# **Gyrokinetic Simulation:** Introduction and Prospect for Astrophysics

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### **Micro Turbulence in Fusion Device**



[Klasky, ORNL; Ethier, Wang, PPPL]



G. McKee et al., Plasma and Fusion Research 2007



### **Micro Turbulence in Fusion Device**

• Source of trouble and reason... why fusion people want to build ever larger machine









- Introduction to gyrokinetic theory
- Issues in gyrokinetic simulation
- Numerical methods for gyrokinetic simulation
- Summary



# Introduction to Gyrokinetic Theory



# **Basic Idea of GK Theory**

GK orderings

T.S. Hahm, Phys. Fluids 31, 2670 (1988) A. Brizard, T.S. Hahm, Rev. Mod. Phys. 79, 421(2007)

- small fluctuation:  $\frac{\delta f}{f_0} \sim \frac{e\delta\phi}{T} \sim \frac{\delta B}{B_0} \sim \epsilon$ 

- low frequency: 
$$\frac{\omega}{\Omega_i} \sim \epsilon$$

Fast MHD waves and cyclotron waves are ruled out (high freq. GK, H. Qin '99)

- anisotropic fluctuation:  $\frac{k_{\parallel}}{k_{\perp}} \sim \epsilon$ ,  $k_{\perp}\rho_i \sim 1$
- mild non-uniformity in plasma profiles, background

magnetic field etc.: 
$$\frac{\rho_i}{L_0} \sim \epsilon \Rightarrow$$

Free energy to drive turbulence (GK with strong gradient, T.S. Hahm '09)



# **Basic Idea of GK Theory (cont'd)**

• Guiding center transformation

particle space  $(\vec{x}, \vec{v}) \leftrightarrow \text{guiding}(\text{gyro})$  center space  $(\vec{R}, v_{\parallel}, \mu, \theta)$ 

 $\theta$ : gyrophase-angle  $\rightarrow$  average out

$$\vec{R} = \vec{x} - \vec{
ho}, \quad \vec{
ho} = \hat{b} \times \frac{\vec{v}}{\Omega'}, \quad \Omega = \frac{eB_0}{mc}$$

$$v_{\parallel} = \hat{b} \cdot \vec{v}, \quad \mu = \frac{v_{\perp}^2}{2B}$$
$$\vec{v} = v_{\parallel}\hat{b} + v_{\perp}\hat{e}_{\perp}$$





# **Basic Idea of GK Theory (cont'd)**

- Schematics of guiding center transformations in GK simulation
  - ✓ Solve Vlasov equation in guiding center space and evaluate ( $n_s$ ,  $j_s$ )
  - ✓ Transform  $(n_s, j_s)$  to particle space
  - ✓ Solve Maxwell equations to obtain EM fields
  - ✓ Transform EM fields to guiding center space





# **Gyrokinetic Vlasov Equation**

- Transform original 6D Vlasov equation in particle space into guiding center space
- Take gyro-angle average to remove  $\theta$

 $\rightarrow$  reduction to 5D  $\bar{f}(\vec{R}, v_{\parallel}, \mu, t)$ , large time step  $\Delta t > 1/\Omega_i$ 

$$\frac{\partial \bar{f}}{\partial t} + \left( \nu_{\parallel} \hat{b}^{*} + \frac{\mu}{B} \, \hat{b} \times \nabla B + \frac{c}{B_{0}} \nabla_{\perp} \hat{b} \times \langle \delta \psi \rangle \right) \cdot \frac{\partial \bar{f}}{\partial \vec{R}} + \frac{q}{m} \left( -\hat{b}^{*} \cdot \mu \nabla B - \hat{b}^{*} \cdot \nabla \langle \delta \phi \rangle - \frac{1}{c} \frac{\partial}{\partial t} \langle \delta A_{\parallel} \rangle \right) \frac{\partial \bar{f}}{\partial \nu_{\parallel}} = 0$$

$$\delta \psi = \delta \phi - \frac{v_{\parallel}}{c} \delta A_{\parallel}$$
$$\hat{b}^* = \hat{b} + \frac{v_{\parallel}}{B} \hat{b} \times \hat{b} \cdot \nabla \hat{b}$$
$$\langle \cdot \rangle = \text{gyro-phase}$$
averaged fluctuations



# **Gyrokinetic Maxwell Equation**

• Solved in particle space i.e. no guiding center transformation

$$-\nabla^2 \delta \phi(\vec{x},t) = 4\pi \sum_s q_s n_s(\vec{x},t)$$

$$-\nabla^2 \delta A_{\parallel}(\vec{x},t) = \frac{4\pi}{c} \sum_s j_s(\vec{x},t)$$

• Evaluation of  $(n_s, j_s)$  in particle space  $\rightarrow$  pull-back transformation of sources (i.e. from guiding center space to particle space) is needed:  $\bar{f_s}(\vec{R}, v_{\parallel}, \mu, t) \rightarrow f_s(\vec{x}, \vec{v}, t)$ 

$$n_{s}(\vec{x},t) = \int B^{*} d^{3} R dv_{\parallel} d\mu d\theta \ \delta\left(\vec{R}+\vec{\rho}-\vec{x}\right) \left\{ \bar{f}_{s} + \frac{q_{s}}{m_{s}B_{0}} (\delta\psi - \langle\delta\psi\rangle) \frac{\partial f_{s}}{\partial\mu} \right\}$$
$$j_{s}(\vec{x},t) = \int B^{*} d^{3} R dv_{\parallel} d\mu d\theta \ \delta\left(\vec{R}+\vec{\rho}-\vec{x}\right) v_{\parallel} q_{s} \left\{ \bar{f}_{s} + \frac{q_{s}}{m_{s}B_{0}} (\delta\psi - \langle\delta\psi\rangle) \frac{\partial \bar{f}_{s}}{\partial\mu} \right\}$$



### **Gyrokinetic Maxwell Equation (cont'd)**

• We need to solve to the following forms:

$$\nabla^{2}\delta\phi\left(\vec{x},t\right) = -4\pi \sum_{s} \left\{ q_{s} \left[ \overline{N}_{s} - \sum_{k} e^{i\vec{k}\cdot\vec{x}} \frac{1 - \Gamma_{0}(b_{s})}{T_{s}} (q_{s}\delta\phi_{k}N_{s} - \frac{1}{c}J_{s}\delta A_{\parallel k}) \right] \right\}$$
$$\nabla^{2}\delta A_{\parallel}(\vec{x},t) = -\frac{4\pi}{c} \sum_{s} \left\{ \left[ \overline{J}_{s} - \sum_{k} e^{i\vec{k}\cdot\vec{x}} \frac{q_{s}(1 - \Gamma_{0}(b_{s}))}{T_{s}} (\delta\phi_{k}J_{s} - \frac{q_{s}}{c} \Pi_{s}\delta A_{\parallel k}) \right] \right\}$$

• If we take long wave length limit, we can simplify these as (long wave length limit  $\rightarrow b_i = (k_{\perp}\rho_i)^2 \ll 1$ ,  $\Gamma_0(b_i) \approx 1 - b_i$ ,  $\Gamma_0(b_e) \approx 1$ )

$$-(1 + \frac{\rho_i^2}{\lambda_{Di}^2})\nabla^2 \delta \phi(\vec{x}, t) = 4\pi \sum_s q_s \overline{N}_s \qquad \overline{N}_s \equiv \int B^* d^3 R dv_{\parallel} d\mu d\theta \ \delta(\vec{R} + \vec{\rho} - \vec{x}) \, \bar{f}_s$$
$$-\nabla_{\perp}^2 \delta A_{\parallel} = \frac{4\pi}{c} \sum_s \bar{J}_s \qquad \overline{J}_s \equiv \int B^* d^3 R dv_{\parallel} d\mu d\theta \ v_{\parallel} q_s \delta(\vec{R} + \vec{\rho} - \vec{x}) \, \bar{f}_s$$

(A. Brizard, T.S. Hahm, Rev. Mod. Phys. 2007)



Gyrokinetic description of magnetized plasmas





# **Elementary Plasma Physics**

•  $\vec{F} \times \vec{B}$  drift motion of charged particle

 $\rightarrow$  drift motion of gyration center in  $\vec{F} \times \vec{B}$  direction





### **Closer look at GK equations**



➔ GK equations of motion are nothing but a combination of familiar drift motions ensuring phase space volume conservation and making them

Hamiltonian flows

$$\frac{\partial}{\partial t}(B^*\bar{f}) + \frac{\partial}{\partial \vec{R}}(\frac{d\vec{R}}{dt}B^*\bar{f}) + \frac{\partial}{\partial v_{\parallel}}(\frac{dv_{\parallel}}{dt}B^*\bar{f}) = 0$$



- What is gyro-average < > and how to compute it?
  - → Gyro-averaged field is nothing but field felt by "charged ring"

Integration can be approximated by a few points sum

$$\left\langle \delta \phi \right\rangle \equiv \frac{1}{2\pi} \int_0^{2\pi} d\theta \int d\vec{x} \,\delta(\vec{X} + \vec{\rho}_i(\theta) - \vec{x}) \delta \phi(\vec{x})$$
  
=  $\frac{1}{2\pi} \int_0^{2\pi} \delta \phi(\vec{X} + \vec{\rho}_i(\theta)) d\theta \cong \frac{1}{N} \sum_{l=1}^N \delta \phi(\vec{X} + \vec{\rho}_i(\theta_l))$ 



or in Fourier space (as is often done in continuum codes)

$$\begin{split} \left\langle \delta\phi \right\rangle &= \frac{1}{2\pi} \int_{0}^{2\pi} d\theta \int d\vec{x} \,\delta(\vec{X} + \vec{\rho}_{i}(\theta) - \vec{x}) \delta\phi(\vec{x}) \\ &= \frac{1}{2\pi} \int_{0}^{2\pi} \delta\phi(\vec{X} + \vec{\rho}_{i}(\theta)) d\theta = \frac{1}{2\pi} \int_{0}^{2\pi} \left\{ \frac{1}{(2\pi)^{3}} \int \delta\hat{\phi}(\vec{k}) e^{i\vec{k}\cdot(\vec{X} + \vec{\rho}_{i}(\theta))} d\vec{k} \right\} d\theta \\ &= \frac{1}{(2\pi)^{3}} \int \left\{ \frac{1}{2\pi} \int_{0}^{2\pi} \delta\hat{\phi}(\vec{k}) e^{ik_{\perp}\rho_{i}\cos\theta} d\theta \right\} e^{i\vec{k}\cdot\vec{X}} d\vec{k} = \frac{1}{(2\pi)^{3}} \int \delta\hat{\phi}(\vec{k}) J_{0}\left(\frac{k_{\perp}v_{\perp}}{\Omega_{i}}\right) e^{i\vec{k}\cdot\vec{X}} d\vec{k} \end{split}$$



• Charged rings have stronger shielding effect than point particles

$$-(1 + \frac{\rho_i^2}{\lambda_{Di}^2})\nabla^2 \delta \phi(\vec{x}, t) = 4\pi \sum_{s} q_s \overline{N_s} \leftarrow \text{Charge density from charged rings}$$

✓ Additional shielding by polarization charges carried by charged rings
 ✓ Significantly enhanced as compared to Debye shielding

 Charged rings have no response to parallel direction i.e. no such thing as polarization current in parallel direction

$$-\nabla_{\perp}^{2}\delta A_{\parallel} = \frac{4\pi}{c}\sum_{s} \bar{J}_{s} \leftarrow \text{Parallel current carried by charged rings}$$



• Gyrokinetic equation for guiding center distribution

$$\frac{\partial}{\partial t}\vec{f} + \frac{d\vec{R}}{dt} \cdot \frac{\partial}{\partial \vec{R}}\vec{f} + \frac{dv_{\parallel}}{dt}\frac{\partial}{\partial v_{\parallel}}\vec{f} = 0$$
$$\frac{d}{dt}\vec{R} = v_{\parallel}\hat{b}^{*} + \frac{\mu}{B}\hat{b} \times \nabla B + c\frac{\hat{b}}{B} \times \nabla\langle\delta\psi\rangle$$
$$\frac{d}{dt}v_{\parallel} = -\hat{b}^{*} \cdot \mu\nabla B - \hat{b}^{*} \cdot \nabla\langle\delta\phi\rangle - \frac{1}{c}\frac{\partial}{\partial t}\langle\deltaA_{\parallel}\rangle$$

Gyrokinetic Maxwell Equation

$$-(1+\frac{\rho_i^2}{\lambda_{Di}^2})\nabla^2 \delta \phi = 4\pi \sum_s q_s \overline{N}_s$$
$$-\nabla_{\perp}^2 \delta A_{\parallel} = \frac{4\pi}{c} \sum_s \overline{J}_{\parallel s}$$



- Standard numerical techniques can be employed
- Issue is mainly problem size and computational cost
- Blind choice of scheme can easily end up with practically unsolvable one



# Where dose it stand?

• Where does it stand?





# Where dose it stand?

- Alfvenic turbulence:  $\omega \sim k_{\parallel} v_A$
- GS scaling of anisotropy:  $k_{\parallel} \propto k_{\perp}^{2/3}$
- $\Rightarrow \omega < \Omega_i \text{ for } k_\perp \rho_i \rightarrow 1$
- ➔ regime of gyrokinetic





Basic plasma physics for the intracluster medium mean free-path for electron-electron & proton-proton collisions  $l_{p-p} \sim l_{e-e} \sim \frac{10^5}{\ln \Lambda} \frac{T^2(K)}{n_e(cm^{-3})} cm \sim a \text{ few kpc}$ = 3.1 × 10<sup>19</sup> m

mean free-path for electron-proton relaxation

$$l_{e-p} \sim l_{p-p} \times \left(\frac{m_p}{m_e}\right)^{\frac{1}{2}} \sim 100 \text{ kpc}$$

gyro-radius of protons

$$r_{\rm gyro,p} \sim \frac{\sqrt{T({
m K})}}{B({
m G})}\,{
m cm} \sim 10^4~{
m km}$$

gyro-radius of elections  

$$r_{\text{gyro,e}} = r_{\text{gyro,p}} \times \frac{m_e}{m_p} \sim 10 \text{ km}$$

$$l_{p-p} < L < l_{e-p} \longrightarrow$$

$$\Delta T_e \neq \Delta T_p$$

$$L < l_{p-p} \longrightarrow$$
viscous regime?

D.S. Ryu, WCI-CNU workshop 2010

# **Merits and Limitations**

- Applicable to small-scale (gyro-radius) turbulence in strongly magnetized plasmas → solar winds, corona, ISM, intracluster etc.
- Describe kinetic cascade in 5D phase space (both space and velocity) → collisionless Landau damping
- Compressional component can be included
- Recover various MHD results for some appropriate limiting cases
- Limitation: fast MHD waves, cyclotron resonance are ruled out (extension to high frequency gyrokinetic theory, H. Qin, PoP'99)



# Issues in Gyrokinetic Simulation



### **Problem Size and Parallelization**

• Though reduced to 5D, problem size is still challenging!

Number of grids:  $N_x \times N_y \times N_z \times N_{\nu\parallel} \times N_{\mu}$  $\geq 256 \times 256 \times 64 \times 128 \times 32 \sim 10^{10}$ 

Electron-proton mass ratio ~ 1:2000 → time scale disparity ~ 45

 Complexity of equations → careful choice of numerical scheme is required i.e. well balanced between good numerical property and simplicity for easy implementation and parallelization



Collisionless Vlasov equation

$$\frac{\partial f}{\partial t} + \frac{d\vec{R}}{dt}\frac{\partial f}{\partial \vec{R}} + \frac{dv_{\parallel}}{dt}\frac{\partial f}{\partial v_{\parallel}} = \frac{\partial f}{\partial t} - \{H, f\} = 0$$

- Characteristic equations  $\Rightarrow$  Hamiltonian flow
- Phase space volume is conserved along the characteristics
- evolution of distribution function with streaming and interactions
  - $\Rightarrow$  finer and finer filamentation in phase space down to sub-grid scales







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This process continues until (neglected) collision can catch up.

(Note that neglected collision term becomes important for smaller velocity space scales)

$$\frac{df}{dt} = \frac{\partial f}{\partial t} - \{H, f\} = \mathcal{C}(f, f) \qquad \mathcal{C}(f, f) \sim f \frac{\partial^2 f}{\partial v^2} \uparrow \text{ as } \Delta v \to 0$$



- Issues in numerical simulation
  - But sufficient grid resolution all the way down to the collisional scale is practically impossible!
  - − Strong gradients in phase space → source of many numerical troubles
  - Careful choice of scheme and/or adding artificial dissipation is needed to minimize non-physical behaviors





# Numerical Simulation of Gyrokinetic Equations



### Particle in Cell (PIC) method (Lagrangian)

Phase space is sampled by a fewer number of particles carrying "weight"

$$\bar{f}(\vec{R}, v_{\parallel}, \mu, t) = \sum_{\rho} w_{\rho} \delta(\vec{R} - \vec{R}_{\rho}(t)) \delta(v_{\parallel} - v_{\parallel \rho}(t)) \delta(\mu - \mu_{\rho}(t))$$







### Particle in Cell (PIC) method (Lagrangian)

- Almost same with conventional PIC simulations ("particles" →
   "charged rings")
- All previous numerical methods developed for PIC can be employed
- Issue of small scale noise (~  $1/\sqrt{N}$ )
- ~ 2000 particles per cell as rule of thumb
- Explicit scheme, larger time step etc. possible
- Easier to parallelize



#### XGC1 performance on 3mm ITER grid



S. Ku and CPES team, ICNSP'11





XGC1 full torus simulation of ITG turbulence (S. Ku et al., EPS'12)



# **Continuum Method (Eulerian)**

Setup grid system for entire phase space (5D) and apply standard method to solve hyperbolic PDE i.e. FDM, FVM, etc



$$M_{IJ}\bar{f}_J^{n+1} = N_{IJ}\bar{f}_J^n$$

Inversion of "huge matrix" is usually required

$$\bar{f}^{n+1} = M^{-1} N \bar{f}^n$$



# **Continuum Method (Eulerian)**



Vlasov simulation of two steam instability (D.K. Jang and D.K. Lee '12)



# **Continuum Method (Eulerian)**

- All advanced schemes developed in hydro communities can be employed
- Some operations are very costly e.g.  $\langle \phi \rangle \sim \int J_0(k\rho_i)\phi_k dk$
- CFL condition often dictates implicit time integration
- Phase space granulation poses high velocity space resolution
   → grid scale dissipation is necessary → poorer conservation than PIC
- Parallelization efficiency is often less than PIC
- Low noise high quality simulation is possible if sufficient resolution is provided
- → development of massively parallel supercomputer makes this possible!



# **Semi-Lagrangian Scheme**

Invariance of distribution function along characteristics



- Find  $f_{now}$  at grid point by tracing back characteristic line and interpolating  $f_{ott}$
- Relatively free from CFL constraint i.e. larger  $\Delta t$
- Interpolation on Eulerian grid  $\rightarrow$  greatly reduce discrete particle noise



### **Numerical Simulation of Gyrokinetic Equation**

- What is  $\delta f$  scheme?
  - Write distribution function as a sum of known  $f_0$  and  $\delta f$
  - Solve only perturbed part  $\delta f$  only

$$\frac{\partial f}{\partial t} + \frac{d\vec{R}}{dt} \cdot \nabla f + \frac{dv_{\parallel}}{dt} \frac{\partial f}{\partial v_{\parallel}} = 0$$
Gyrokinetic equation in  $\delta f$  form  
(W.W. Lee CPC'87)
$$\stackrel{\partial}{\partial t} \delta f + \frac{d\vec{R}}{dt} \cdot \nabla \delta f + \frac{dv_{\parallel}}{dt} \frac{\partial}{\partial v_{\parallel}} \delta f = -\frac{d\vec{R}}{dt} \cdot \nabla f_0 - \frac{dv_{\parallel}}{dt} \frac{\partial f_0}{\partial v_{\parallel}}$$

$$f(\vec{R}, v_{\parallel}, \mu, t) = \sum_p w_p \delta(\vec{R} - \vec{R}_p(t)) \delta(v_{\parallel} - v_{\parallel p}(t)) \delta(\mu - \mu_p(t))$$

$$\stackrel{\partial}{\longrightarrow} \delta f(\vec{R}, v_{\parallel}, \mu, t) = \sum_p w_p(t) \delta(\vec{R} - \vec{R}_p(t)) \delta(v_{\parallel} - v_{\parallel p}(t)) \delta(\mu - \mu_p(t))$$

$$\stackrel{d}{\longrightarrow} w_p(t) = -(1 - w_p) \left[ \frac{d\vec{R}}{dt} \cdot \frac{\nabla f_0}{f_0} + \frac{dv_{\parallel}}{dt} \frac{\partial f_0}{f_0 \partial v_{\parallel}} \right]$$



### **Numerical Simulation of Gyrokinetic Equation**

• Why  $\delta f$  scheme?

For PIC method  $\varepsilon \propto \frac{1}{\sqrt{N}} \sqrt{\langle w^2 \rangle} \ll \frac{1}{\sqrt{N}} \quad \text{for } \langle w^2 \rangle \equiv \frac{1}{N} \sum_{p=1}^N w_p^2 \sim (\partial f / f_0)^2 \ll 1$ 

Simulation noise is reduced by  $\delta f/f_0$ 

• Why not  $\delta f$  scheme?

But... what if  $\langle w^2 \rangle$  increases during simulation?

We lose the merit  $\Rightarrow$  actually, it can become large in

- ✓ Short time by phase space filamentation (granulation)
- $\checkmark$  Longer time by equilibrium evolution

$$\frac{d}{dt} \left\langle w^2 \right\rangle = D \left( \frac{\partial}{\partial x} f_0 \right)^2 - v \left\langle w^2 \right\rangle \qquad \left\langle w^2 \right\rangle \sim \int \delta f^2 dx dv \ (\propto -H : \text{entropy})$$

In collisionless simulation (v=0), particle weights grow linearly in time and  $\delta f$  scheme stops to work



# Summary

- Gyrokinetic simulation is a well developed tool to study low frequency micro-scale turbulence. Serious validation efforts are also ongoing in fusion community.
- With careful examination of parameter regime, it can be applied to astrophysical environments such as ISM, intracluster medium etc.
  - microscopic turbulence with kinetic processes e.g. collisionless Landau damping
  - sub-grid transport model for global simulation studies
  - stimulate the extension of gyrokinetic model beyond present limit
- Careful choice of numerical scheme is absolutely critical
  - beneficial for both communities to expand present simulation capabilities

