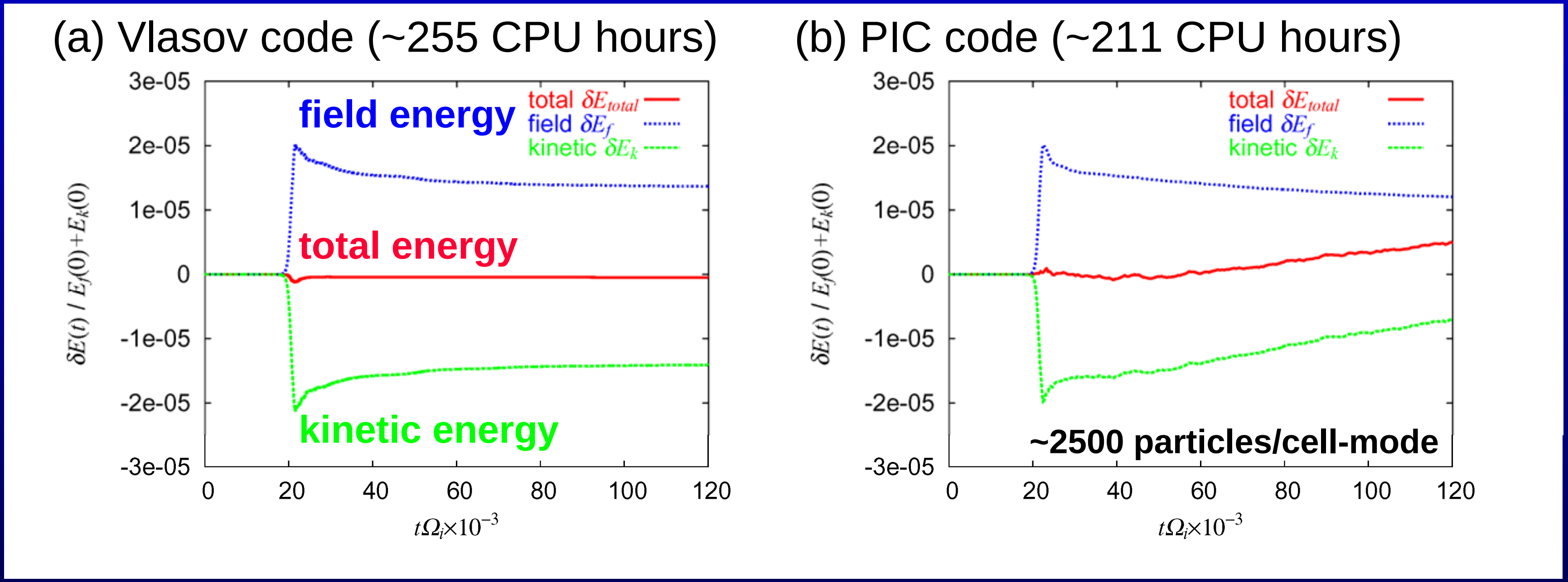
Non-dissipative gyrokinetic simulation

- ITG turbulence simulation
  G5D code (Idomura,JCP07)
  – FVM: 2nd order centered finite difference
  – Morinishi: 2nd order Morinishi scheme



Comparison between Vlasov and PIC simulations

- Gyrokinetic simulations of slab ion temperature gradient turbulence
  G3D/G5D (Idomura,POP00,JCP07), $L_x=2L_y=32\rho_{ti}$, $L_z=8000\rho_{ti}$, $L_x/L_n=0$, $L_x/L_{ti}=0.86$



- Results show quantitative agreement up to saturation phase
- PIC simulation show spurious heating due to numerical noise
- Secular accumulation of error is not observed in Vlasov simulation (Memory usage was ~5 times larger in Vlasov simulation)

Summary of Mesh/Eulerian approach

- Semi-Lagrangian approach
  - Vlasov simulation was initiated by splitting method
  - Splitting method works as symplectic integrator for Vlasov Eq.
  - Semi-Lagrangian method is used for Gyrokinetic Eq.
- Dissipative upwind finite difference approach
  - Suppress numerical oscillations by numerical dissipation
  - Less dissipative higher order schemes are available
- Non-dissipative finite difference approach
  - Suppress numerical oscillations by conserving f and f^2
  - Conserve phase space volume, f, and f^2
- Equivalence of Vlasov and PIC simulations
  - Converged Vlasov and PIC simulations give the same results
  - Vlasov code may be advantageous in long time simulation

6. Collisionless gyrokinetic simulation

Collisionless gyrokinetic simulation?

- Collisionless gyrokinetic equation

$$\frac{\partial f}{\partial t} + \{f, H\} = 0$$

  - Similar to Euler equation which describes ideal fluids ($Re=\infty$)
  - Where does turbulent field energy go?
- One possible scenario in micro-turbulence simulations

Excitation of micro-instabilities

↓

Nonlinear energy transfer in configuration space

↓

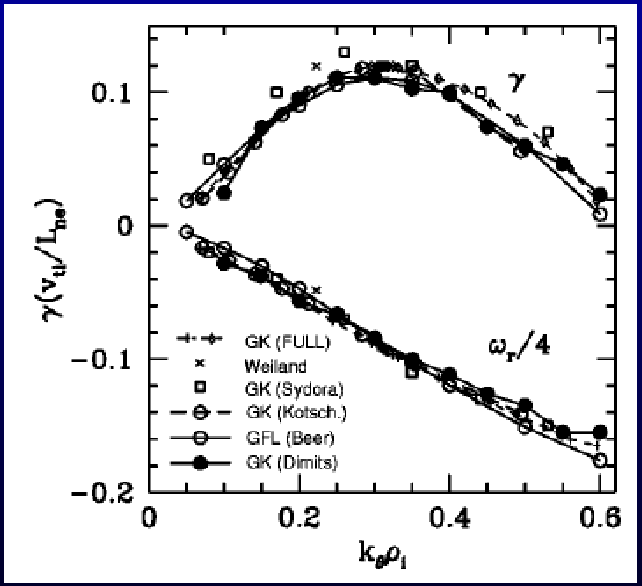
Energy sink (Landau damping) at ρ_i scale

↓

Phase mixing in velocity space

↓

?



ITG ω,γ-spectrum (Dimits,POP00)

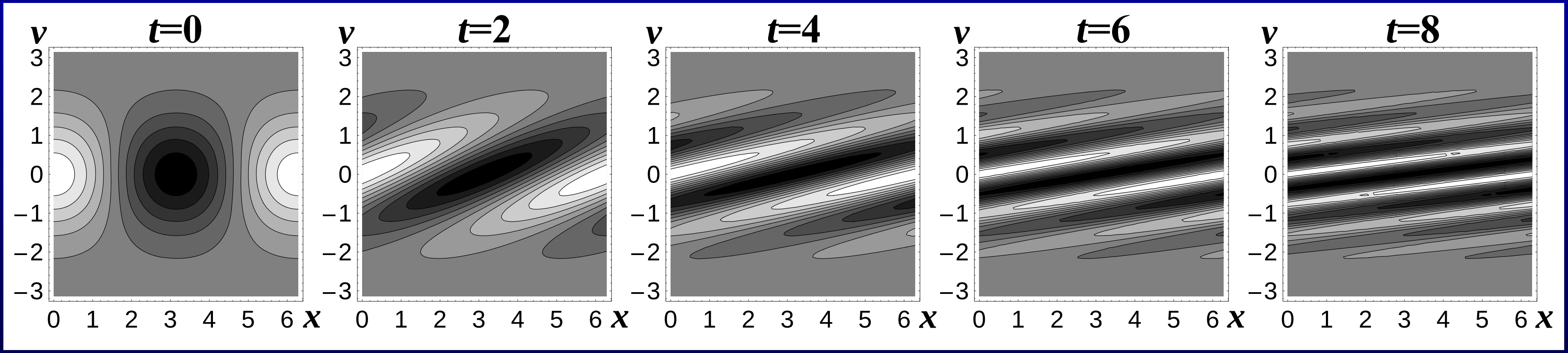
Phase mixing due to parallel streaming motion

- Free streaming starting from $f(x,v,0)=(2\pi)^{-1/2}\exp(-v^2/2)\cos(kx)$

$$\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}=0$$

$$f(x,v,t)=f(x-vt,v,0)=(2\pi)^{-1/2}\exp\left(-v^2/2\right)\cos\left(k[x-vt]\right)$$

$$n(x,t)=\int f(x,v,t)dv=\exp\left(-k^2t^2/2\right)\cos(kx)$$



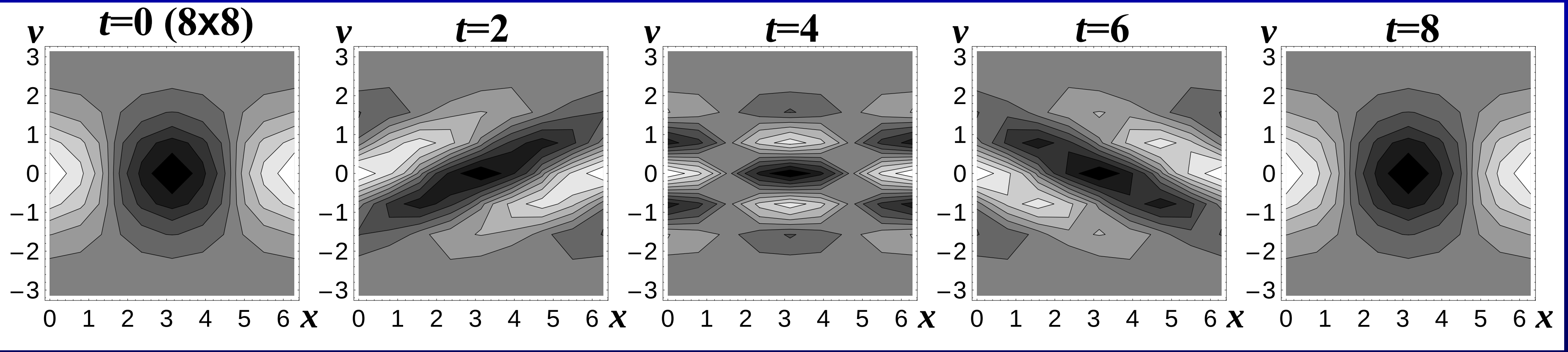
- n damps away with conserving f
- Fine scale structures are continuously produced
- In reality, weak collisions, $\propto \partial_v^2 f$, smear out fine structures

Phase mixing in numerical simulations

- Free streaming on discrete phase space grids $(x_i,v_j)=(i\Delta x,j\Delta v)$

$$f(x_i,v_j,t)=f(x_i-v_jt,v_j,0)=(2\pi)^{-1/2}\exp\left(-(j\Delta v)^2/2\right)\cos\left(k[i\Delta x-j\Delta vt]\right)$$

$$f(x_i,v_j,t)=f(x_i,v_j,t+T_R),\quad T_R=\frac{2\pi}{k\Delta v}$$



  – Spurious recurrence phenomena occurs due to aliasing error
  – Purely collisionless simulation is limited for $t<T_R/2$
  – Most of GK simulations go further with numerical dissipation

  How the numerical dissipation affect simulation results?

Entropy balance relation in gyrokientic equation

- Slab gyrokinetic equation (drop $O(\rho^*)$, local limit $T, \nabla T \to const.$)

$$\frac{\partial \delta f}{\partial t} + \left[v_{//}\mathbf{b} + \frac{c}{B}\mathbf{b}\times\nabla\langle\phi\rangle_\alpha \right]\cdot\nabla\delta f = -\frac{c}{B}\mathbf{b}\times\nabla\langle\phi\rangle_\alpha\cdot\nabla f_0 + \frac{e}{m}\mathbf{b}\cdot\nabla\langle\phi\rangle_\alpha \frac{\partial f_0}{\partial v_{//}} + C(f)$$

$$\frac{1}{\lambda_{Di}^2}\left(\phi - \langle\bar{\phi}\rangle_\alpha\right) + \frac{1}{\lambda_{De}^2}\left(\phi - \langle\phi\rangle_{flux}\right) = 4\pi e n_0 \int \delta f \delta[(\mathbf{R}+\boldsymbol{\rho}) - \mathbf{q}] m^2 B_{//}^* d\mathbf{Z}$$

- Balance relation of fluctuation entropy δS

  (Lee,PF88, Krommes,POP94, Sugama,POP96)

$$\underbrace{\frac{d\delta S}{dt}}_{\text{entropy}} + \underbrace{\frac{dW}{dt}}_{\text{field energy}} = \underbrace{Q}_{\text{heat flux}} + \underbrace{D}_{\text{dissipation}}$$

$$\delta S \equiv \int \frac{\delta f^2}{2 f_0} m^2 B d\mathbf{Z} = \int [f \ln f - f_0 \ln f_0] m^2 B d\mathbf{Z} + O(\delta f^3)$$

$$W = \frac{1}{2}\sum_{\mathbf{k}} \left[1 - I_0(k_\perp^2\rho_{ts}^2)\exp(-k_\perp^2\rho_{ts}^2)\right]\left|\frac{e\phi_{\mathbf{k}}}{T}\right|^2 n_0 + \frac{1}{2}\sum_{k_{//}\neq 0}\left|\frac{e\phi_{\mathbf{k}}}{T}\right|^2 n_0$$

$$Q = -\frac{1}{2T}\left[\int \frac{c}{B}\mathbf{b}\times\nabla\langle\phi\rangle_\alpha n_0 \delta T d\mathbf{R}\right]\cdot\nabla\ln T, \quad D = \int C(f)\frac{\delta f}{f_0} m^2 B d\mathbf{Z}$$

Three distinct statistical states of entropy balance

(Watanabe-Sugama,POP02, POP04)

- Collisionless limit with zonal flows
  - Turbulence is quenched by zonal flows

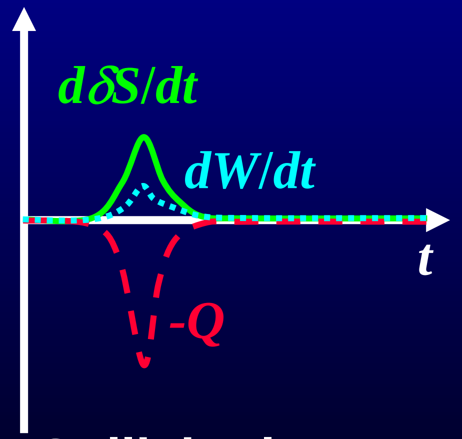
$$\frac{d\delta S}{dt} = 0, \frac{dW}{dt} = 0, Q = D = 0$$

- Collisionless limit without zonal flows
  - Quasi-steady W,Q with increasing δS

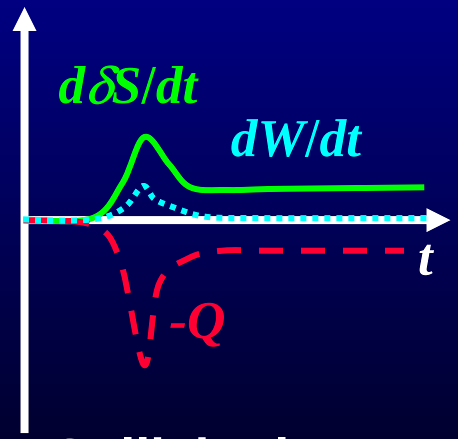
$$\frac{dW}{dt} = 0, \frac{d\delta S}{dt} + Q = 0, D = 0$$

- Collisional case without zonal flows
  - Steady state with balanced Q and D

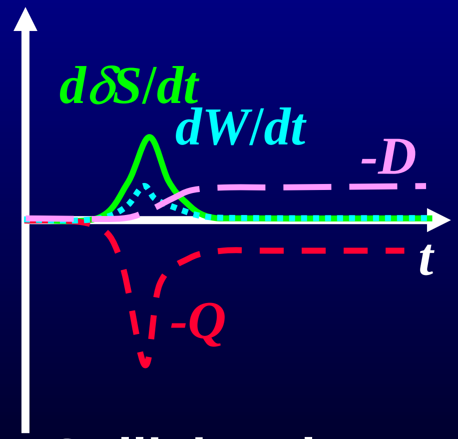
$$\frac{d\delta S}{dt} = 0, \frac{dW}{dt} = 0, Q + D = 0$$



Collisionless with zonal flows



Collisionless w/o zonal flows



Collisional w/o zonal flows

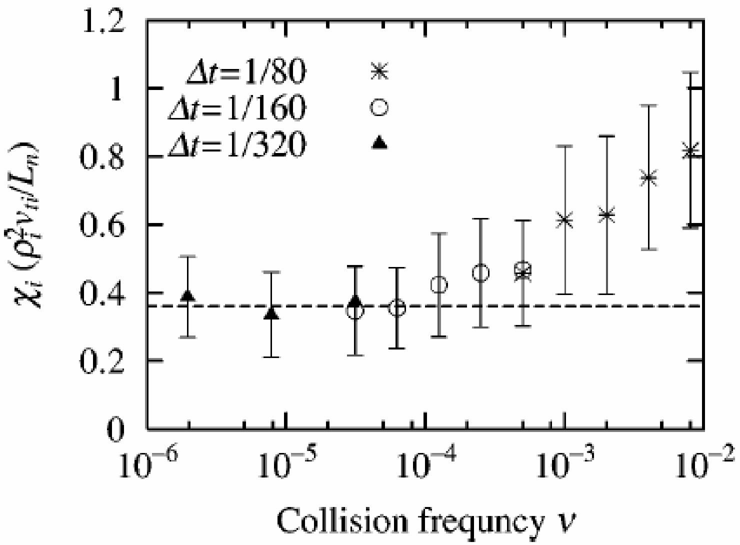
Asymptotic behavior of Q in weak collisional limit

- Relevant steady state determined by $Q+D=0$
  - Is Q determined by forcing (gradients) or dissipation?
- Collisionality ν dependence of diffusivity χ in weak collisional limit

Slab ITG turbulence simulation

(Watanabe-Sugama,POP04)

- χ approaches to collisionless limit asymptotically
- χ is independent of ν for $\nu<10^{-4}$
- Q ($=D$) is determined by forcing



  - Collisionless simulation is possible with finite but small enough numerical or physical dissipation
  - Convergence study for numerical dissipation is important

    Grid number, particle number, hyper diffusivity, etc…

Summary of entropy balance relation

- Phase mixing in velocity space
  - Parallel streaming continuously produce fine scale structures
  - n damps away with conserving f (phase mixing damping)
  - Discrete system shows spurious recurrence effect
  - To avoid recurrence numerical/physical dissipation is needed
- Collisionless limit in gyrokinetic simulations
  - Steady solution of entropy balance is given by $Q+D=0$
  - χ approaches to collisionless limit asymptotically with $\nu \rightarrow 0$
  - Forcing determines heat flux Q at weakly collisional regime
  - Collisionless simulation is possible with finite but small enough numerical or physical dissipation