Introduction to Kinetic Simulation of Magnetized Plasma

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2018 EASW8

July 30 – Aug 3, 2018

Outline

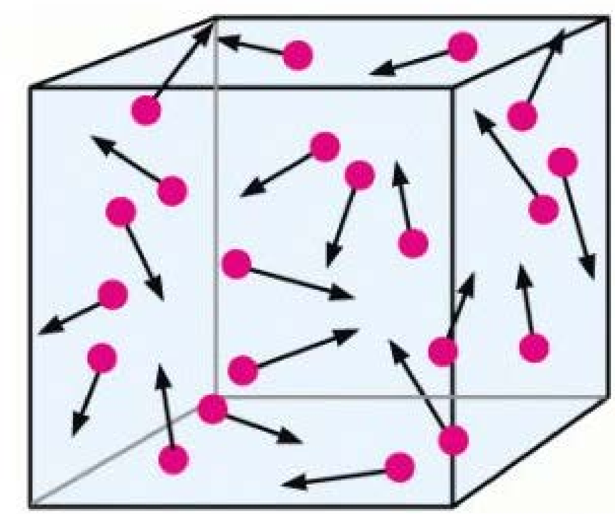
- Introduction to kinetic plasma model
  - Very brief on essential things to understand kinetic simulation
- Reduced kinetic models for magnetized plasma
  - 5D gyrokinetic, 4D bounce-averaged kinetic, 3D fluid with kinetic closure
- Numerical methods for kinetic simulation of magnetized plasma
  - Particle-in-Cell methods, and related numerical issues
- Help students understand the basic idea behind the models and read related literatures for further studies

Introduction to Kinetic Plasma Model

Kinetic Plasma Model

- The most general description of physical system with many particles
- Each particle satisfies the following equations of motion

$$\frac{d\vec{x}}{dt} = \vec{v}, \qquad m\frac{d\vec{v}}{dt} = \vec{F}(x,t) = q\vec{E} + \frac{\vec{v}}{c} \times \vec{B}$$



- Number of particles in $d^3x d^3v$

$$f(\vec{x}, \vec{v}, t)\, d^3x d^3v$$

Klimontovich Equation

- Exact description of classical particles interacting with self-consistent electromagnetic forces

$$F(x,v,t)=\sum_{p=1}^{N}\delta\left[x-X_p(t)\right]\delta\left[v-V_p(t)\right]$$

$$\frac{d}{dt}X_p(t)=V_p(t), \qquad m_s\frac{d}{dt}V_p(t)=qE^m\left[X_p(t),t\right]+\frac{q}{c}V_p(t)\times B^m\left[X_p(t),t\right]$$

- Then, F satisfies

$$\frac{\partial}{\partial t}F+v\cdot\nabla F+\frac{q}{m}\left(E^m+\frac{v}{c}\times B^m\right)\cdot\nabla_v F=0$$

- Note that this equation contains whole spatio-temporal scales all the way down to particle distances.

Klimontovich Equation

- Since we are not interested in physical phenomena occurring in super micro-scales (actually, the equation itself is not valid in such scales),
- We separate quantities into two scales i.e. smooth part in large scale and non-smooth part in small scale, and
- We keep only the smooth part in left hand side and through out all the remaining into the right hand side and call them “collision”

$$F = f + \delta f, \qquad E^m = E + \delta E, \qquad B^m = B + \delta B$$

$$\frac{\partial}{\partial t} f + v \cdot \nabla f + \frac{q}{m}\left(E + \frac{v}{c} \times B\right) \cdot \nabla_v f = -\frac{q}{m}\left\langle\left(\delta E + \frac{v}{c} \times \delta B\right) \cdot \nabla_v \delta f\right\rangle \equiv C$$

$$\rho = \sum_s q_s \int f_s d\vec{v} \qquad \vec{j} = \sum_s q_s \int f_s \vec{v} d\vec{v}$$

$$\nabla \cdot \vec{B} = 0 \qquad \frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} \qquad \nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0} \qquad \frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{B} - \mu_0 \vec{j}$$

Collision Operator

- Collision term can be derived by following BBGKY hierarchy and truncating higher order interaction terms (Introduction to Plasma Theory, Nicholson)

$$C(f) = -\nabla_v \cdot \left[\vec{A} f(\vec{v})\right] + \frac{1}{2}\nabla_v \nabla_v : \left[\overleftrightarrow{B} f(\vec{v})\right]$$

$$A(\vec{v}, t) \equiv \frac{8\pi n_0 e^4 ln\Lambda}{m_e^2} \nabla_v \int d\vec{v}' \frac{f(\vec{v}', t)}{|\vec{v} - \vec{v}'|}$$

$$B(\vec{v}, t) \equiv \frac{4\pi n_0 e^4 ln\Lambda}{m_e^2} \nabla_v \nabla_v \int d\vec{v}' |\vec{v} - \vec{v}'| f(\vec{v}', t)$$

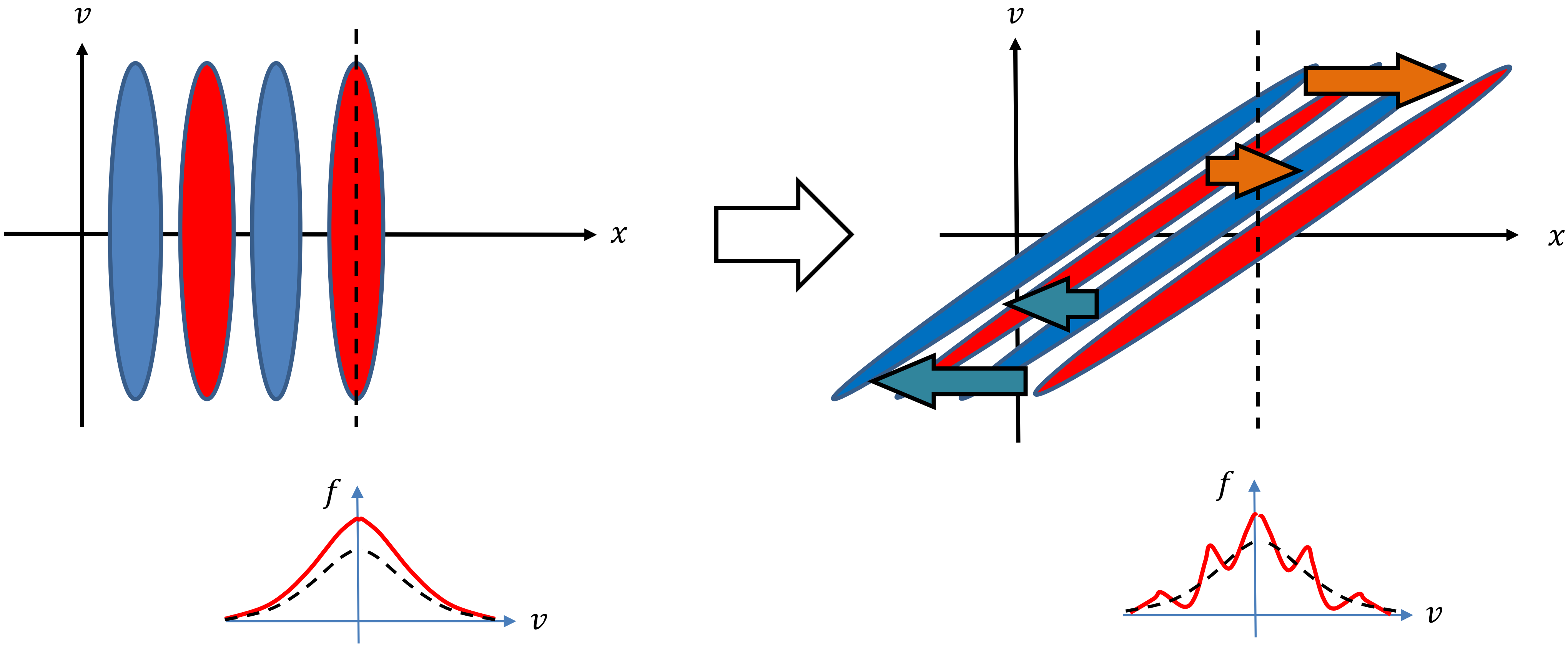
- For high temperature plasmas, the collision frequency becomes very small

$$\nu_{coll} \propto n/T^{3/2}$$

In tokamak plasma $\nu_{coll}^{-1} = 10 \sim 100\, ms$ → collisionless

Kinetic Phase Mixing

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



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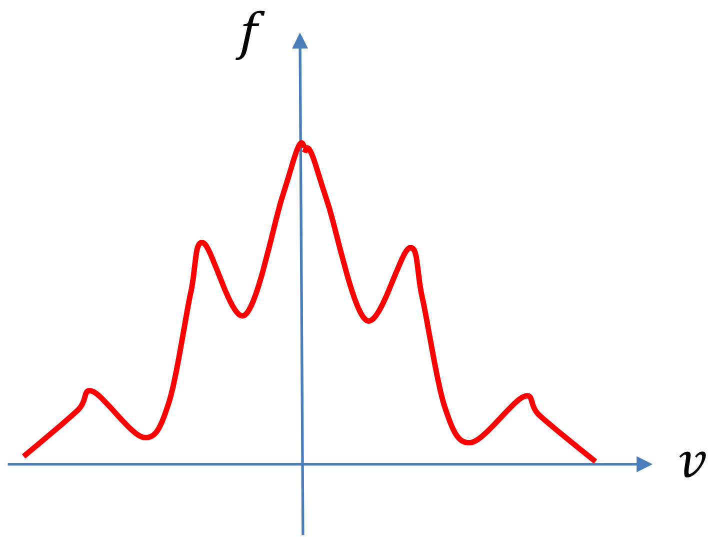
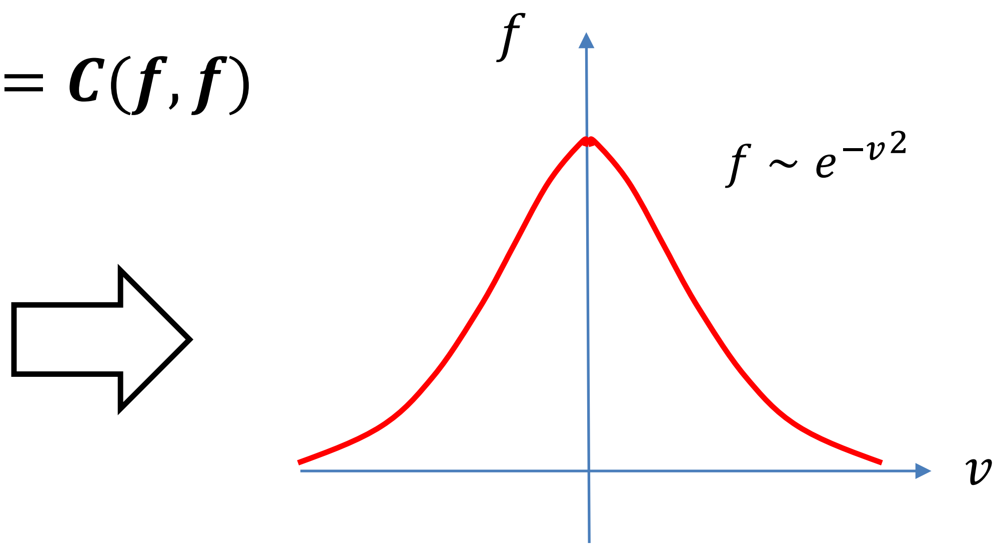
Collisionless ≠ No Collision

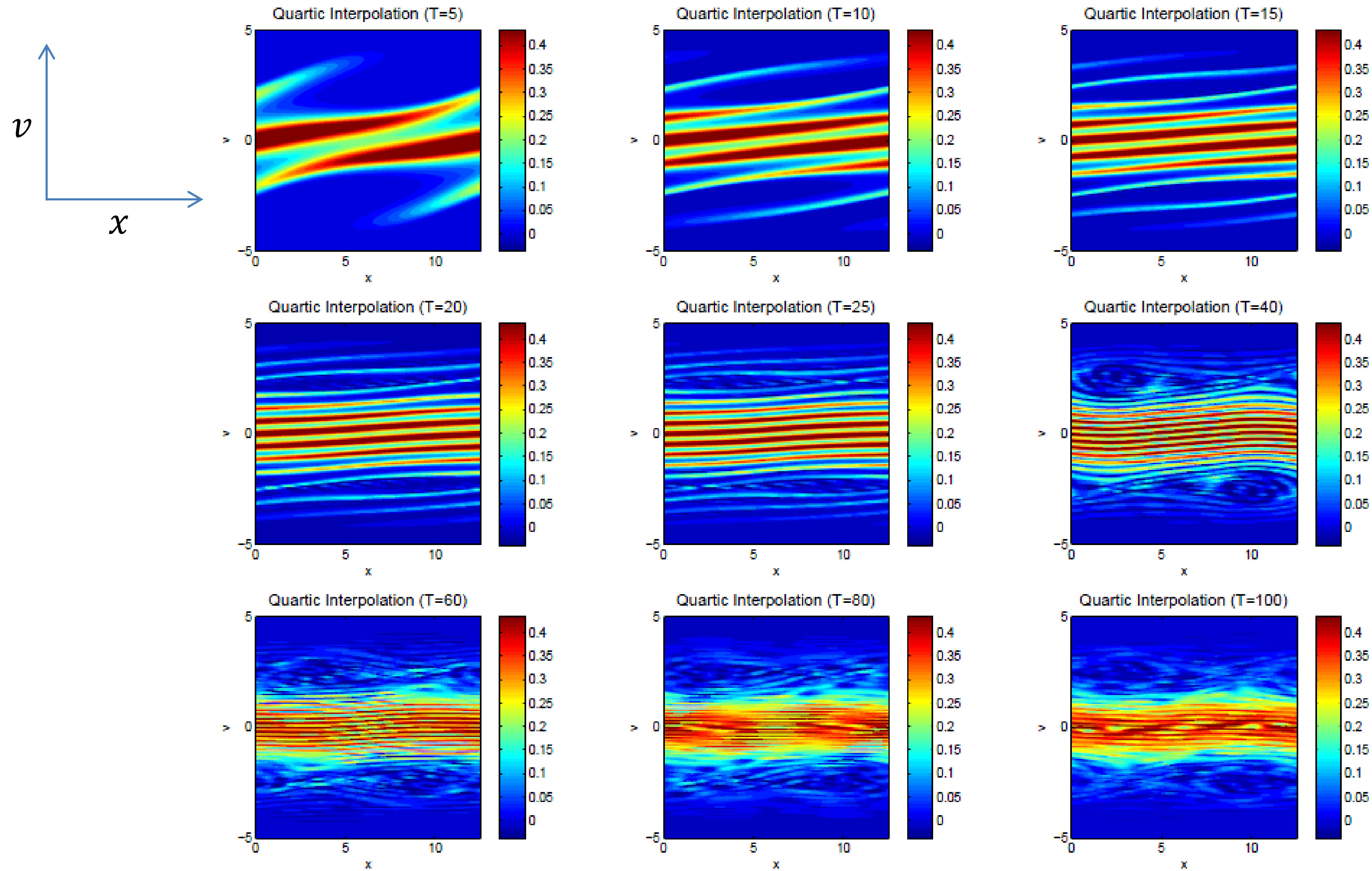


$$\frac{\partial f}{\partial t} = C(f,f)$$



- As $\Delta v \to 0$, $C(f,f) \sim \frac{\partial^2 f}{\partial v^2}$ increases faster than streaming term $\sim \frac{\partial f}{\partial v}$
- Collision becomes important as fine scale structures are developed in velocity space

Kinetic Phase Mixing

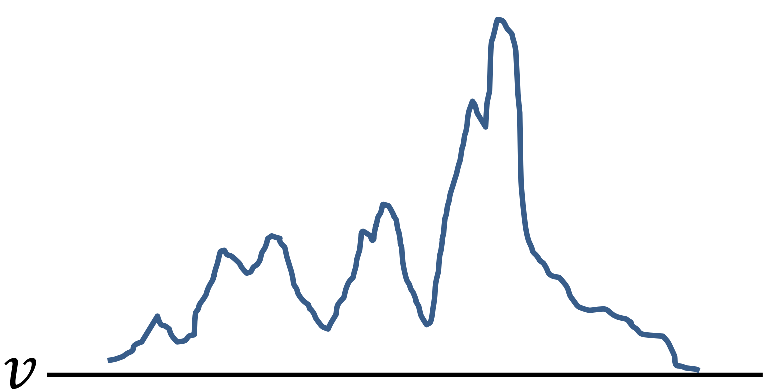


Kinetic Plasma Model

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla f + \frac{\vec{F}}{m}\cdot\nabla_v f = C(f,f)$$

Streaming motions of particles + Mutual interactions in large scales

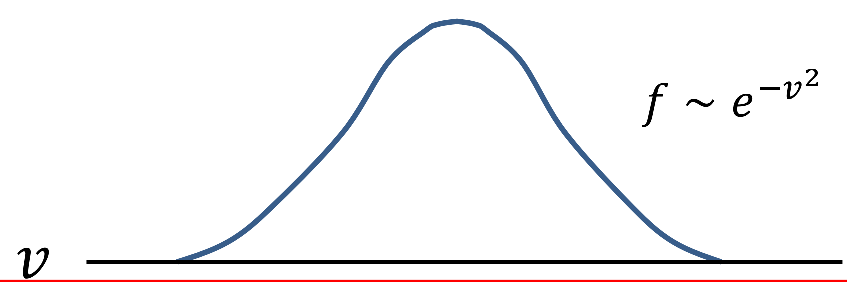
Tend to drive complicated phase space structures



Mutual interactions in very short scales ~ Random collision

Tend to erase fine scale phase space structures

Weaker for small density and high temperature system. Stronger for smaller velocity space scales

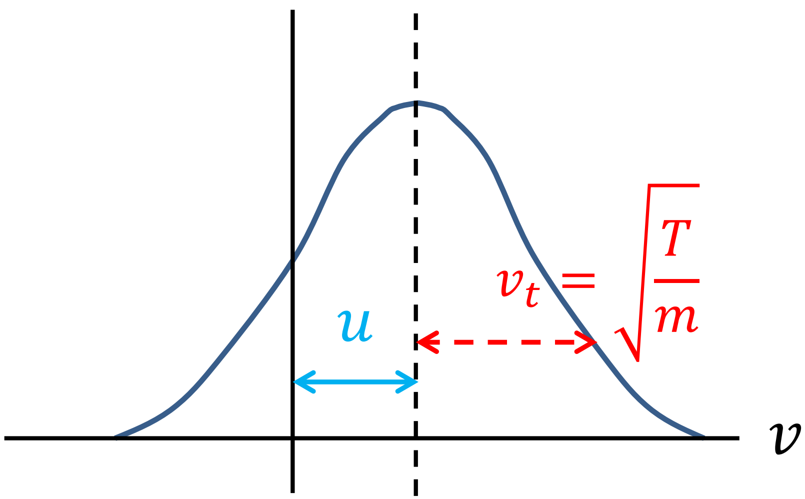


Kinetic vs Fluid

Shifted Gaussian distribution function

$$f(x,v,t) = \frac{\boldsymbol{n}(\vec{x})}{(2\pi)^{3/2}\left(\frac{\boldsymbol{T}(\vec{x})}{m}\right)^{3/2}} \exp\left[-\frac{m(\vec{v}-\vec{\boldsymbol{u}}(\vec{\boldsymbol{x}}))^2}{2\boldsymbol{T}(\vec{\boldsymbol{x}})}\right]$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\vec{v} f \quad = \boldsymbol{n}$$

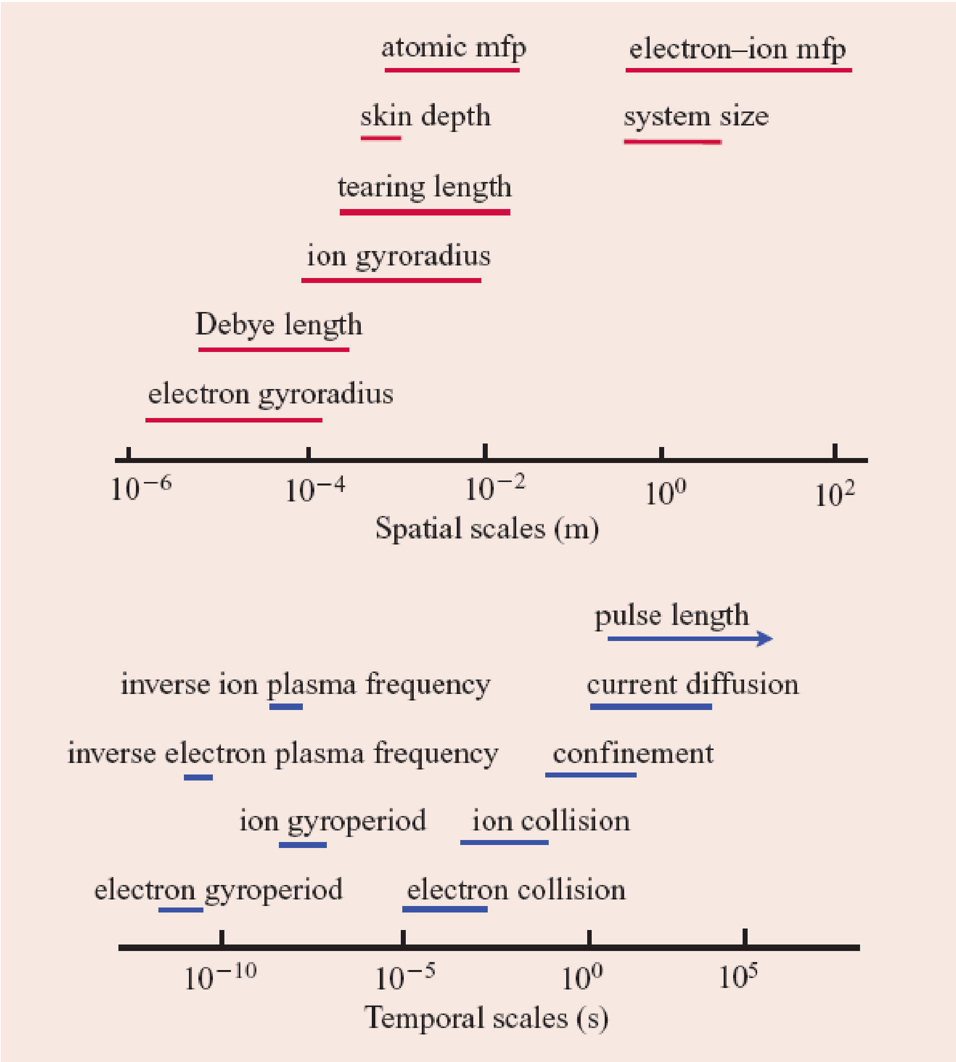


Navier-Stokes (Fluid) Equation

$$n\left(\frac{\partial\vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u}\right) = -\nabla p + \mu\nabla^2\vec{u}$$

$$p = nT$$

Spatio-Temporal Scales of Fusion Plasma

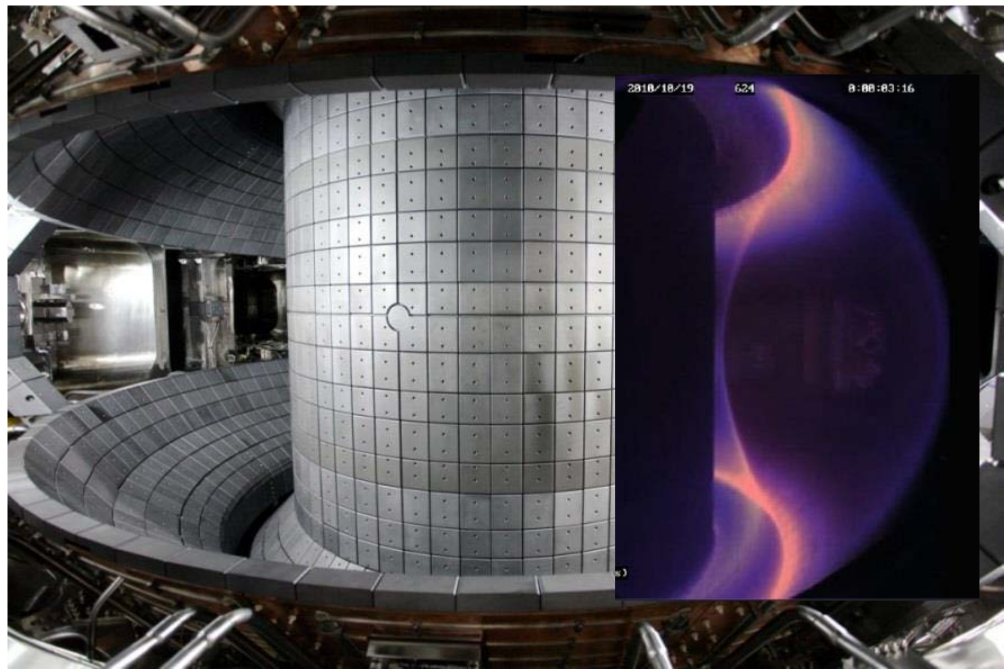


S.Either et al, IBM J. RES. & DEV. Vol. 52 2008

Turbulence in Fusion Device

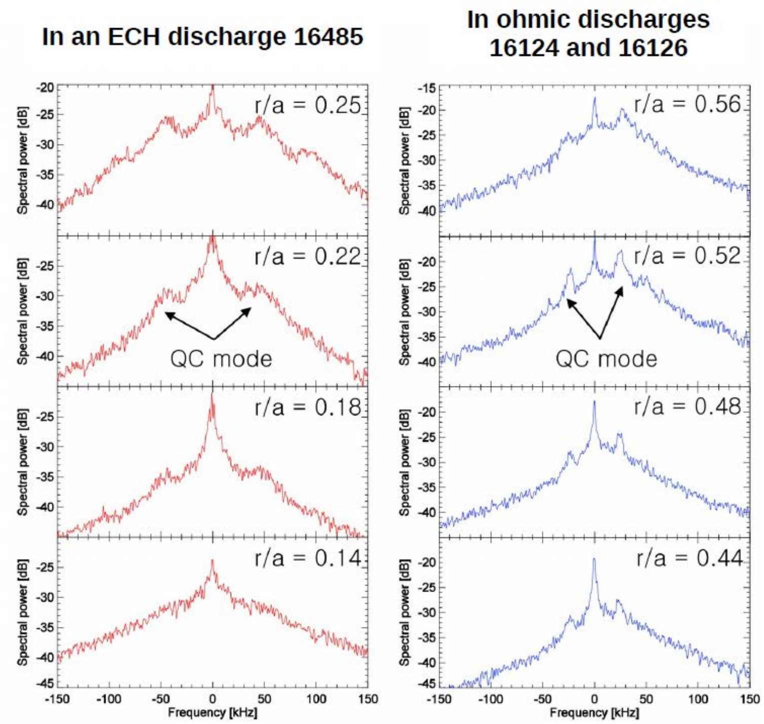
- Fusion plasma confined by external magnetic field

  → strongly magnetized plasma $\rho \ll R$

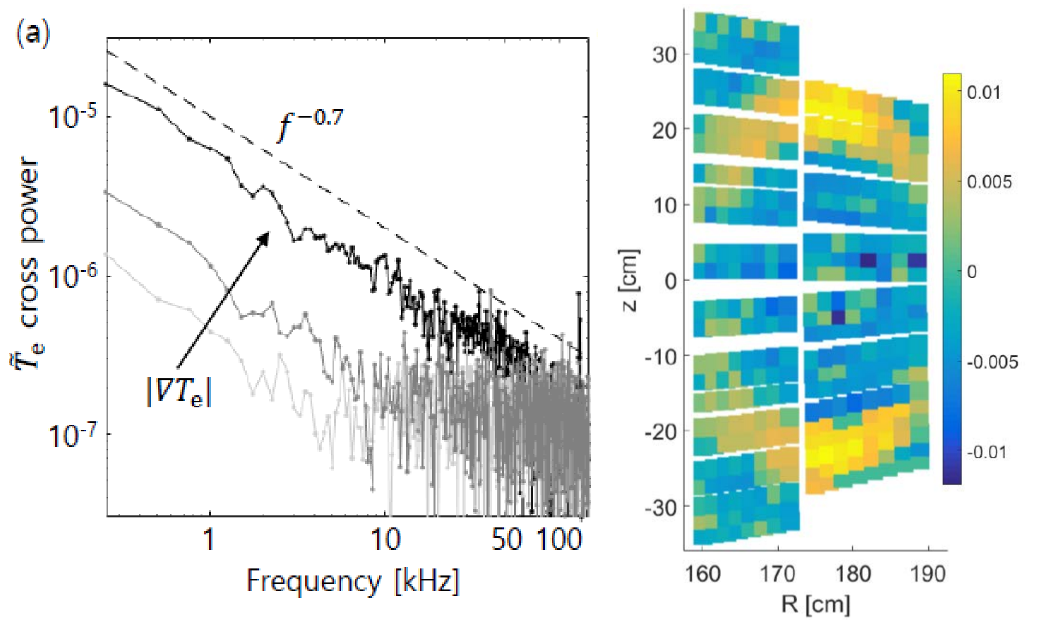


Turbulence in Fusion Device

- In Tokamak, anomalous heat and particle transport driven by micro-scale fluctuations with relatively low frequency $f \leq 300\ kHz$ and $k_{\perp}\rho_i \leq 1$
- Collisionless plasma $\nu_c/f \ll 1$



MIR measured n_e fluctuation on KSTAR L-mode
(J.A. Lee et al, PoP 25, 022513(2018))



ECEI measured T_e fluctuation with $f \leq 100\ kHz$ (M.J. Choi, 2018)

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Kinetic Plasma Model: Problem Size

- Problem size for KSTAR plasma

Number of grids: $N_x \times N_y \times N_z \times N_{v_x} \times N_{v_y} \times N_{v_z}$

$\geq 256 \times 256 \times 256 \times 128 \times 128 \times 128 \sim 10^{13}$

Electron-Ion mass ratio ~ 1:3600

➔ time scale disparity ~ 100

- Even for limited spatio-temporal scales, simulations based on brute-force approaches are practically impossible

- Reduced models are essential

Model Hierarchy for Magnetized Plasma

6D Boltzmann

$$\frac{\partial f_s}{\partial t} + \vec{v}\cdot\nabla f_s + \frac{q_s}{m_s}\left(\vec{E} + \vec{v}\times\vec{B}\right)\cdot\nabla_v f_s = C(f_s)$$

$$\rho = \sum_s q_s \int f_s d\vec{v} \qquad \vec{j} = \sum_s q_s \int f_s \vec{v} d\vec{v}$$

$$\nabla\cdot\vec{B} = 0 \qquad \frac{\partial \vec{B}}{\partial t} = -\nabla\times\vec{E}$$

$$\nabla\cdot\vec{E} = \frac{\rho}{\epsilon_0} \qquad \frac{\partial \vec{E}}{\partial t} = \nabla\times\vec{B} - \mu_0\vec{j}$$

→

5D Gyrokinetic (4D Kinetic)

↓

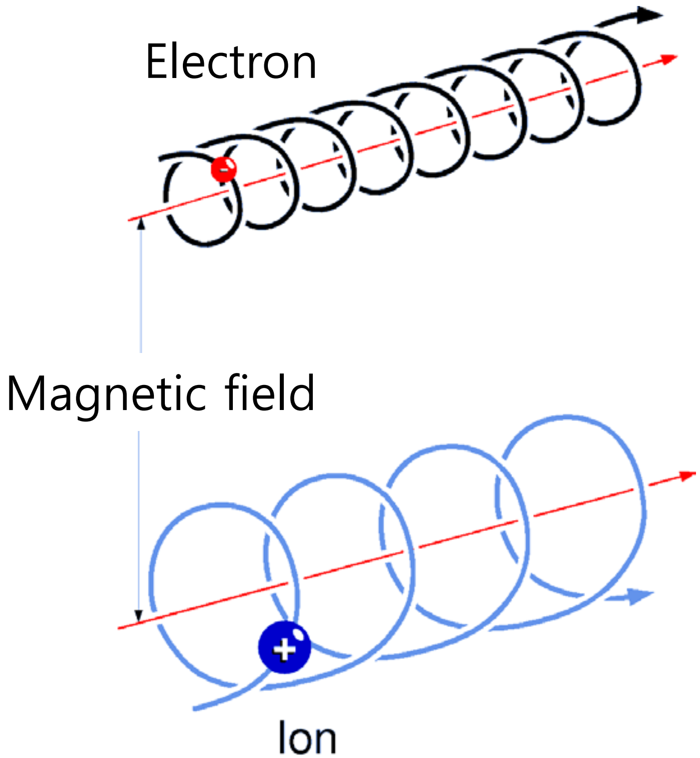
3D Fluid (Gyro-Landau-Fluid, MHD)

↓

1D Diffusion

5D Gyrokinetic Model

Gyro Motion in Magnetized Plasma



[Klasky, ORNL; Ethier, Wang, PPPL]

$\mu \propto \frac{v_\perp^2}{\Omega_i}$ ➔ **Adiabatic invariant of motion for time scales slower than Ω_i^{-1}**

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Basic Idea of Gyrokinetic Model

Frieman, Chen, Phys. Fluids 25, 502(1982)
Hahm, Lee et al, Phys. Fluids 31, 1940(1988)
Hahm, Phys. Fluids 31, 2670(1988)
Brizard, Hahm, Rev. Mod. Phys. 79, 421(2007)

- Gyrokinetic orderings
  - Small fluctuation: $\frac{\delta f}{f_0} \sim \frac{e\delta\phi}{T} \sim \frac{\delta B}{B_0} \ll 1$
  - Low frequency: $\frac{\omega}{\Omega_i} \ll 1$ ➡ Fast MHD waves and cyclotron waves are ruled out (high freq. GK; *Kolesnikov et al, Phys. Plasmas 14, 072506(2007)*)
  - Anisotropic fluctuation: $\frac{k_\parallel}{k_\perp} \ll 1,\ k_\perp \rho_i \sim 1$
  - Mild non-uniformity in plasma profiles, background magnetic field: $\frac{\rho_i}{L_{T,n}} \ll 1$
    - ⬇ Free energy to drive turbulence (GK with strong gradient; *Hahm et al, Phys. Plasmas 16, 022305(2009)*)
  - Low beta: $\beta \ll 1$
    - ⬇ Shear Alfven wave only (GK with Compressional Alfven; *Brizard, Hahm '07*)

Basic Idea of Gyrokinetic Model

- Guiding center transformation

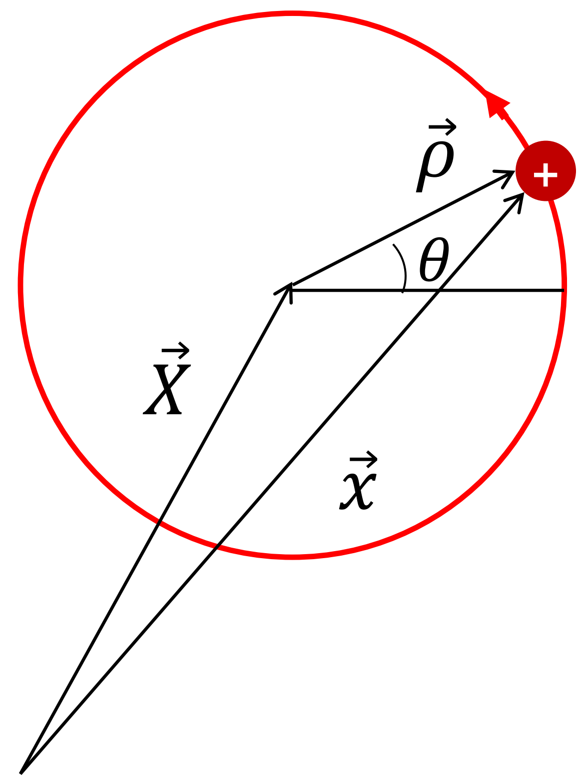
particle space $(\vec{x}, \vec{v}) \leftrightarrow$ guiding center space $(\vec{X}, v_\parallel, \mu, \theta)$

θ: gyro-angle $\rightarrow$ average out

$$\vec{X} = \vec{x} - \vec{\rho} \qquad \vec{\rho} = \hat{b} \times \frac{\vec{v}}{\Omega} \qquad \Omega = \frac{eB_0}{mc}$$

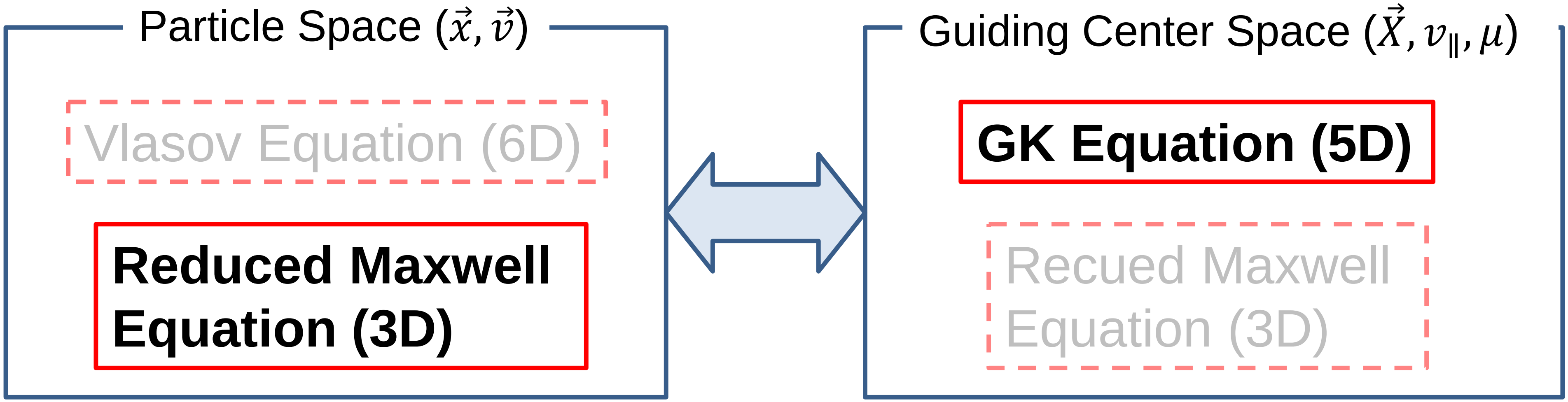
$$v_\parallel = \hat{b} \cdot \vec{v} \qquad \mu = \frac{v_\perp^2}{2B}$$

$$\vec{v} = v_\parallel \hat{b} + v_\perp \hat{e}_\perp$$



Basic Idea of Gyrokinetic Model

- Schematics of guiding center transformation in Gyrokinetic model



- ✓ Solve Vlasov equation in guiding center space and evaluate sources (n_s, j_s)
- ✓ Transform sources (n_s, j_s) to particle space
- ✓ Solve recued Maxwell equations to obtain EM fields
- ✓ Transform EM fields to guiding center space

Gyrokinetic Vlasov Equation for Low-β Plasma

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

$\rightarrow$ reduction to 5D $\bar{f}(\vec{X}, v_\parallel, \mu, t)$, retaining only slow time scales $\Delta t \ll 1/\Omega_i$

$$\frac{\partial \bar{f}}{\partial t} + \left(v_\parallel \hat{b}^* + \frac{\mu}{B}\,\hat{b} \times \nabla B + \frac{c}{B_0}\hat{b} \times \nabla\langle\delta\psi\rangle \right) \cdot \frac{\partial \bar{f}}{\partial \vec{X}} + \frac{q}{m}\left(-\hat{b}^* \cdot \mu \nabla B - \hat{b}^* \cdot \nabla\langle\delta\phi\rangle - \frac{1}{c}\frac{\partial}{\partial t}\langle\delta A_\parallel\rangle \right)\frac{\partial \bar{f}}{\partial v_\parallel} = 0$$

$$\delta\psi = \delta\phi - \frac{v_\parallel}{c}\delta A_\parallel$$

$$\hat{b}^* = \hat{b} + \frac{v_\parallel}{B}\hat{b} \times \hat{b} \cdot \nabla \hat{b}$$

$\langle \cdot \rangle$ = gyro-phase averaged fluctuations

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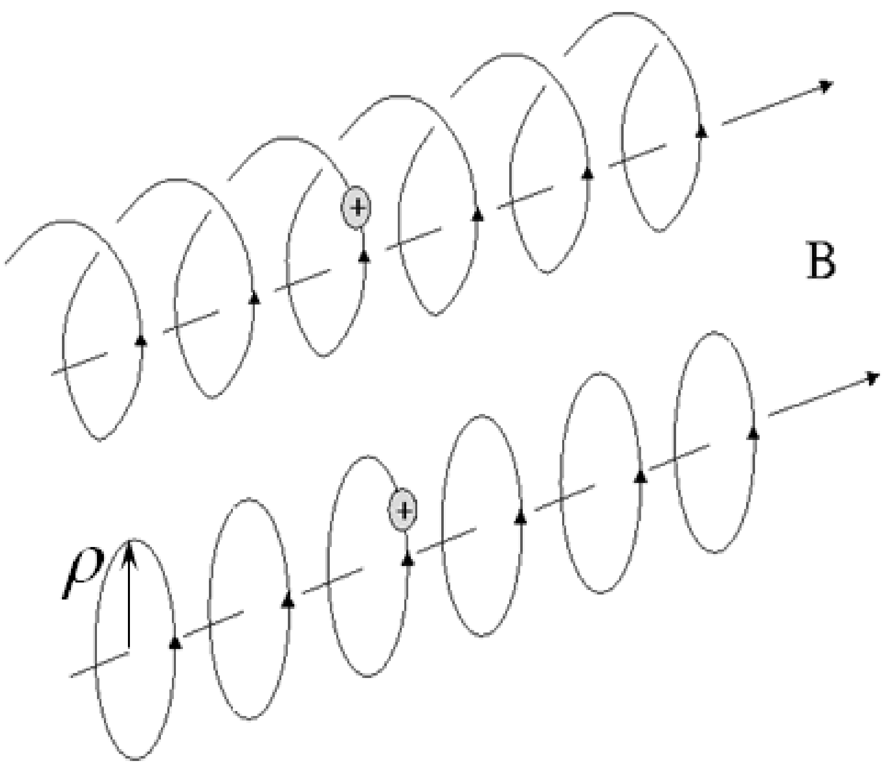
Gyrokinetic Model – Simple View

- Gyrokinetic description of magnetized plasmas



Motion of charged particle

$$\frac{d}{dt}\vec{x} = \vec{v}$$

$$\frac{d}{dt}\vec{v} = -\frac{q}{m}\nabla\delta\phi + \frac{q}{mc}\vec{v}\times\left(\vec{B}_0 + \delta\vec{B}\right)$$

Motion of charged ring centered at $\vec{X}$

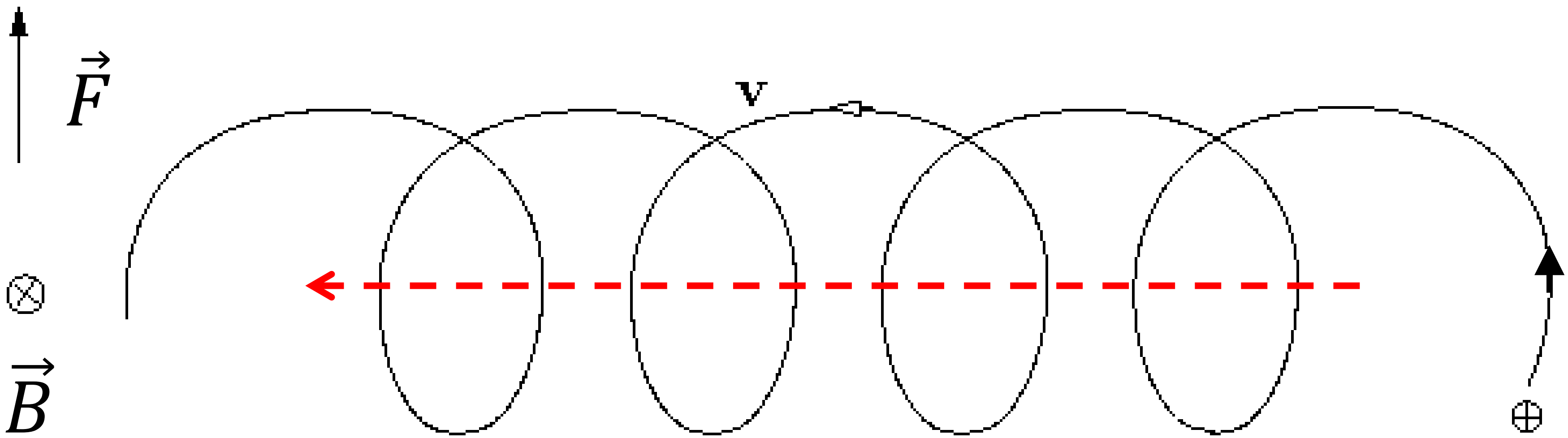
$$\frac{d\vec{X}}{dt} = v_{\parallel}\hat{b}^* + \frac{\mu}{B}\hat{b}\times\nabla B + \frac{c}{B_0}\hat{b}\times\nabla\langle\delta\psi\rangle$$

$$\frac{dv_{\parallel}}{dt} = -\frac{q}{m}\left(\hat{b}^*\cdot\mu\nabla B + \hat{b}^*\cdot\nabla\langle\delta\phi\rangle + \frac{1}{c}\frac{\partial}{\partial t}\langle\delta A_{\parallel}\rangle\right)$$

Gyrokinetic Model – Simple View

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

  ➔ drift motion of gyro-center in $\vec{F} \times \vec{B}$ direction



Gyrokinetic Model – Simple View

Grad-B + Curvature drift

$$\frac{d\vec{X}}{dt} \approx v_\parallel \left[\hat{b} + \frac{\nabla\delta A_\parallel \times \hat{b}}{cB}\right] + \left(mv_\parallel^2 + \mu B\right)\frac{\hat{b}\times\nabla B}{qB^2} + \frac{c}{B_0}\hat{b}\times\nabla\delta\phi$$

ExB drift

Parallel motion along perturbed magnetic field

$$\frac{dv_\parallel}{dt} \approx -\frac{q}{m}\left(\mu\hat{b}\cdot\nabla B + \hat{b}\cdot\nabla\langle\delta\phi\rangle + \frac{1}{c}\frac{\partial}{\partial t}\delta A_\parallel\right)$$

Parallel E-field

mirror force

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

$$\frac{\partial}{\partial t}\left(B_\parallel^* \bar{f}\right) + \frac{\partial}{\partial\vec{X}}\left(\frac{d\vec{X}}{dt}B_\parallel^*\bar{f}\right) + \frac{\partial}{\partial v_\parallel}\left(\frac{dv_\parallel}{dt}B_\parallel^*\bar{f}\right) = 0$$

Gyrokinetic Model – Simple View

- Poisson equation with enhanced polarization shielding

$$-\left(1+\frac{\rho_i^2}{\lambda_{Di}^2}\right)\nabla^2\delta\phi(\vec{x},t) = 4\pi\sum_s q_s \bar{N}_s$$

← Density from charged rings

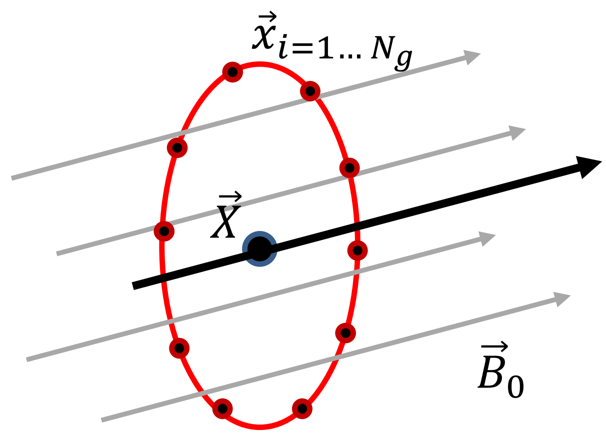
  - ✓ Additional shielding by polarization charges carried by charged rings
  - ✓ Significantly enhanced compared to Debye shielding

- Ampere equation without displacement current, also for $\delta\vec{A} = \hat{b}\delta A_{\parallel}$ for low-β

$$\nabla\times\delta\vec{B} \approx \nabla\times\nabla\times\left(\hat{b}\delta A_{\parallel}\right) \approx \frac{4\pi}{c}\sum_s \vec{J}_s$$

$$\Rightarrow \quad -\nabla_{\perp}^2\delta A_{\parallel} = \frac{4\pi}{c}\sum_s \bar{J}_{\parallel s}$$

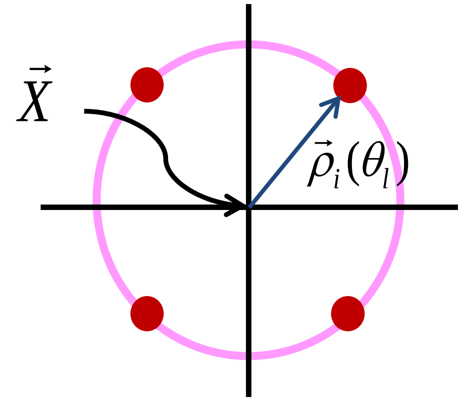
← Parallel current carried by charged rings



Gyrokinetic Model – Simple View

- Gyro-averaged potentials $\langle\delta\phi\rangle$, $\langle\delta A_{\|}\rangle$ 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)

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

$$=\frac{1}{2\pi}\int_0^{2\pi}\delta\phi(\vec{X}+\vec{\rho}_i(\theta))d\theta = \frac{1}{2\pi}\int_0^{2\pi}\left\{\frac{1}{(2\pi)^3}\int \delta\hat{\phi}(\vec{k})e^{i\vec{k}\cdot\left(\vec{X}+\vec{\rho}_i(\theta)\right)}d\vec{k}\right\}d\theta$$

$$=\frac{1}{(2\pi)^3}\int\left\{\frac{1}{2\pi}\int_0^{2\pi}\delta\hat{\phi}(\vec{k})e^{ik_\perp\rho_i\cos\theta}d\theta\right\}e^{i\vec{k}\cdot\vec{X}}d\vec{k} = \frac{1}{(2\pi)^3}\int\delta\hat{\phi}(\vec{k})J_0\left(\frac{k_\perp v_\perp}{\Omega_i}\right)e^{i\vec{k}\cdot\vec{X}}d\vec{k}$$

Reduced Problem Size

- Problem size for KSTAR plasma

Number of grids: $N_x \times N_y \times N_z \times N_{v_x} \times N_{v_y} \times N_{v_z}$

$$\geq 256 \times 256 \times 256 \times 128 \times 128 \times 128 \sim 10^{13}$$

Number of grids: $N_x \times N_y \times N_z \times N_{v_\parallel} \times N_\mu$

$$\geq 256 \times 256 \times 256 \times 128 \times 16 \sim 10^{10}$$

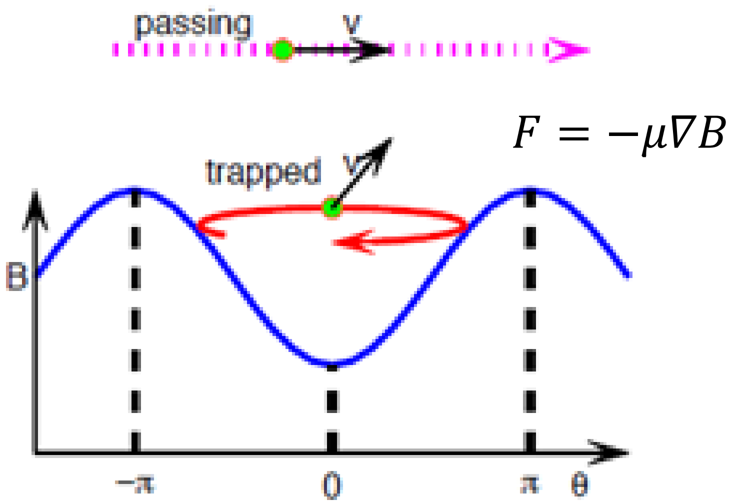
Electron-Ion mass ratio ~ 1:3600

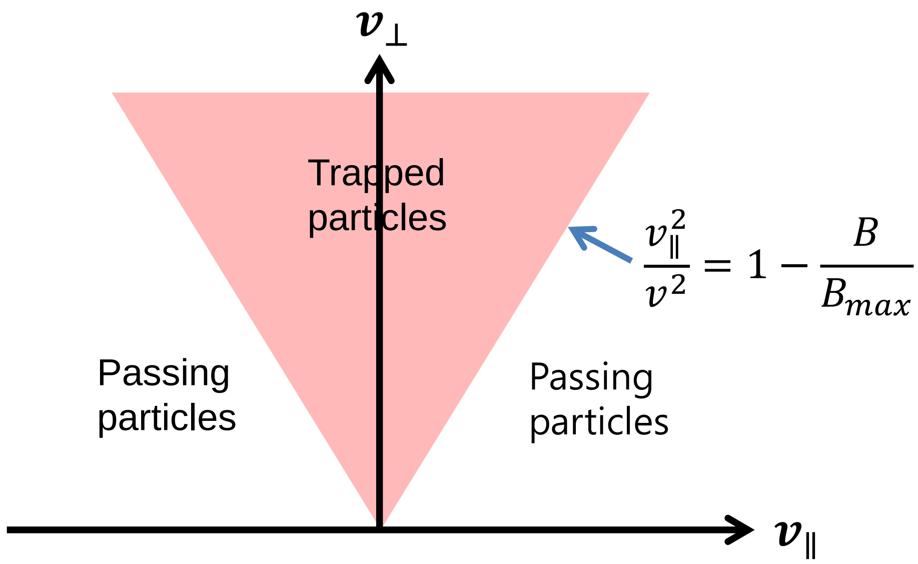
➔ Time scale disparity ~ 100

Fluid Model?

4D Bounce-Averaged Kinetic Model

Bounce Motion in Magnetized Plasma



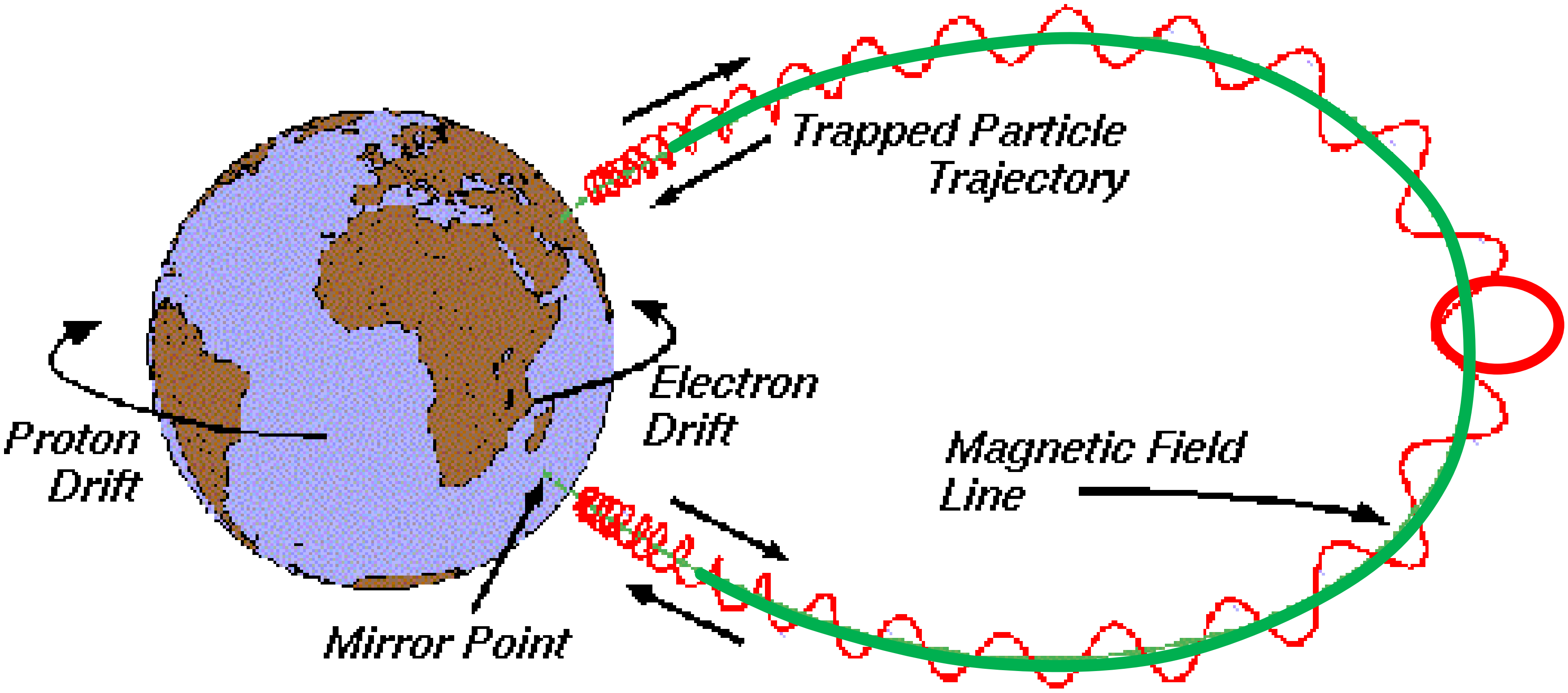


- Passing and trapped particles behave very differently
  - Passing particles move freely along magnetic field line

    → For slow perturbation, fluid model works well
  - Trapped particles show non-trivial responses to slow perturbations

    → Hard to capture in fluid model

Bounce Motion in Magnetized Plasma



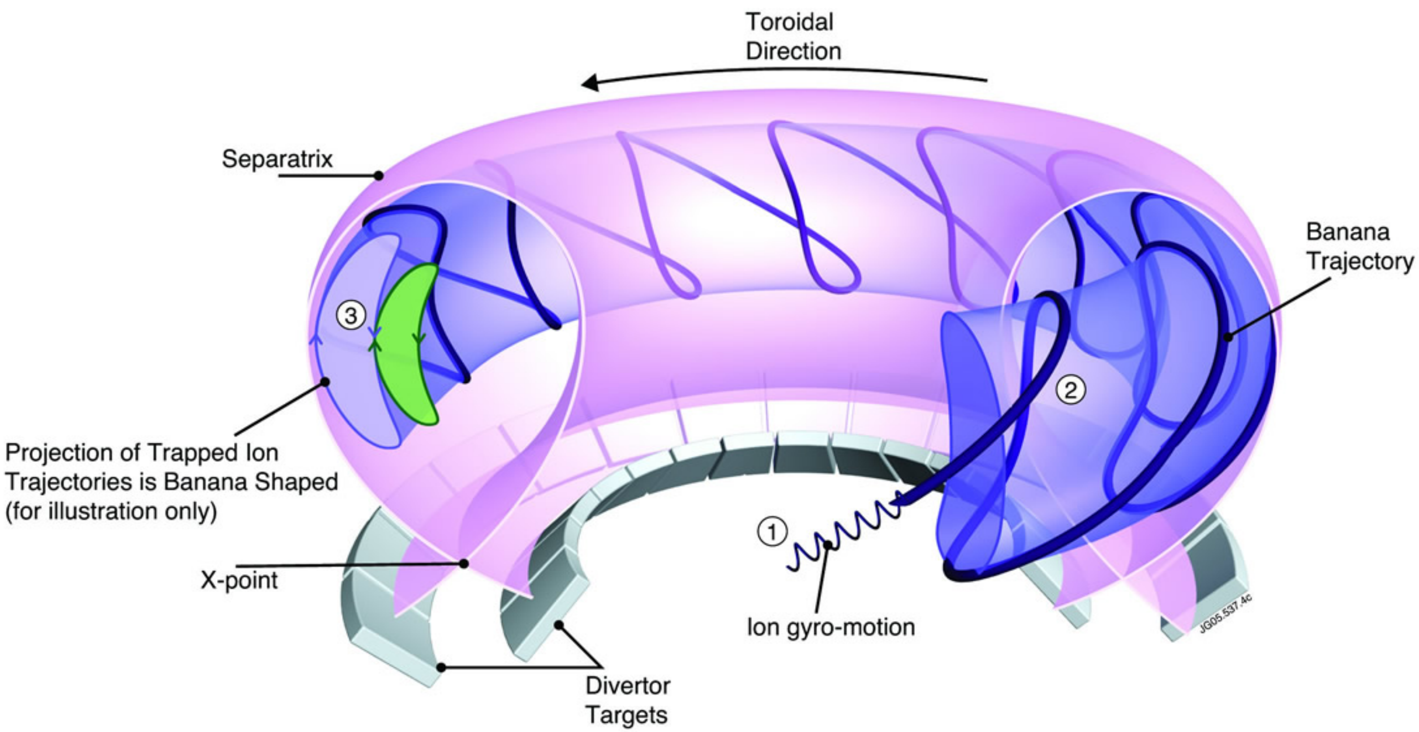
$$J_1 = \oint \vec{P}_\perp \cdot d\vec{l} = \oint \left(m v_\perp - \frac{1}{2} q B R \right) R d\theta = \frac{\pi m v_\perp^2}{\Omega} \propto \mu$$

$$J_2 = \oint P_\parallel dl \approx \oint m v_z dz = \oint m v_z^2 dt = \frac{\pi m \hat{v}_z^2}{\omega_b}, \quad v_z = \hat{v}_z \cos \omega_b t$$

Figure from Geomagnetism, Nathani Basavaiah

Bounce Motion in Magnetized Plasma

- Trapped electrons in fusion device
  - Motions along banana are very fast → detailed position is negligible
  - Toroidal precession motions are slow → comparable with ion transit motions
- Trapped electron bounce-centers behave like ions → resonate with ion scale turbulence

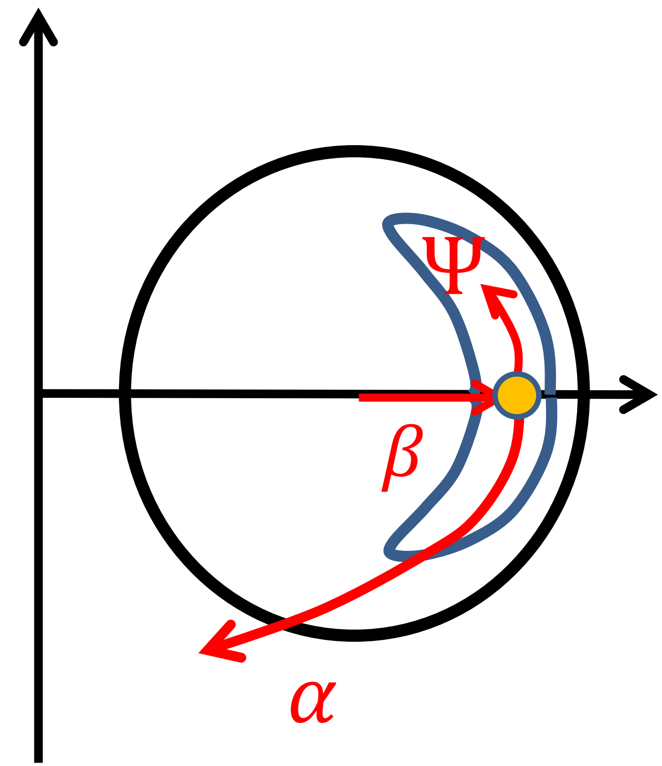


https://www.euro-fusion.org/wpcms/wp-content/uploads/2011/09/jg05-537-4c.jpg

Bounce-Averaged Kinetic Model

- Bounce-center coordinate
  - Radial position of bounce center: $\beta = r$
  - Toroidal angle of bounce center at outer mid-plane: $\alpha = \zeta$
  - Bounce phase: $\Psi = \pi + sgn(v_{||})\left[\sin^{-1}\left(\frac{\sin(\theta/2)}{\kappa_p}\right) + \pi/2\right]$

    ➔ Ignorable variable, averaged out
  - Bounce invariant: $I \cong 2qR_0\sqrt{m\varepsilon\mu B_0}\kappa_p^2$
- Further reduction of 5D gyrokinetic equation to 4D bounce-averaged kinetic model



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Kwon, Qi, Yi, Hahm, Comput. Phys. Commun. 177, 775(2017)

Bounce-Averaged Kinetic Model

- Hamiltonian and equations of motion:

$$H(\beta,\alpha,I,\mu) = \mu B_0\left(1+\Delta-\varepsilon+\frac{\kappa^2}{2q^2}\varepsilon^2\right)+\frac{\sqrt{\varepsilon\mu B_0}}{qR_0\sqrt{m}}I+q_s\langle\phi\rangle_b$$

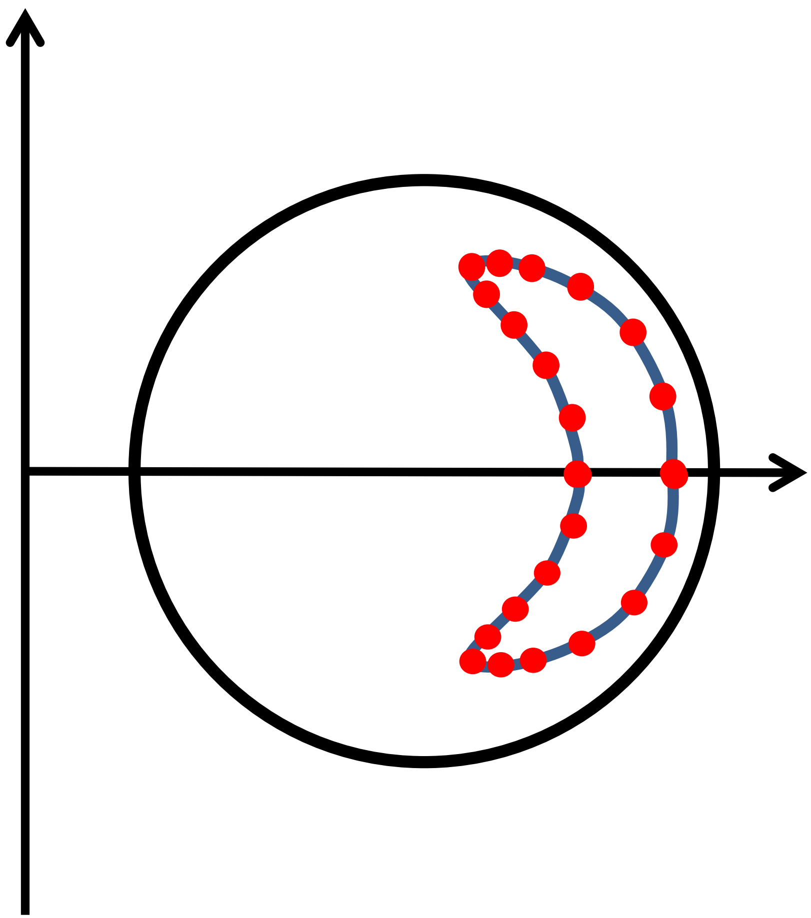
$$\frac{d\beta}{dt}=c\frac{\partial\langle\phi\rangle_b}{\partial\alpha} \qquad \frac{d\alpha}{dt}=-\frac{c}{e}\frac{\partial H_0}{\partial\beta}-c\frac{\partial\langle\phi\rangle_b}{\partial\beta} \qquad \frac{dI}{dt}=0 \qquad \frac{d\mu}{dt}=0$$

- Bounce averaged kinetic equation:

$$\frac{dF}{dt}=\frac{\partial F}{\partial t}+\frac{d\beta}{dt}\frac{\partial F}{\partial\beta}+\frac{d\alpha}{dt}\frac{\partial F}{\partial\alpha}=0$$

Bounce-Averaged Kinetic Model

- Numerical calculation of bounce average



$$\langle\phi\rangle_b \equiv \frac{\oint \phi \frac{dl}{\dot{l}}}{\oint \frac{dl}{\dot{l}}} = \frac{1}{T}\oint \phi \frac{dl}{\dot{l}}$$

Approximation of bounce orbit by unperturbed guiding center motion

Reduced Problem Size

- Problem size for KSTAR plasma

Number of grids: $N_x \times N_y \times N_z \times N_{v_x} \times N_{v_y} \times N_{v_z}$

$\geq 256 \times 256 \times 256 \times 128 \times 128 \times 128 \sim 10^{13}$

Number of grids: $N_x \times N_y \times N_z \times N_{v_\parallel} \times N_\mu$

$\geq 256 \times 256 \times 256 \times 32 \times 16 \sim 10^{9}$

Electron-Ion mass ratio ~ 1:3600

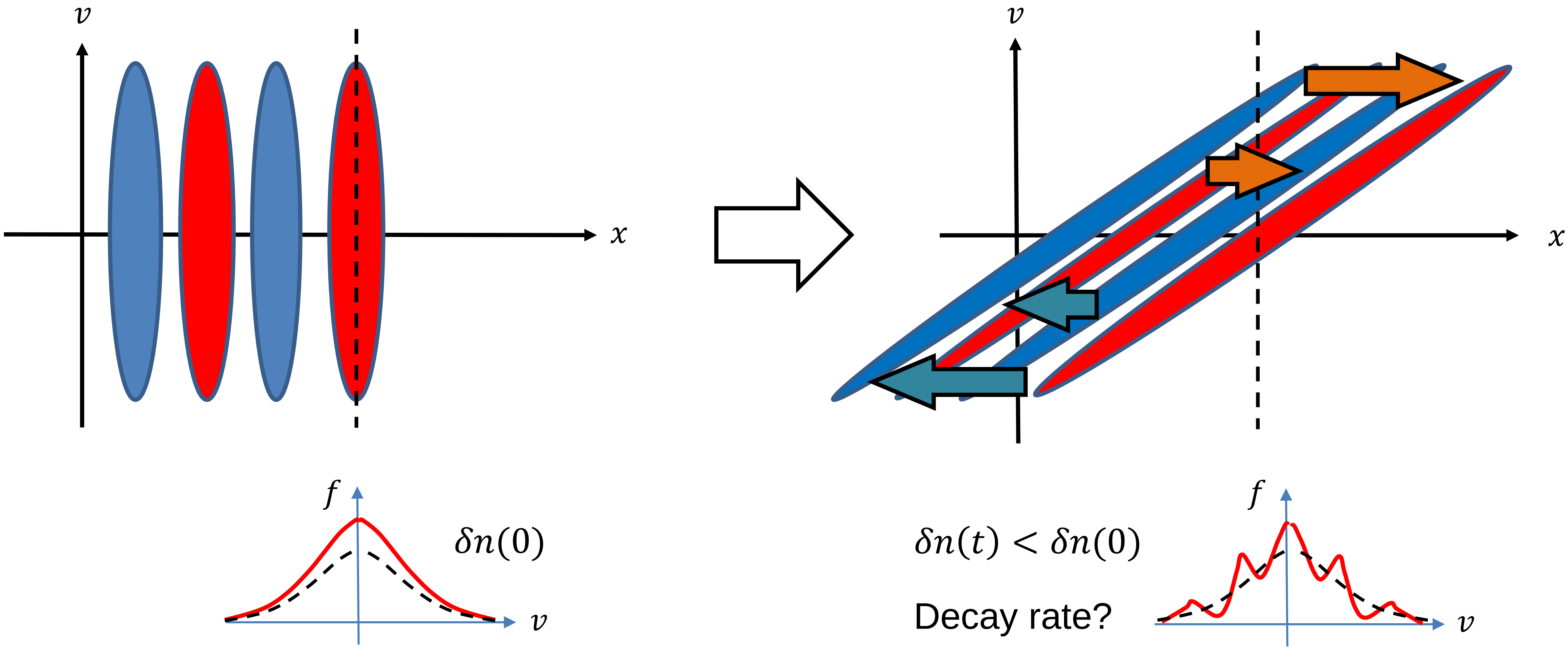
➔ time scale disparity ~ 100

$\Delta t_{CFL} \sim \Delta t$ for ions only

Fluid Model with Kinetic Closure

Kinetic Phase Mixing

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



Kinetic Closure: How to mimic kinetic process?

- Fluid Model
  - For neutral gas $\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(Vn) = 0$ with particle flux $\Gamma = nV = -D\frac{\partial n}{\partial x}$ (Fick's law)
  - Then, we have $\frac{\partial n}{\partial t} = D\frac{\partial^2}{\partial x^2}n$
  - Let's assume a stationary solution $n(x,t) = n_0$ and put a perturbation at $t = 0$ as $\delta n(x,0) = n_1 e^{ikx}$.
  - Then, the solution of the equation becomes $\delta n(x,t) = \delta n(x,0)e^{-Dk^2 t}$

Kinetic Closure: How to mimic kinetic process?

- Kinetic Model
  - For neutral gas $\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0$
  - With a stationary solution, $f_0(v) = \frac{n_0}{\sqrt{2\pi v_t^2}}\, e^{-\frac{v^2}{2v_t^2}}$ (note that $\int_{-\infty}^{+\infty} dv f_0 = n_0$)
  - Let's put a perturbation at $t = 0$, $f_1(x, v) = \frac{n_1 e^{ikx}}{\sqrt{2\pi v_t^2}}\, e^{-\frac{v^2}{2v_t^2}}$ (note that $\int_{-\infty}^{+\infty} dv f_1 = n_1 e^{ikx}$)
  - Then the solution of the kinetic equation becomes

$$f(x, v, t) = \left(n_0 + n_1 e^{ik(x-vt)}\right) \frac{1}{\sqrt{2\pi v_t^2}}\, e^{-v^2/2v_t^2}$$

Kinetic Closure: How to mimic kinetic process?

- Kinetic Model
  - $f(x,v,t) = \left(n_0 + n_1 e^{ik(x-vt)}\right) \frac{1}{\sqrt{2\pi v_t^2}} e^{-v^2/2v_t^2}$
  - The density evolution becomes

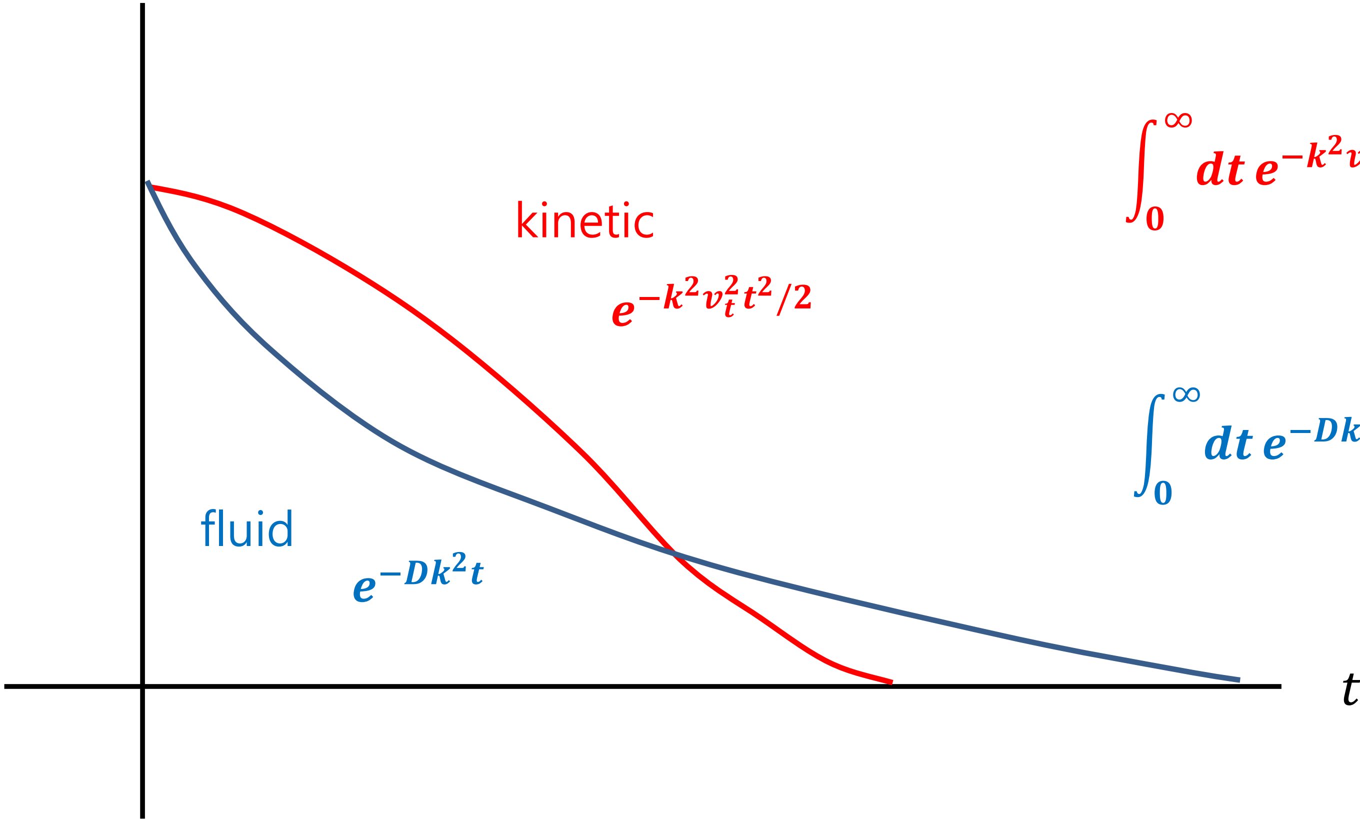
$$n(x,t) = \int dvf = n_0 + n_1 \frac{e^{ikx}}{\sqrt{2\pi v_t^2}} \int dv e^{-ikvt} e^{-\frac{v^2}{2v_t^2}} = n_0 + n_1 e^{ikx} e^{-k^2 v_t^2 t^2/2}$$

i.e. $\delta n(x,t) = \delta n(x,0) e^{-k^2 v_t^2 t^2/2}$

- Kinetic vs Fluid

kinetic	fluid
$e^{-k^2 v_t^2 t^2/2}$	$e^{-Dk^2 t}$

Kinetic Closure: How to mimic kinetic process?



$$\int_0^\infty dt\, e^{-k^2 v_t^2 t^2/2} = \frac{1}{\sqrt{k^2 v_t^2}}\sqrt{\frac{\pi}{2}}$$

$$\int_0^\infty dt\, e^{-Dk^2 t} = \frac{1}{Dk^2}$$

Match two time responses ~ match the two areas → $D = \sqrt{\frac{2}{\pi}}\frac{v_t}{|k|}$

Hammett et al, Phy Rev Lett 64, 3019(1990)
Hammett et al, Phys Fluids B 4, 2052(1992)

Kinetic Closure: How to mimic kinetic process?

- With $D_k = \sqrt{\frac{2}{\pi}}\frac{v_t}{|k|}$, the particle flux can be written as $\Gamma_k = -D_k i k n_k$
- In real space, $\Gamma = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dk e^{ikx}\Gamma_k = -\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dk e^{ikx} n_k \frac{ik}{|k|}$
- Using delta function identities

$$\frac{1}{|k|} = \int_{-\infty}^{+\infty}\delta(kx')dx', \;\; \delta(kx') = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{\epsilon^2+k^2x'^2}$$

- $\Gamma = -\frac{\sqrt{2}v_t}{\pi^{3/2}}\int_0^{\infty} dx' \frac{n(x+x')-n(x-x')}{x'}$ (c.f. conventional closure $\Gamma = -D\frac{\partial n}{\partial x}$)

i.e. D_k is a non-local integral operator

- **4-moment (3 parallel, 1 perpendicular) equations:**

$$\frac{dn}{dt} + f_{ut}\nabla_{\|}u_{\|} - i\left(1 + \frac{\eta_\perp}{2}\nabla_\perp^2\right)\omega_*\Psi + i\left(2 + \frac{1}{2}\nabla_\perp^2\right)\omega_d\Psi + i\omega_d\left(p_{\|} + p_\perp\right) = 0$$

$$\frac{dp_{\|}}{dt} + |k_{\|}|\chi_{\|}\left(f_{ut}p_{\|} - n\right) + f_{ut}3\nabla_{\|}u_{\|} - i\left(1 + \eta_{\|} + \frac{\eta_\perp}{2}\nabla_\perp^2\right)\omega_*\Psi + i\left(4 + \frac{1}{2}\nabla_\perp^2\right)\omega_d\Psi$$
$$+ i\omega_d\left(7p_{\|} + p_\perp - 4n\right) + 2|\omega_d|\left(\nu_1 T_{\|} + \nu_2 T_\perp\right) = 0$$

$$\frac{dp_\perp}{dt} + |k_{\|}|\chi_\perp\left(f_{ut}p_\perp - n\right) + f_{ut}\nabla_{\|}u_{\|} - i\left[1 + \frac{1}{2}\nabla_\perp^2 + \eta_\perp\left(1 + \frac{1}{2}\nabla_\perp^2 + \nabla_\perp^2\right)\right]\omega_*\Psi$$
$$+ i\omega_d\left(3 + \frac{3}{2}\nabla_\perp^2 + \nabla_\perp^2\right)\Psi + i\omega_d\left(5p_\perp + p_{\|} - 3n\right) + 2|\omega_d|\left(\nu_3 T_{\|} + \nu_4 T_\perp\right) = 0$$

$$\frac{du_{\|}}{dt} + \nabla_{\|}\left(p_{\|} + \psi\right) + 4i\omega_d u_{\|} + 2|\omega_d|\nu_5 u_{\|} = 0 \qquad f_{ut} = 1 - f_t$$

- **Closure coefficients:**

$\nu_1 = (1.232, 0.437)$ $\nu2 = (-0.912, 0.362)$ $\nu3 = (-1.164, 0.294)$

$\nu4 = (0.478, -1.926)$ $\nu_5 = (0.515, -0.958)$

Hammett et al, Phys Fluids B 4, 2052(1992)
Beer, Hammett, Phys. Plasmas 3, 4046(1996)
P. Snyder, Ph.D. Thesis (1999)

Numerical Methods for Kinetic Plasma Simulation

- Continuum (Eulerian) Method
  - Discretize 5D/4D phase space, and apply FDM, FVM, FEM
  - Computationally expensive, but enable high quality simulation
- Particle-in-Cell (Lagrangian) Method
  - Computationally cheap (relative to continuum method)
  - Noise issues
- Semi-Lagrangian Method

Particle-in-Cell Method

for Kinetic Simulation

C.K. Birdsall and A.B. Langdon, "Plasma Physics via Computer Simulation", McGraw-Hill, 1985
R.W. Hockney and J.W. Eastwood, "Computer Simulation using Particles", IPP, 1988
W.W. Lee, J. Comput. Phys. 72, 243 (1987)

From Klimontovich Equation to PIC

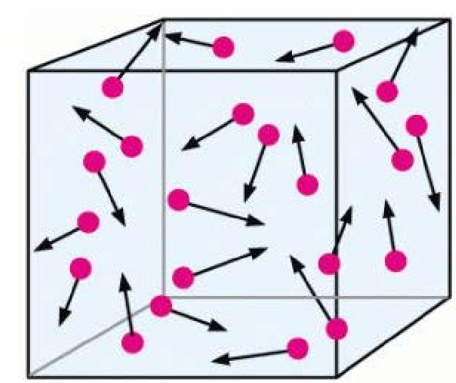
$$\frac{\partial}{\partial t}F + v \cdot \nabla F + \frac{q}{m}\left(E^m + \frac{v}{c} \times B^m\right) \cdot \nabla_v F = 0 \qquad F(x, v, t) = \sum_{p=1}^{N} \delta[x - X_p(t)]\delta[v - V_p(t)]$$

$$\frac{d}{dt}X_p(t) = V_p(t) \qquad m_s \frac{d}{dt}V_p(t) = qE^m[X_p(t), t] + \frac{q}{c} V_p(t) \times B^m[X_p(t), t]$$

- We want simulate N-particle system with $N_s \ll N$, $G = \sum_{p=1}^{N_s} \delta[x - X_p(t)]\delta[v - V_p(t)]$

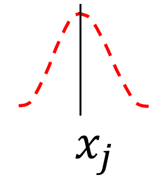
$$F \approx W(x, v)G = \sum_{p=1}^{N_s} W_p\, \delta[x - X_p(t)]\delta[v - V_p(t)]$$

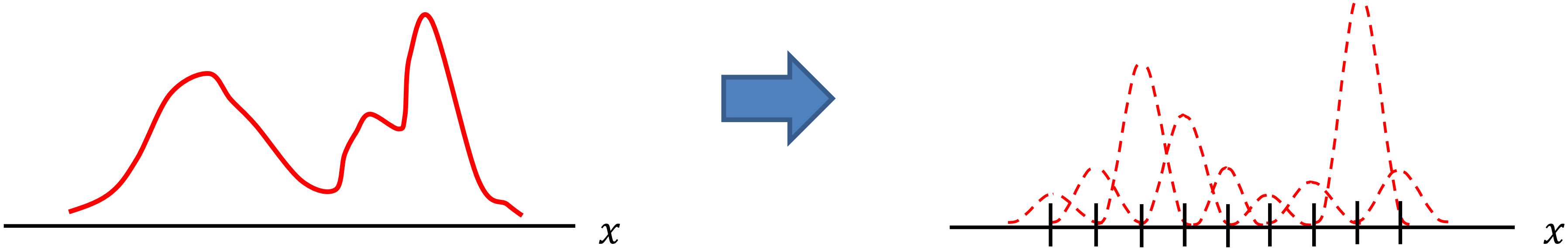
- $\{W_p\}$ depends on marker particle loading scheme i.e. how to set $\{X_p(0),\ V_p(0)\}$
  - For example, if $G(x, v, t = 0) \propto F(x, v, t = 0)$ ➔ $W_p = \frac{N}{N_s}$
  - More sophisticated schemes to minimize loading noise: quite starting scheme, optimal loading scheme etc. (J. Denavit and J.M. Walsh, Plasma Phys. Control. Fusion 6, 209 (1981))



Poisson Equation: $-\nabla^2\phi = 4\pi e\int dvf$

$$\phi(x,t) = \sum_j \hat{\phi}_j(t)S_j(x) = \sum_j \hat{\phi}_j(t)S(x - x_j)$$





- If we write electrostatic potential as $\phi(x,t) = \sum_j \hat{\phi}_j(t)S_j(x)$ using a set of basis function $\{S_j(x)\}$, the Poisson equation becomes

$$-\sum_j \hat{\phi}_j(t)\nabla^2 S_j(x) = 4\pi e\int dv\, F(x,v,t) = 4\pi e\int dv \sum_{p=0}^{N} W_p\delta[x - X_p(t)]\delta[v - V_p(t)]$$

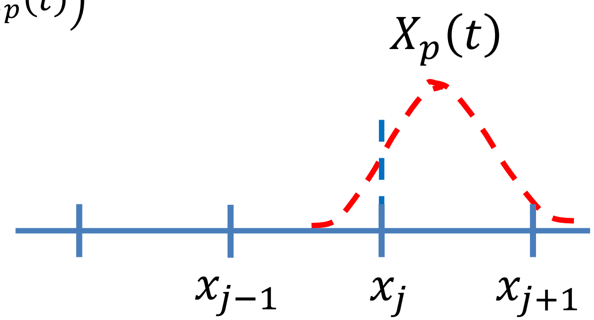
P.M. Prenter, “Splines and Variational Methods”, John Wiley & Sons

Poisson Equation: $-\nabla^2\phi = 4\pi e \int dv f$

$$-\sum_j \hat{\phi}_j(t)\nabla^2 S_j(x) = 4\pi e \int dv\, F(x,v,t) = 4\pi e \int dv \sum_{p=0}^{N} W_p \delta[x - X_p(t)]\delta[v - V_p(t)]$$

- Appling $\int dx\, S_i(x)$ on both sides,

$$\sum_j \left[\int dx\, \nabla S_i(x)\cdot\nabla S_j(x)\right]\hat{\phi}_j(t) = 4\pi e \sum_p W_p S_i\left(X_p(t)\right)$$



- Note that if S is spline function, it satisfies $S_x(y) = S_y(x)$

$$\sum_p W_p S_i\left(X_p(t)\right) = \sum_p W_p S_{X_p(t)}(x_i) = \int dv \sum_p W_p S_{X_p(t)}(x_i)\delta[x - X_p(t)]\delta[v - V_p(t)]$$

i.e. the distribution function can be interpreted as a set of particles with spatial shape $S(x)$

P.M. Prenter, "Splines and Variational Methods", John Wiley & Sons

Collision in PIC Simulation

- Fokker-Planck equation

$$\frac{\partial}{\partial t}f(v,t) = -\frac{\partial}{\partial v}\left[\alpha(v)f(v,t)\right] + \frac{\partial^2}{\partial v^2}\left[\beta(v)f(v,t)\right]$$

- It can be interpreted as a distribution function for particles with characteristic equation

$$\frac{dv}{dt} = \alpha(v,t) + \beta(v,t)\xi(t), \qquad \langle \xi(t')\xi(t)\rangle = \delta(t'-t)$$

- Due to the drag and diffusion on the right hand side, particle trajectories are scattered as

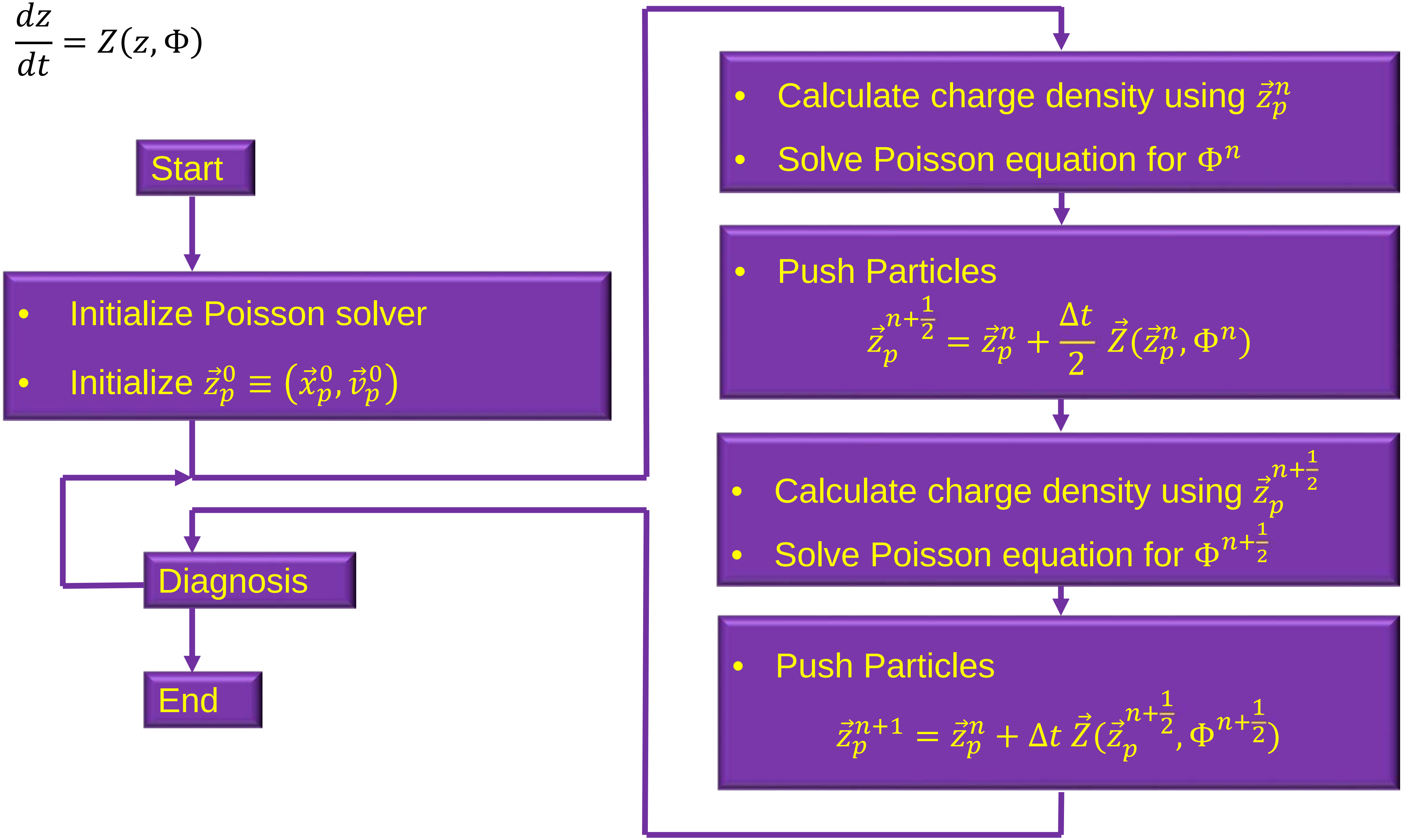
$$\Delta v = \alpha\Delta t + 2\sqrt{3}\,(R-0.5)\sqrt{2\beta\Delta t}$$

R is a random number in [0, 1]

J. Grasman and O.A. van Herwaarden,
“Asymptotic Methods for the Fokker-Planck Equation and the Exit Problem in Applications”, Springer

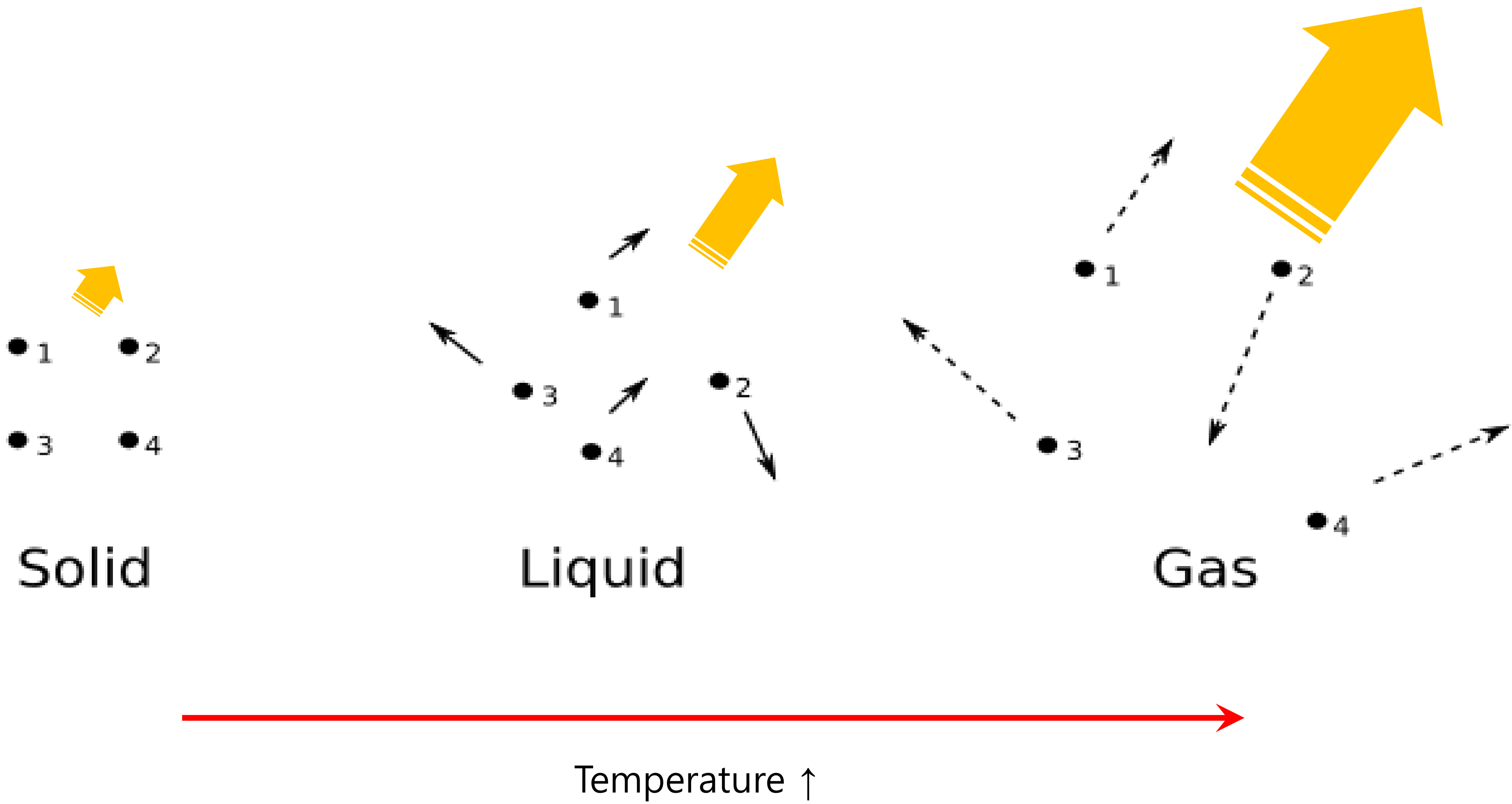
Example: 2nd order Runge-Kutta

$$\frac{dz}{dt} = Z(z, \Phi)$$



Numerical Issues in PIC Simulation

N-Particle System



N-Particle System

- Fourier representation of potential and distribution function

$$\Phi(x) = \sum_k e^{ikx}\widetilde{\Phi}_k, \qquad \widetilde{\Phi}_k = \frac{1}{L}\int dx e^{-ikx}\Phi(x)$$

$$f(x,v,t) = \sum_p w_p \delta(x - x_p)\delta(v - v_p), \qquad \tilde{f}_k(t) = \frac{1}{L}\int dx e^{-ikx} f(x,v,t) = \frac{1}{L}\sum_p w_p e^{-ikx_p}\delta(v - v_p)$$

- Poisson equation in Fourier space

$$-\nabla^2\Phi = 4\pi\rho = 4\pi e\int dv f$$

$$k^2\widetilde{\Phi}_k = \frac{4\pi e}{L}\sum_p w_p e^{-ikx_p}$$

- Apply a filter S_k on RHS

$$k^2\widetilde{\Phi}_k = \frac{4\pi e}{L} S_k \sum_p w_p e^{-ikx_p}$$

$$\therefore \left|\widetilde{\Phi}_k\right|^2 = \left(\frac{4\pi e}{Lk^2}\right)^2 S_k^2 \sum_p \sum_{p'} w_p w_{p'} e^{-ik(x_p - x_{p'})}$$

N-Particle System

$$\left|\tilde{\Phi}_k\right|^2 = \left(\frac{4\pi e}{Lk^2}\right)^2 S_k^2 \sum_p \sum_{p'} w_p w_{p'} e^{-ik(x_p - x_{p'})}$$

- For randomly scattered particles and $N \gg 1$, we can simplify RHS

$$\left|\tilde{\Phi}_k\right|^2 \approx \left(\frac{4\pi e}{Lk^2}\right)^2 S_k^2 \sum_p w_p^2 = \left(\frac{4\pi e}{Lk^2}\right)^2 S_k^2 \langle w^2 \rangle N$$

$$\left|\frac{e\tilde{\Phi}_k}{T}\right|^2 \approx \left(\frac{4\pi e^2}{LTk^2}\right)^2 S_k^2 \langle w^2 \rangle N = \left(\frac{4\pi n e^2}{T}\right)^2 \frac{1}{n^2 L^2 k^4} S_k^2 \langle w^2 \rangle N = \frac{S_k^2}{\lambda_D^4 k^4} \frac{\langle w^2 \rangle}{N}$$

$$\frac{fluctuation\ energy}{thermal\ energy} \sim \frac{1}{\sqrt{N}}$$

Dielectric Response Function and Fluctuation Dissipation Theorem

- Suppose we put an external test charge

$$\hat{\rho}_{ext}(x,t) = \sum_{k,\omega} \rho_{ext}(k,\omega) \exp[i(kx - \omega t)]$$

- Then, plasma will respond to this external perturbation and generate density fluctuation $\rho(k,\omega)$
- If we write the total charge density as $\rho_{tot}(k,w)$, dielectric response function is defined as

$$\rho_{tot}(k,\omega) = \rho_{ext}(k,\omega) + \rho(k,\omega) \equiv \frac{\rho_{ext}(k,\omega)}{\epsilon(k,\omega)}, \qquad \epsilon(k,\omega)\rho_{tot}(k,\omega) = \rho_{ext}(k,\omega)$$

- Fluctuation Dissipation Theorem tells us how system responds to small fluctuations and provides useful information for fluctuation spectrum

$$\frac{L}{2\pi}|\delta E(\omega,k)|^2 = -\frac{T}{\omega}\, Im \frac{1}{\epsilon(k,\omega)}$$

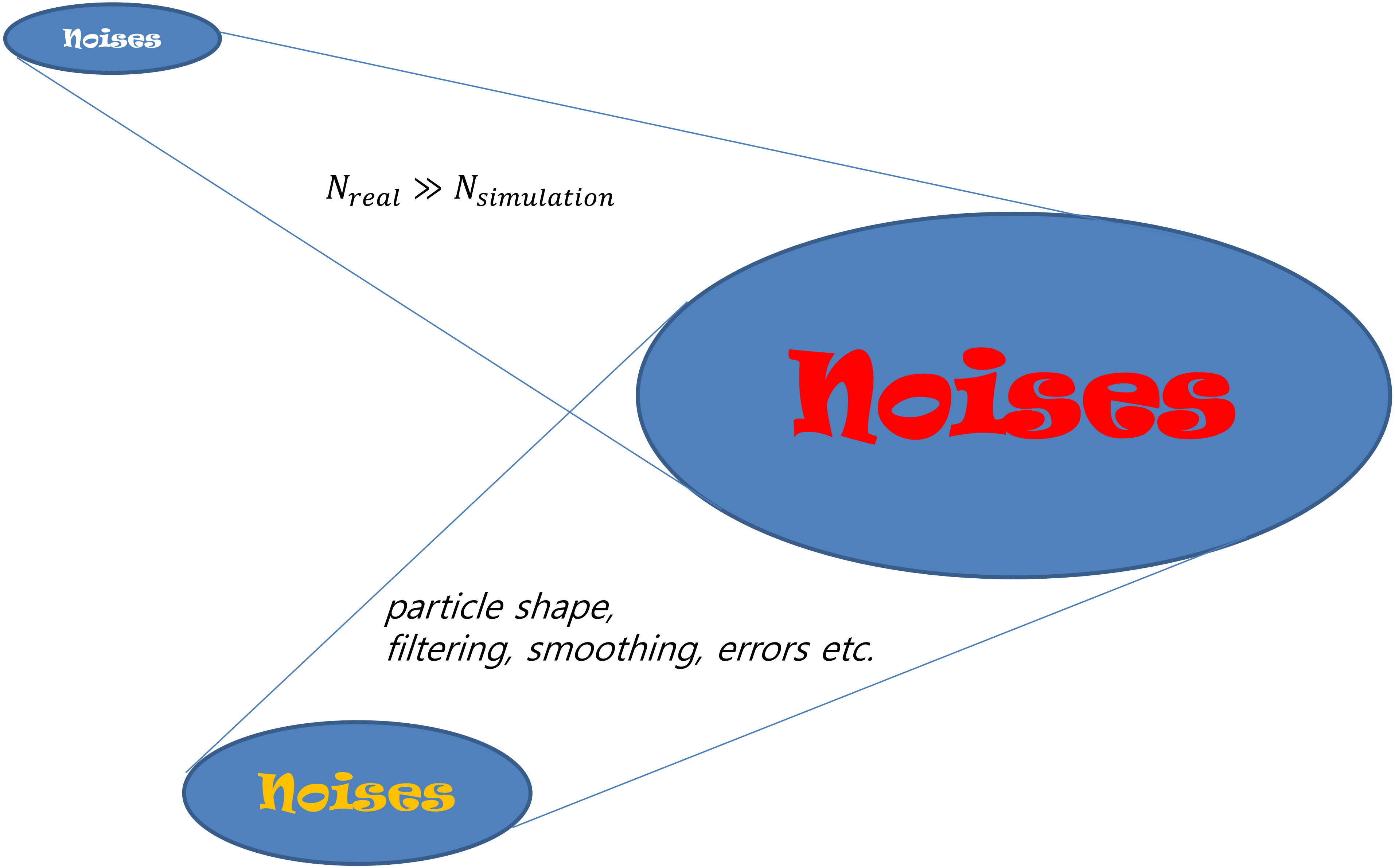
➔ Lower bound of **fluctuation (or noise)** for N-body system

Fluctuation and Dissipation Theorem: Implication for PIC simulation

- PIC simulation employs finite number of particles, actually far fewer than the real number of particles (e.g. in medium fusion device $N_{real} \sim 10^{21} \gg N_{sim} = 10^{9} \sim 10^{12}$)
- Fluctuation (or noise) from simulation should be much bigger than physical ones
- However, we have numerical tools to control too big fluctuation (or noise):
  - Number of particles
  - Particle shape function S_k
  - Spatio-temporal discretization $\Delta x, \Delta t$

$$\left|\frac{e\tilde{\Phi}_k}{T}\right|^2 \approx \frac{S_k^2}{\lambda_D^4 k^4}\frac{\langle w^2 \rangle}{N}$$

- The strategy is to employ these to suppress noise to a level not to affect key physics


Noises
$N_{real} \gg N_{simulation}$
Noises
particle shape,
filtering, smoothing, errors etc.
Noises

Summary

- Reduced kinetic models for magnetized plasma
  - 5D gyrokinetic, 4D bounce-averaged kinetic, 3D fluid with kinetic closure
  - These enable us to perform kinetic simulation with reasonable computing cost
- Numerical methods for kinetic simulation of magnetized plasma
  - Particle-in-Cell method
  - Fluctuation dissipation theorem to understand discrete particle noise
- Verification and benchmark test are necessary, and experimental validation should be the next step → very active area of on-going research in fusion