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 $(\vec{R}, v_{\parallel}, \mu, \theta)$

 θ : 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 θ

 \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 × 10¹⁹ 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 Δt
- Interpolation on Eulerian grid \rightarrow greatly reduce discrete particle noise

Numerical Simulation of Gyrokinetic Equation

- What is δf scheme?
 - Write distribution function as a sum of known f_0 and δf
 - Solve only perturbed part δf 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 δf 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 δf 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 δf 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 δf 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

