Introduction to particle-in-cell simulation of plasmas

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Particle-in-cell simulation of plasmas

- Motivations for direct numerical simulation
  - lack of analytical theory: nonlinear problem, large number of degrees of freedom
  - beyond the validity regime of analytic theory
- Classes of direct numerical simulations
  - kinetic: particle-in-cell (Lagrangian), Vlasov (Eulerian, continuum), Monte-Carlo, molecular dynamics simulation
  - fluid: MHD, two fluid, gyrofluid
  - hybrid
- Advantages of particle-in-cell simulation
  - faithful for kinetic effects: resonance, trapping
  - computational: explicit, local, scalable on parallel computers

Outline

- Particle simulation method
- Effects of spatial grid and finite size particle
- Effects of finite time step
- Kinetic theory of numerical noise
- Perturbative (δf) simulation method
- Other topics (not covered): collision, implicit scheme, quiet start, multipole model, orbit-average scheme

where

$$C = -\frac{q}{m}\langle[(\tilde{\mathbf{E}} - \mathbf{E}) + \mathbf{v} \times (\tilde{\mathbf{B}} - \mathbf{B})] \cdot \nabla_{\mathbf{v}}(\tilde{f} - f)\rangle \qquad (2.7)$$

represents the discreteness effects of point particle, i.e., collisions. In ideal plasmas, we can neglect the collisions when we are only interested in collective phenomena. Then the evolution of plasma is governed by the Vlasov equation:

$$\frac{\partial}{\partial t}f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q}{m}[\mathbf{E} + \mathbf{v} \times \mathbf{B}] \cdot \nabla_{\mathbf{v}} f = 0 \qquad (2.8)$$

The Vlasov equation is closed by the Maxwell equation,

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \sigma && (2.9) \\ \nabla \times \mathbf{B} &= \frac{\partial \mathbf{E}}{\partial t} + \mathbf{j} && (2.10) \\ \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} && (2.11) \\ \nabla \cdot \mathbf{B} &= 0 && (2.12) \end{aligned}$$

the charge density and current density is obtained from the appropriate moments of the distribution function,

$$\begin{aligned} \sigma &= \sum_s q \int f d^3\mathbf{v} && (2.13) \\ \mathbf{j} &= \sum_s q \int \mathbf{v} f d^3\mathbf{v} && (2.14) \end{aligned}$$

Particle simulations solve Vlasov-Maxwell system, Eqs. 2.8 - 2.14 using characteristic method.

Particle Simulation Method

Particle simulation

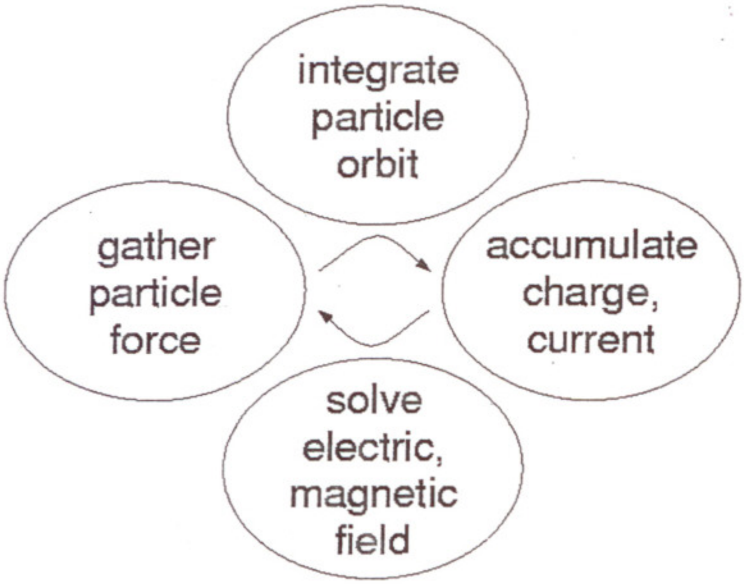
In particle simulation, we calculate the trajectories, using Eqs. 2.2 and 2.3, of a group of particles. The density function of these particles, Eq 2.1, obviously evolves according to Eq. 2.4. When collision is suppressed, we are simulating the Vlasov equation, Eq. 2.8.

- Vlasov equation is solved in Lagrangian coordinates
  - nonlinear PDE becomes linear ODE

The charge density and current density, Eq. 2.13 and 2.14, are deposited on a mesh of spatial grids. The self-consistent electric and magnetic field are then calculated on the grids using Eqs. 2.9-2.12

- Maxwell equations are solved in Eulerian coordinates
  - linear PDE
  - number of computation $\propto N_g \log N_g$ grid
- Collisions can be treated as sub-grid phenomena using Monte-Carlo method

Computational circle



We use one-dimensional electrostatic simulation as an example to illustrate the detailed procedure.

- Maxwell equation reduces to Poisson equation

$$\nabla^2\phi = -\sigma \tag{3.1}$$

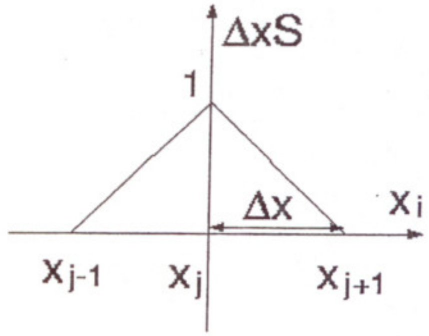
Deposition of particle charge

We need a scheme to calculate the charge density on the discrete spatial grids from the continuous particle position

- nearest grid point (NGP), linear interpolation (CIC,PIC), • • •

In 1-D linear interpolation scheme, the assignment $\sigma_j(x_i)$ of a point particle charge at x_i to a grid point x_j is

$$\sigma_j(x_i) = q \quad \max[0, 1 - \frac{|x_j - x_i|}{\Delta x}] \tag{3.2}$$



The observed density $\sigma_j(x_i)$ for a point particle by the grids suggests that the particle has a nonzero width of charge cloud, or a finite size particle.

- particles can pass through each other, short range collision eliminated

The charge density of the cloud is denotes as $qS(x_j\text{-}x_i)$, where the shape function S is,

$$S(x_j - x_i) = \max[0, 1 - \frac{|x_j - x_i|}{\Delta x}] \tag{3.3}$$

Summing up all particle, the charge density on the grid j is,

$$\sigma_j(x_j) = \int dx S(x_j - x)\sigma_i(x) \tag{3.4}$$

where the continuous particle charge density is

$$\sigma_i(x) = \sum_s \sum_i q\delta(x - x_i) \tag{3.5}$$

The same interpolation scheme is also used for gathering electric field on particle position x_i from the grids, i.e,

$$E_i(x_i) = \int dx S(x - x_i) E_j(x) \tag{3.6}$$

Since these relation are convolution, we take Fourier transform of S,

$$S(k) = \int e^{-ikx} S(x) dx \tag{3.7}$$

Then

$$\sigma_j(k) = S(k)\sigma_i(k) \tag{3.8}$$

$$E_i(k) = S(-k)E_j(k) \tag{3.9}$$

For linear interpolation,

$$S(k) = (\frac{\sin\theta}{\theta})^2, \qquad \theta = \frac{k\Delta x}{2} \tag{3.10}$$

Solution of Poisson equation

For periodic system, Fast Fourier Transform (FFT) is commonly used to solve the Poisson equation, Eq 3.1,

$$\phi_k = \frac{\sigma_k}{k^2} \qquad \text{or} \qquad E_k = \frac{i\sigma_k}{k} \tag{3.11}$$

where 1/N

$$\phi_k = \frac{\Delta x}{L} \sum_{j=0}^{N_g - 1} \phi(x_j) e^{-ikx_j} \tag{3.12}$$

The inverse transform gives the desired potential in real space,i.e,

$$\phi(x_j) = \sum_{n=-N_g/2}^{n=N_g/2} \phi_k e^{ink_0 x_j} \tag{3.13}$$

where $k_0 = 2\pi/L$ is the lowest wave vector of the system.

[illegible]

Finite difference and finite element are often used in more complicated geometry. Let's examine the accuracy of 1-D finite difference for solving Eq. 3.1.

$$E_j = \frac{\phi_{j-1} - \phi_{j+1}}{2\Delta x} \tag{3.14}$$

$$\frac{\phi_{j-1} - 2\phi_j + \phi_{j+1}}{(\Delta x)^2} = -\sigma_j \tag{3.15}$$

after Fourier transform,

$$E_k = ik(\frac{\sin k\Delta x}{k\Delta x})\phi_k \tag{3.16}$$

$$\phi_k = \frac{\sigma_k}{k^2}(\frac{\sin k\Delta x/2}{k\Delta x/2})^2 \tag{3.17}$$

We recover the exact solution in the limit of $k\Delta x \to 0$

Integration of particle orbit

Leap-frog method is a popular choice for time stepping because of its simplicity and accuracy. We integrate an oscillator to illustrate the procedure and accuracy.

$$\begin{cases} \frac{dx}{dt} = v \\ \frac{dv}{dt} = -\omega_0^2 x \end{cases} \tag{3.18}$$

In finite difference form, it becomes

$$\begin{cases} \frac{x_t - x_{x-\Delta t}}{\Delta t} = v_{t-\Delta t/2} \\ \frac{x_{x+\Delta t} - x_t}{\Delta t} = v_{t+\Delta t/2} \\ \frac{v_{t+\Delta t/2} - v_{t-\Delta t/2}}{\Delta t} = -\omega_0^2 x_t \end{cases} \tag{3.19}$$

So we have

$$\frac{x_{t+\Delta t} - 2x_t + x_{t-\Delta t}}{(\Delta t)^2} = -\omega_0^2 x_t \tag{3.20}$$

Assuming

$$x_t = Ae^{-i\omega t} \tag{3.21}$$

then we have

$$\sin(\frac{\omega\Delta t}{2}) = \pm\frac{\omega_0 t}{2} \tag{3.22}$$

The solution $\omega = \omega_0 + \delta\omega + i\gamma$ is,

$$\begin{cases} \frac{\delta\gamma}{\omega_0} = \frac{1}{6}(\frac{\omega_0\delta t}{2})^2 \\ \frac{\gamma}{\omega_0} = 0 \qquad \text{for} \qquad \frac{\omega\Delta t}{2} \le 1 \end{cases} \tag{3.23}$$

?

- second order accuracy
- stable for $\omega\Delta t/2 \le 1$

Leap-frog scheme is not applicable in more complicated situation, e.g., collisions of guiding center motion. A more general, but less accurate method is Runge-Kutta method. We can redo the oscillator problem using 2nd order Runge-Kutta method. First step finite difference equation is,

$$\begin{cases} x_{t+\Delta t/2} - x_t = \frac{1}{2}\Delta t v_t \\ v_{t+\Delta t/2} - v_t = -\frac{1}{2}\omega_0^2\Delta t x_t \end{cases} \tag{3.24}$$

Second step equation is,

$$\begin{cases} x_{t+\Delta t} - x_t = \Delta t v_{t+\Delta t/2} \\ v_{t+\Delta t} - v_t = -\omega_0^2\Delta t x_{t+\Delta t/2} \end{cases} \tag{3.25}$$

Follow similar procedure in deriving Eq. 3.22, we have the dispersion relation for 2nd Runge-Kutta method,

$$(\omega\Delta t)^2 - 4\sin^2(\frac{\omega\Delta t}{2}) = -\frac{1}{4}(\omega\Delta t)^4 e^{i\omega t} \tag{3.26}$$

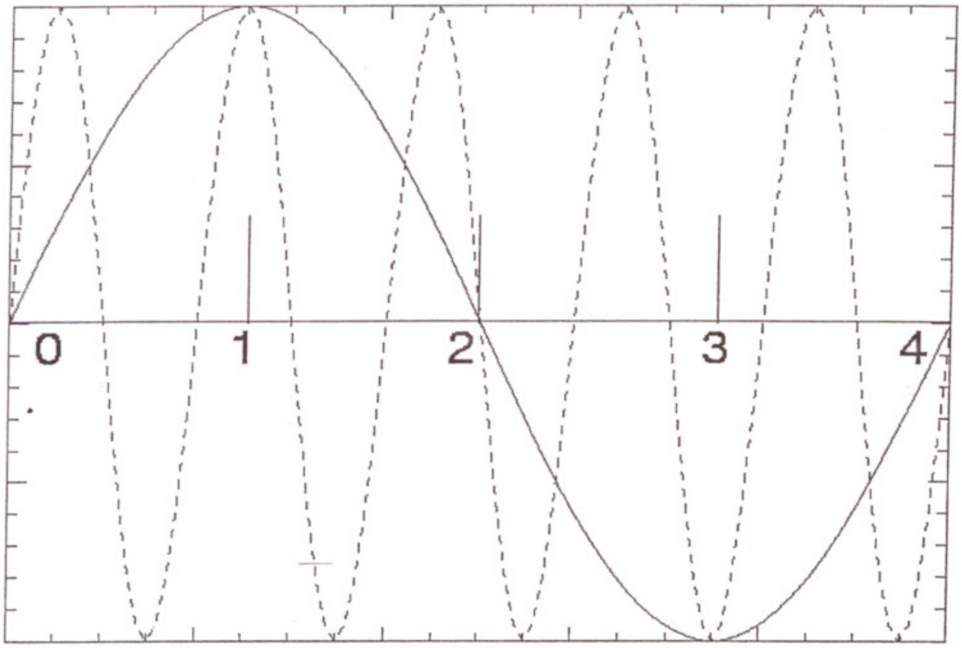
For $\omega\Delta t/2 \ll 1$, we have

$$\frac{\gamma}{\omega_0} = (\omega_0\Delta t/2)^3 \tag{3.27}$$

i.e., there is absolute numerical instability.

Effects of Discretization

Aliasing



Effects of Spatial Grids

The particle charge cloud density in Fourier space as observed by the grids is described by Eq. 3.8. Here $\sigma_j(k)$ contains all harmonics, i.e., $-\infty < k < +\infty$.

The grid charge density is

$$\sigma_g(x_j) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi}\sigma_j(k)e^{ikx_j} \qquad (4.1)$$

$$= \int_{-k_g/2}^{k_g/2} \frac{dk}{2\pi}e^{ikx_j} \sum_{p=-\infty}^{+\infty} \sigma_j(k_p) \qquad (4.2)$$

where k_g=k-pk_g, $k_g = 2\pi/\Delta x$. Thus the Fourier modes $\sigma(k)$ of the grid charge density $\sigma_g(x_j)$ is,

$$\sigma_g(k) = \sum_p S(k_p)\sigma_i(k_p) \qquad (4.3)$$

Therefore the spectral density with frequency higher than the Nyquist frequency is falsely translated into the frequency range $-k_c < k < k_c$, i.e., aliasing effects. This is due to the fact that we use finite sampling points x_j's to represent continuous function $\sigma_i(x_i)$.

We examine the dispersion relation of a Maxwellian plasma.

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + E\frac{\partial f}{\partial v} = 0 \tag{4.4}$$

Let

$$f = F_m + \delta f, \qquad \delta f = \delta f_k e^{ikx} \tag{4.5}$$

then particle cloud charge is,

$$\sigma_k = \sum_s q\phi \int k\frac{\partial f_0/\partial v}{\omega - kv}dv \tag{4.6}$$

The corresponding grid charge is

$$\sigma_g(k) = \sum_p S(k_p)\sigma_{\cancel{g}}(k_p) \qquad \sigma(k) \tag{4.7}$$

If we solve Poisson equation using FFT, $k_p = k - p\frac{2\pi}{\Delta x}$

$$k^2\phi(k) = \sigma_g(k) \tag{4.8}$$

$$k^2\phi(k) = \sigma_g(k) = \sum_p S(k_p)\sigma(k_p) = \sum_p S(k_p)\phi S(-k_p)\int k_p\frac{\partial f/\partial v}{\omega - k_p v}dv \tag{4.9}$$

Using Eq. 3.9, we have the linear dispersion relation,

$$\epsilon(\omega, k) = 1 - \frac{\omega_p^2}{2k^2v_t^2}\sum_p |S|^2\frac{kk_p}{k_p^2}Z\left(\frac{\omega}{\sqrt{2}|k_p|v_t}\right) = 0 \tag{4.10}$$

where Z is plasma dispersion function. The principal effects of aliasing is coupled perturbations of different wavelength. In particular, short wavelength (smaller than grid spacing) fluctuations can drive longer wavelength mode. For weakly damped modes, Performing Landau integral yields,

$$\mathrm{Im}\epsilon = -\pi\frac{\omega_p^2}{k^2}\sum_p S^2(k_p)\frac{kk_p}{k_p^2}\frac{\partial f_0(\omega/k_p)}{\partial v} \tag{4.11}$$

Numerical solution shows that $\mathrm{Im}\epsilon < 0$, i.e., nonphysical instability, for $\Delta x \sim \lambda_D$. The instability arise when and undamped mode, $\omega/k \gg v_t$, is coupled through aliasing to a shorter mode which has wave particle resonance $\omega/k_p \sim v_t$. grid size restriction: $\Delta x < \lambda_D$

Effects of Finite Time Step

Linear dispersion relation with finite time step can be obtained by calculating the deflection of particle from unperturbed orbit caused by an external field

$$\delta E(x,t) = E_k e^{i(kx-\omega t)} \tag{4.12}$$

We use Leap-frog method as an example to study the effects of finite time step.

$$v_{n+1/2} - v_{n-1/2} = \Delta t a_n x_{n+1} - x_{n-1} = \Delta t v_{n+1/2} \tag{4.13}$$

Linearized

$$x = x^{(0)} + \delta x \tag{4.14}$$

$$\delta x_{n+1} - 2\delta x_n + \delta x_{n-1} = \Delta t^2 \frac{q}{m} E e^{-i\omega_d t_n} \tag{4.15}$$

where $\omega_d = \omega - kv^{(0)}$ is the Doppler shifted frequency, Assuming $\boldsymbol{x} = \boldsymbol{x} e^{-i\omega_d t}$,

$$\delta x(x_n^{(0)}, v_n^{(0)}, t_n) = [\frac{\Delta t/2}{\sin \omega_d \Delta t/2}]^2 \frac{q}{m} \delta E \tag{4.16}$$

Dipole density

$$P(x,t) = n_0 q \int dv f_0(v) \delta x(x^{(0)}, v^{(0)}, t) \tag{4.17}$$

Charge density

$$-\nabla^2 \phi = \delta\sigma = -\nabla \cdot \mathbf{P} \tag{4.18}$$

Dispersion relation

$$\epsilon = 1 + \frac{\omega_p^2}{k^2} \int dv k \frac{\partial f_0}{\partial v} \sum_{-\infty}^{+\infty} \frac{1}{\omega - kv - q\omega_g} \tag{4.19}$$

where $\omega_g = 2\pi/\Delta t$ is the Nyquist frequency. This is the aliasing on the temporal grid. Numerical instability can occur when $\omega_p\Delta t > 1$, similar to the problem of integrating the simple oscillator.

- time step restriction $\omega_p\Delta t < 1$ for numerical stability
- $k v_{\mathrm{th}}\Delta t < 1$ for accuracy in plasma response

Dispersion relation with both spatial grids and finite time step

$$\epsilon = 1 + \frac{\omega_p^2}{k^2}\sum_p S^2(k_p)\int dv k_p \frac{\partial f_0}{\partial v}\sum_q \frac{1}{\omega - k_p v - q\omega_g} \tag{4.20}$$

Kinetic Theory of Numerical Noise

Linear response of the plasmas to a external test charge,

$$\phi(k,\omega) = \frac{\sigma_e}{k^2\epsilon} \tag{4.21}$$

where the dielectric function is define by Eq. 4.20

Zero order position of particle i at time $t_n = n\Delta t$,

$$x_n^{(0)} = x_0 + v t_n \tag{4.22}$$

and the Fourier transform number density

$$n^0(k,\omega) = 2\pi\sum_i e^{(-ikx_0)}\sum_q \delta(\omega - q\omega_g) \tag{4.23}$$

Density autocorrelation function,

$$(\sigma^2)_{k,\omega} = \frac{2\pi\sigma_0 q}{|\epsilon(k,\omega)|^2}\sum_p S^2(k_p)\int dv f_0(v)\sum_q \delta(\omega - k_p v - q\omega_g) \tag{4.24}$$

Energy density spectrum in a energy conserving model is

$$(\frac{1}{2}\sigma\phi)_{k,\omega} = \frac{(\sigma^2)_{k,\omega}}{2k^2} \tag{4.25}$$

Spatial spectrum

$$(\frac{1}{2}\sigma\phi)_k = \int \frac{d\omega}{2\pi}(\frac{1}{2}\sigma\phi)_{k,\omega} = \frac{T}{2}\frac{\sum S^2}{\sum S^2 + k^2\lambda_D^2} \qquad (4.26)$$

Enhanced numerical noise

$$\frac{\delta n}{n} = \frac{1}{\sqrt{N_p}k\lambda_D} \qquad (4.27)$$

- Required number of particle: noise (thermal fluctuation level) smaller than signal (turbulence level)

Perturbative δf Simulation Method

Heuristic derivation of δf method

Rewrite Vlasov equation, Eq. 2.8,

$$\frac{df}{dt} = 0 \qquad (5.1)$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} + \frac{q}{m}[\mathbf{E} + \mathbf{v}\times\mathbf{B}]\cdot\nabla_{\mathbf{v}} \qquad (5.2)$$

Separate distribution function $f = f_0 + \delta f$

f_0: equilibrium (``known") part; δf perturbed part

Define particle weight $w = \delta f / f$,

$$w_i = w(\mathbf{x}_i, \mathbf{v}_i) \qquad (5.3)$$

$$\delta f = \sum_i w_i \delta(\mathbf{x} - \mathbf{x}_i)\delta(\mathbf{v} - \mathbf{v}_i), \qquad (5.4)$$

$$\frac{1}{f_0+\delta f} = \frac{(f_0-\delta f)}{f_0} - (1-w) = \frac{df_0}{dt}$$

Weight evolution equation

$$\frac{dw}{dt} = \frac{1}{f}\frac{d\delta f}{dt} = -(1-w)\frac{df_0}{f_0 dt} \tag{5.5}$$?

For 1-D electrostatic simulation,

$$\frac{dw}{dt} = (1-w)\frac{qvE}{T} \tag{5.6}$$?

Monte Carlo interpretation of particle simulation

The particles in the simulation can be interpreted as markers of the phase space.

Each marker *i* represents a volume element $\Delta\tilde{A}_i$ in phase space and evolves according to the dynamics of real particles. The marker information can be used to calculate moments of distribution function.

(TO BE COMPLETED)

Kinetic theory of sampling noise

Intensity of discrete particle noise reduced by $(\delta f/f)^2$

(TO BE COMPLETED)

Split Weight Scheme

Split Weight Perturbative (δf) Particle Simulation Scheme

Let $f_e = f_{0e} + (e\phi/T_e)f_{0e} + \delta h_e$,

$$\frac{d\delta h_e}{dt} = -\frac{\partial}{\partial t}\frac{e\phi}{T_e}f_{0e} + \frac{\mathbf{v}}{2}\cdot\left[\frac{\partial}{\partial \mathbf{x}}\left(\frac{e\phi}{T_e}\right)^2\right]f_{0e} \tag{5.7}$$

For $w^{NA} = \delta h_e/f$,

$$\frac{dw^{NA}}{dt} = \frac{1-w^{NA}}{1+e\phi/T_e}\left[-\frac{\partial}{\partial t}\frac{e\phi}{T_e} + \frac{\mathbf{v}}{2}\cdot\frac{\partial}{\partial \mathbf{x}}\left(\frac{e\phi}{T_e}\right)^2\right]. \tag{5.8}$$

Modified Poisson's equation and Charge Conservation

$$\left(\lambda_D^2 \nabla^2 - 1\right) \frac{e\phi}{T_e} = \int \delta h_e d\mathbf{v} - \delta n_i, \tag{5.9}$$

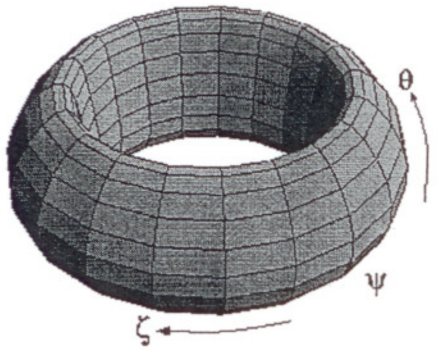
$$\lambda_D^2 \nabla^2 \left(\frac{\partial}{\partial t} \frac{e\phi}{T_e}\right) = -\frac{\partial}{\partial \mathbf{x}} \cdot \int \mathbf{v} \delta h_e d\mathbf{v}, \tag{5.10}$$

$$\delta h_e = \sum_i w_j^{NA} \delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{v} - \mathbf{v}_i), \tag{5.11}$$

Gyrokinetic Simulation of Magnetized Plasmas

Introduction

- In fusion experiment, gas of charged particles (plasma) is created and heated to 10^8 F
- Plasma is confined by magnetic field which forms nested surfaces in a fusion device (tokamak)



- Electric field produced by these charged particles is unstable: fluctuation grows exponentially
- Charged particle motion becomes chaotic: confinement of plasma is lost
- The ability to control turbulence is important in order to make fusion a long term energy source

- Time scale (s)

$$10^{-12} \quad \leftrightarrow \quad 10^{-8} \quad \leftrightarrow \quad 10^{-5} \quad \leftrightarrow \quad 1$$

$$plasma\ oscillation \quad gyromotion \quad fluctuation \quad confinement$$

- Length scale (m)

$$10^{-5} \quad \leftrightarrow \quad 10^{-3} \quad \leftrightarrow \quad 10^{-2} \quad \leftrightarrow \quad 1$$

$$Debye\ length \quad gyroradius \quad eddy\ size \quad device\ size$$

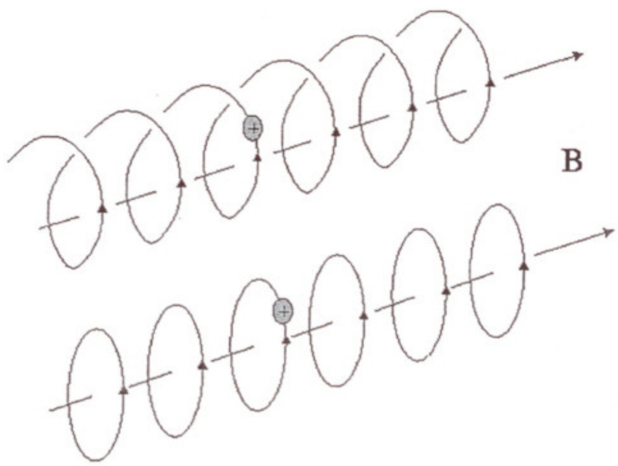
Nonlinear gyrokinetic theory

- Low frequency, short wavelength microturbulence believed to be responsible for transport
- Gyrokinetic ordering

$$\frac{\omega}{\Omega} \sim \frac{\rho}{L} \sim k_{||}\rho \sim \frac{e\Phi}{T} \sim \epsilon$$

$$k_{\perp}\rho \sim 1$$

We gyrophase-average Vlasov-Maxwell equations for low frequency microinstabilities. The spiral motion of a charged particle is modified as a rotating charged ring subject to guiding center electric and magnetic drift motion as well as parallel acceleration.



We arrive at the gyrokinetic Vlasov-Poisson system for simple (ion-electron) plasmas in slab geometry which (by neglecting nonlinear polarization effect and terms of the order of $\vartheta(k_\perp \rho)^4$) takes the form of

$$\frac{\partial f}{\partial t} + v_\| \hat{b} \cdot \frac{\partial f}{\partial \mathbf{R}} - \frac{q}{m\Omega} \frac{\partial \bar{\Phi}}{\partial \mathbf{R}} \times \hat{b} \cdot \frac{\partial f}{\partial \mathbf{R}} - \frac{q}{m} \frac{\partial \bar{\Phi}}{\partial \mathbf{R}} \cdot \hat{b} \frac{\partial f}{\partial v_\|} = 0 \,, \qquad (6.1)$$

and

$$\frac{\tau}{\lambda_D^2}(\Phi - \tilde{\Phi}) = 4\pi e(\bar{n}_i - n_e) \,. \qquad (6.2)$$

Here, $F(\mathbf{R}, \mu, v_\|, t)$ is the gyrocenter distribution function, which is independent of gyrophase, $\mathbf{R} \equiv \mathbf{x} - \rho$, $\rho \equiv -v_\perp \times \hat{\mathbf{b}}/\Omega$, $\Omega \equiv qB/mc$, $\hat{\mathbf{b}} \equiv \mathbf{B}/B$, $\mathbf{B}$ is the external magnetic field, $\mu \equiv v_\perp^2/2$, $\mathbf{v}_\| = v_\| \hat{\mathbf{b}}$, q is the signed charge, $\lambda_D \equiv \sqrt{T_e/4\pi n_0 e^2}$ is the Debye length, $\tau \equiv T_e/T_i$, subscripts e and i denote species, $\Phi(\mathbf{x}, t)$ is the electrostatic potential, $\bar{\Phi}$ represents the gyrophase averaged potential, and $\tilde{\Phi}$ is defined as the second gyrophase-averaged potential. Specifically,

$$\bar{\Phi}(\mathbf{R}) = \frac{1}{2\pi} \int \Phi(\mathbf{x}) \delta(\mathbf{x} - \mathbf{R} - \rho) d\mathbf{x} d\alpha \,, \qquad (6.3)$$

where α is the gyrophase angle and $\mathbf{R}$ is held fixed in the integration, and

$$\tilde{\Phi}(\mathbf{x}) = \frac{1}{2\pi} \int \bar{\Phi}(\mathbf{R}) f_{Mi}(\epsilon \mathbf{R}, \mu, v_\|) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} d\mu dv_\| d\alpha \qquad (6.4)$$

with $\mathbf{x}$ now held fixed in the integration. In Eq. (6.4), F_{Mi} is assumed to be Maxwellian in $v_\perp$ and spatially slowly varying, i.e., $\epsilon \ll 1$. The gyrophase averaged ion number density is defined as

$$\bar{n}_i(\mathbf{x}) = \frac{1}{2\pi n_0} \int f_i(\mathbf{R}) \delta(\mathbf{R} - \mathbf{x} + \rho) d\mathbf{R} d\mu dv_\| d\alpha, \qquad (6.5)$$

and, likewise, n_e is the electron number density from F_e in the limit of $\rho \to 0$. The background number density n_0 comes from F_e assuming $\epsilon \mathbf{x} \approx \epsilon \mathbf{R}$.

Numerical properties of gyrokinetic plasmas

Numerical Properties of a Gyrokinetic Plasma

Grid spacing imposed by cold electron response

$$\Delta x < \rho_s; \quad (\rho_s/\lambda_D \approx 100) \tag{6.6}$$

$(\omega_H \equiv \frac{k_\|}{k_\perp}\frac{\lambda_D}{\rho_s}\omega_{pe}) = \frac{k_y}{k_\perp}(\frac{m_i}{m_e})^{1/2}\Omega_i$

Time step imposed by cold electron response

$$\omega_H \Delta t \ll 1; \quad (\omega_{pe}/\omega_H \approx 1000) \tag{6.7}$$

Time step restricted by streaming of thermal electrons:

$$k_{||} v_{te} \Delta < 1 \tag{6.8}$$

Noise enhanced by ω_H:

$$\delta n/n \approx 1/\sqrt{N}(k\rho_s). \tag{6.9}$$

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Gyrokinetic particle simulation

Debye shielding is replaced by polarization shielding in the gyrokinetic model giving rise to quasineutral simulation,

$$\nabla^2 \phi = -4\pi\rho \quad \Rightarrow \quad (\frac{\rho_s}{\lambda_D})^2 \nabla_\perp^2 \phi = -4\pi e(\overline{n}_i - n_e), \tag{6.10}$$

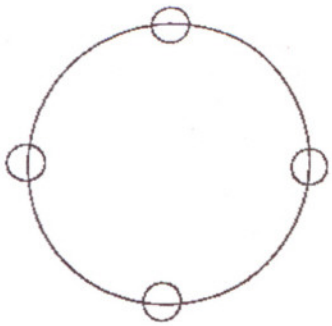
Equations of Motion

$$\frac{d\mathbf{R}}{dt} = U\hat{\mathbf{b}} + \mathbf{v}_d - \frac{c}{B}\frac{\partial\overline{\phi}}{\partial\mathbf{R}} \times \hat{\mathbf{b}}, \quad \frac{\mu}{B} \equiv \frac{v_\perp^2}{2B} = const., \tag{6.11}$$

$$\frac{dU}{dt} = -[\hat{\mathbf{b}} + \frac{U}{\Omega}\hat{\mathbf{b}} \times (\hat{\mathbf{b}} \cdot \frac{\partial}{\partial\mathbf{R}})\hat{\mathbf{b}}] \cdot (\mu\frac{\partial}{\partial\mathbf{R}}\ln B + \frac{q}{m}\frac{\partial\overline{\phi}}{\partial\mathbf{R}}), \tag{6.12}$$

Gyroaveraging

The charge ring is further approximated by 4-point average, valid for $k_\perp \rho_i \leq 2$.



(TO BE COMPLETED

Gyrokinetic Poisson equation solver

The gyrophase-averaged distribution function is a function of gyrocenter variables, i.e., $F = F(\mathbf{R}, \mu, v_{\|}, t)$, while the electrostatic potential is defined in the particle or laboratory coordinates, $\Phi = \Phi(\mathbf{x}, t)$. Thus, to solve the gyrokinetic Vlasov-Poisson system, one has to develop a numerical algorithm to expedite the transformation. In the Fourier space, the coordinate transformation can simply be carried out by using

$$\Phi(\mathbf{x}) = \sum_k \Phi_k e^{i\mathbf{k}\cdot\mathbf{x}} \tag{6.13}$$

and applying it to Eq. (6.3) to obtain

$$\bar{\Phi}(\mathbf{R}) = \sum_k \Phi_k J_0(\frac{k_\perp v_\perp}{\Omega}) e^{i\mathbf{k}\cdot\mathbf{R}}, \tag{6.14}$$

where J_0 is the ordinary Bessel function, and

$$\int_0^{2\pi} exp(\pm i\mathbf{k}\cdot\rho) d\alpha/2\pi = J_0(k_\perp v_\perp/\Omega) \tag{6.15}$$

is utilized in this transformation. Likewise, $\tilde{\bar{\Phi}}$in Eq. (6.4) can be calculated in the Fourier space by assuming a spatially independent Maxwellian distribution function for the ion species and it becomes

$$\tilde{\Phi}(\mathbf{x}) = \sum_k \Phi_k \Gamma_0(b) e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{6.16}$$

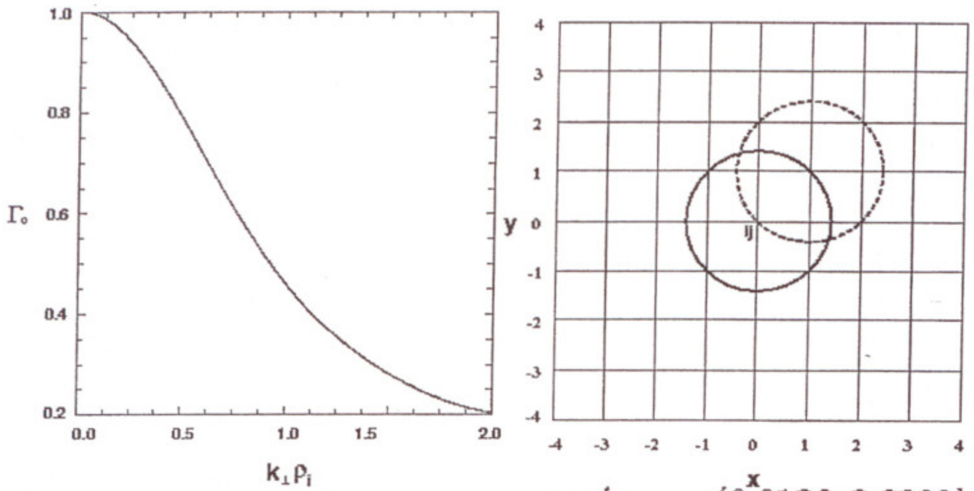
where $\Gamma_0(b) = I_0(b)e^{-b}$, $b \equiv (k_\perp \rho_{th})^2$, $\rho_{th} \equiv \sqrt{T_i/m_i}/\Omega_i$, and I_0 is the modified Bessel function. The term Γ_0 comes from

$$\Gamma_0(b) = \int J_0^2\left(\frac{k_\perp v_\perp}{\Omega}\right) f_{mi}(\mu) d\mu \,, \tag{6.17}$$

which is the result of two gyrophase averaging processes with respect to a Maxwellian background. Since the Debye shielding term in the gyrokinetic Poisson equation is usually neglected for the gyrokinetic particle simulations of low-frequency physics, the resulting equation is an integral equation.

Replace Maxwellian by a sum of finite series of delta functions

$$\Gamma_0(b) = \sum_i c_i J_0^2(k_\perp \rho_i) \tag{6.18}$$



Two rings with c=(0.7194,0.2806) and $v_\perp/v_{thi} = (0.9130, 2.2339)$ can fit Eq. (6.18) very well (less than one percent error) up to $k_\perp \rho_i \simeq 1.5$.

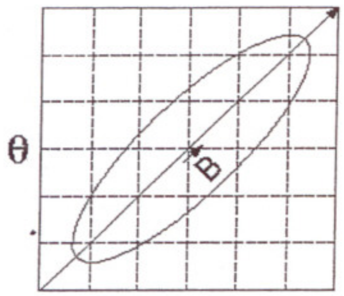
Global Field Line Following Coordinates

- Microinstability wavelength: $\lambda_\perp \propto \rho_i$, $\lambda_{||} \propto qR$
  - grid $\# N \propto a^2$, a: minor radius
- Most global codes: w/o field-line coordinates

- o grid $^{\#}N \propto a^3$
- GTC global code: use field-line coordinates

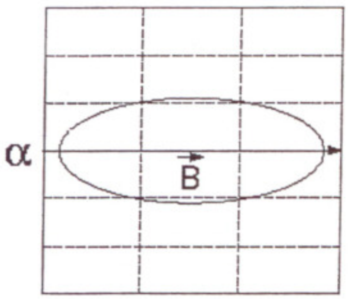
$$(\psi, \alpha, \zeta), \qquad \alpha = \theta - \zeta/q \tag{7.1}$$

  - o grid $^{\#}N \propto a^2$
  - o larger time step: no high $k_{||}$ modes
  - o order of magnitude saving of computing time for reactor size simulations



ζ

$\Delta\zeta \propto \rho$



ζ

$\Delta\zeta \propto R$

Parallel Computing

- PIC code calculates particle-field interaction

$$n(\mathbf{x}) = \sum_j \delta(\mathbf{x} - \mathbf{x}_j)$$

  - o scattering:

$$\mathbf{A_j} = \mathbf{E}(\mathbf{x}_j)$$

  - o gathering:
- Domain decomposition:
  - o each processor holds part of the field array