Perturbative Particle Simulation and Other Schemes -

- Linearized trajectory method: reduce noise lineraly

- Delta-f methods: reduce noise nonlinearly
  - Weight evolution method
  - Perturbed moments method

- Split-weight method: developing a scheme based on the knowledge from linear dispersions:
  - Quasineutral model

- Other innovative schemes
  - Adiabatic pusher, subcycling and orbit averaging
  - Drift Kinetic Model

Linearized Trajectory Method

[J. Byers, Fourth Conference on Numerical Simulation of Plasmas, 1970]

- In my opinion, this paper is the forerunner of the modern-day delta-f schemes.

$$\mathbf{x}_{\alpha j} = \mathbf{x}_{\alpha j0} + \mathbf{x}_{\alpha j1}\,, \qquad \mathbf{v}_{\alpha j} = \mathbf{v}_{\alpha j0} + \mathbf{v}_{\alpha j1}$$

$$F_{\alpha 0} = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_{\alpha j0})\delta(\mathbf{v} - \mathbf{v}_{\alpha j0})$$

$$\delta f_\alpha = -\sum_{j=1}^{N} \left(\mathbf{x}_{\alpha j1} \cdot \frac{\partial}{\partial \mathbf{x}} + \mathbf{v}_{\alpha j1} \cdot \frac{\partial}{\partial \mathbf{v}} \right) \delta(\mathbf{x} - \mathbf{x}_{\alpha j0})\delta(\mathbf{v} - \mathbf{v}_{\alpha j0})$$

$$\frac{d\mathbf{x}_{\alpha j0}}{dt} = \mathbf{v}_{\alpha j0}, \qquad \frac{d\mathbf{v}_{\alpha j0}}{dt} = 0,$$

$$\frac{d\mathbf{x}_{\alpha j1}}{dt} = \mathbf{v}_{\alpha j1}, \qquad \frac{d\mathbf{v}_{\alpha j1}}{dt} = \frac{q_\alpha}{m_\alpha}\mathbf{E}(\mathbf{x}_{\alpha j0})$$

$$\delta n_\alpha = -\frac{\partial}{\partial \mathbf{x}} \cdot \sum_{j=1}^{N} \mathbf{x}_{\alpha j1} \delta(\mathbf{x} - \mathbf{x}_{\alpha j0})$$

$$\nabla \cdot \mathbf{E} = 4\pi \sum_\alpha q_\alpha \delta n_\alpha$$

$$\delta n_\alpha = -\frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{x}_{\alpha 1} \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_{\alpha j0}) = -\frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{x}_{\alpha 1} n_{\alpha 0}$$

$$\frac{\partial}{\partial t}\delta n_\alpha = -\frac{\partial}{\partial \mathbf{x}} \cdot \left(\frac{\partial \mathbf{x}_{\alpha 1}}{\partial t} n_{\alpha 0} \right) = -\frac{\partial}{\partial \mathbf{x}} \cdot \sum_{j=1}^{N} \mathbf{v}_{\alpha j1} \delta(\mathbf{x} - \mathbf{x}_{\alpha j0})$$

$$\nabla^2 \frac{\partial \phi}{\partial t} = 4\pi \sum_\alpha q_\alpha \frac{\partial}{\partial \mathbf{x}} \cdot \sum_{j=1}^{N} \mathbf{v}_{\alpha j1} \delta(\mathbf{x} - \mathbf{x}_{\alpha j0})$$

Compare this later to the split-weight scheme

Delta-f : Weight Evolution Method

[Dimits and Lee JCP ‘ 93; Parker and Lee Phys. Fluids ‘93]

- One Dimensional Vlasov-Poisson System of Equations

$$\frac{dF}{dt} \equiv \frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} + \frac{q}{m}E\frac{\partial F}{\partial v} = 0,$$

$$\frac{\partial E}{\partial x} = 4\pi\rho$$

- Let $\boxed{F = F_0 + \delta f}$ but the perturbed part is not necessarily small.

- Take the time derivatives $\frac{d\delta f}{dt} = -\frac{dF_0}{dt} \longrightarrow \frac{d\delta f}{dt} = -\frac{q}{m}E\frac{\partial F_0}{\partial v}$

- Let $w \equiv \frac{\delta f}{F}$ -- the particle weight

- Klimonmtovich - Dupree representation

$$F(x,v,t) = \sum_{j=1}^{N} \delta[x - x_j(t)]\delta[v - v_j(t)]$$

$$\delta f_(x,v,t) = \sum_{j=1}^{N} w_j \delta[x - x_j(t)]\delta[v - v_j(t)]$$

Delta-f : Weight Evolution Method (cont.)

- Nonlinear Scheme:

$$\left.\begin{aligned} \frac{dx_j}{dt} &= v_j \\ \frac{dv_j}{dt} &= E(x_j) \end{aligned}\right\}$$

-- particle pushing remains the same as the original total F scheme

$$\frac{dw_j}{dt} = -(1 - w_j)\frac{q}{m}E\,\frac{\partial F_0}{\partial v}\,\frac{1}{F_0}\bigg|_{x_j,v_j} = (1 - w_j)\frac{q}{T}v_j E(x_j)$$

-- Weight equation

- Poisson's equation takes account only the perturbed part of the distribution

$$\left.\begin{aligned} \frac{\partial E}{\partial x} &= 4\pi \sum_\alpha q_\alpha \int_N \delta f_\alpha dv \\ &= 4\pi \sum_\alpha q_\alpha \sum_{j=1} w_{\alpha j}\delta(x - x_{\alpha j}) \end{aligned}\right\} \xrightarrow[\text{total F scheme}]{} \begin{aligned} \frac{\partial E}{\partial x} &= 4\pi \sum_\alpha q_\alpha \int_N F_\alpha dv \\ &= 4\pi \sum_\alpha q_\alpha \sum_{j=1} \delta(x - x_{\alpha j}) \end{aligned}$$

- Linear Scheme to solve: $\dfrac{\partial \delta f}{\partial t} + v\dfrac{\partial \delta f}{\partial x} = -\dfrac{q}{m}E\dfrac{\partial F_0}{\partial v}$

$$\frac{dx_j}{dt} = v_j \quad , \qquad \frac{dv_j}{dt} = 0$$

$$\frac{dw_j}{dt} = -(1 - \cancel{w_j})\frac{q}{m}E\,\frac{\partial F_0}{\partial v}\,\frac{1}{F_0}\bigg|_{x_j,v_j} = (1 - \cancel{w_j})\frac{q}{T}v_j E(x_j)$$

Delta-f : Perturbed Moments Method

[Aydemir, Phys. Fluids ‘94]

$$\delta f(x,v,t) = F(x,v,t) - F_0(x,v,t)$$

$$\Big\downarrow \quad \text{Klimontovich -Dupree Representation}$$

$$\delta f(x,v,t) = \sum_{j=1}^{N} (\delta[x - x_j(t)]\delta[v - v_j(t)] - F_0[x_j(t), v_j(t)])$$

- *Fo* is the zeroth order distribution.

- However, δf is singular in phase space.

- We can only calculate the velocity moments such as

$$\delta n = \sum_{j=1}^{N} \delta[x - x_j(t)] - \int F_0[x_j(t), v_j(t)] dv$$

- This method is noisier than the weight evolution method in the linear stage.

- But, it does not have the so-called growing weight problem with the weight evolution method, which is the concern by some people.

Delta-h: Split-Weight Evolution Method

[Manuilskiy and Lee, PoP '00]

- One Dimensional Vlasov-Poisson System of Equations

$$\frac{dF}{dt} \equiv \frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} + \frac{q}{m}E\frac{\partial F}{\partial v} = 0, \qquad \frac{\partial E}{\partial x} = 4\pi\rho$$

- Delta-f : $F = F_0 + \delta f \qquad w \equiv \frac{\delta f}{F}$

$$\frac{dw}{dt} = (1-w)\frac{q}{T}vE \qquad \text{or} \qquad \frac{dw}{dt} \equiv \frac{\partial w}{\partial t} + v\frac{\partial w}{\partial x} = -(1-w)\frac{q}{T}v\frac{\partial \phi}{\partial x}$$

- Warm response : $|\omega/kv_t| \ll 1$

$$w \approx -(1-w)\frac{q\phi}{T} \qquad \text{or} \qquad \delta f \approx -\frac{q\phi}{T}F_0$$

-- aka adiabatic response

- Total response : $\boxed{F = (1-\frac{q\phi}{T})F_0 + \delta h}$

- From *dF / dt = 0*, to the lowest order, we obtain: $\frac{d\delta h}{dt} = \frac{q}{T}\frac{\partial \phi}{\partial t}F_0$

- Let $\boxed{w^{NA} = \frac{\delta h}{F}}$, we then have $\boxed{\frac{dw^{NA}}{dt} = \frac{q}{T}(1-w^{NA})\frac{\partial \phi}{\partial t}}$

$$\delta h = \sum_{j=1}^{N} w_j^{NA}\delta(x-x_j)\delta(v-v_j)$$

A Quasineutral Simulation Model

- Let $F_i = F_{0i} + \delta f_i \qquad F_e = (1 + \frac{e\phi}{T_e})F_{0e} + \delta h_e$

- Poisson's equation becomes

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\phi}{\lambda_{De}^2} = -4\pi e \int (\delta f_i - \delta h_e) dv$$

- We need another equation, i.e.,

$$\frac{\partial^2}{\partial x^2}\frac{\partial \phi}{\partial t} = 4\pi e \frac{\partial}{\partial x}\int v(\delta f_i - \delta h_e) dv$$

- Advantages:

-- δf scheme minimize the noise

-- In addition, δh scheme gets rid of the plasma waves and we can use larger time steps and the restriction on grid size also disappears.

-- Thus, this model is an improvement of the original PIC model in terms of noise, time step and grid size.

-- There is some resemblemce between the current equation above and the Poisson's equation for the linearized trajectory method

Advantages of Perturbative Particle Simulation Methods: δf & δh

- δf method

-- w is the averaged weight of the particles

$$\frac{|E(k)|^2}{8\pi} \approx w^2 \frac{T}{2}$$

$$|e\Phi(k, w_{pe})/T_e|_{th} = \frac{w}{\sqrt{N} k \lambda_{De}} \qquad |e\Phi(k, w_s)/T_e|_{th} = \frac{w}{\sqrt{N}}$$

-- For $w \approx 10^{-6} \ll 1$, noise is greatly reduced at t = 0.

-- When w grows and approaches *1*, the noise will be resides in normal modes -- it's part of the equilibrium thermodynamics, but it is not the short wavelength white noise.

- δh method

-- Plasma waves are no longer in the simulation - can be shown with the resulting equations

-- Only the quasi-neutral waves are in the simulation for $k^2 \lambda_{De}^2 \ll 1$

$$\boxed{\frac{\partial^2 \phi}{\partial x^2}} - \frac{\phi}{\lambda_{De}^2} = -4\pi e \int (\delta f_i - \delta h_e) dv$$

-- Noise is reduced to the ion acoustic level and time step is no longer restricted by $\omega_{pe} \Delta t \ll 1$

-- Grid size can be $\Delta x \gg \lambda_{De}$

Other innovative schemes

- Adiabatic pusher, subcycling and orbit averaging:

-- Take the advantage that the electron moves much faster than the ions

-- Take the advantage the nature of low frequency waves

- Mode expansion method

-- Take the advantage that only a few modes are of interest

- Schemes for Magnetized Plasmas

-- The leap-frog scheme [Buneman, JCP 67]

-- The three-step scheme [Boris, Proc. of the 4th Conference on Numerical Simulation of Plasmas]

-- The guiding-center model [Taylor and McNamara, PF, 71]

-- The low-frequency model - drift kinetic electrons and gyration ions [Lee and Okuda, JCP 78]

-- The gyrokinetic model [Lee, PF ’83]

Simulation of Magnetized Plasmas

- Vlasov Equation

$$\frac{dF}{dt} \equiv \frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}\right) \cdot \frac{\partial F}{\partial \mathbf{v}} = 0$$

$$\boxed{\nabla_{\mathbf{v}} \cdot [\mathbf{v} \times \mathbf{B}(\mathbf{x})] = 0 \ ?}$$

-- Particle codes: j - particle

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v_j} \ , \qquad \frac{d\mathbf{v}_j}{dt} = \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}_j \times \mathbf{B}\right)_{\mathbf{x}_j}$$

1. Leap-frog method [Buneman, JCP '67],
2. Three-step method [Boris, 4th CNSP '70]

$$F = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j)\delta(\mathbf{v} - \mathbf{v}_j)$$ -- Klimontovich and Dupree representation

-- Continuum codes: many ways to solve the equation, -- e.g.,

$$\frac{d\mathbf{x}_g}{dt} = \mathbf{v}_g, \qquad \frac{d\mathbf{v}_g}{dt} = \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}_g \times \mathbf{B}\right)_{\mathbf{x}_g}$$

$$F(\mathbf{x}_g + d\mathbf{x}_g, \mathbf{v}_g + d\mathbf{v}_g, t + dt) = F(\mathbf{x}_g, \mathbf{v}_g, t)$$

1. Semi-Lagrangian method [Cheng and Knorr, JCP '76],
2. Fourier Transform method [Denavit and Kruer, Phys. Fluids '72],
3. Finite-Difference method.

- Poisson's Equation: same for both

$$\nabla^2\phi = -4\pi e \int (F_i - F_e) d\mathbf{v}, \quad \mathbf{E} = -\nabla\phi$$

-- Poisson's equation can be solved on a spatial grid

-- It can also be solved through direct calculations using particles.

Linear Dispersion Relations for Magnetized Plasmas

- integration along unperturbed orbit [Krall & Trivelpiece, '74]

$$X_n(\xi) = I_n(\xi)e^{-\xi}$$

$$\epsilon = 1 + \sum_\alpha \frac{1}{k^2\lambda_{D\alpha}^2}\left[1 + \frac{\omega}{\sqrt{2}k_\parallel v_{t\alpha}} \sum_n X_n\left(\frac{k_\perp^2 v_{t\alpha}^2}{\Omega_\alpha^2}\right) Z\left(\frac{\omega - n\Omega_\alpha}{\sqrt{2}k_\parallel v_{t\alpha}}\right)\right] = 0$$

$$\Omega \equiv qB/mc$$

$$\mathbf{k} = \mathbf{k}_\parallel + \mathbf{k}_\perp$$

I_n- Bessel function

$$\lambda_{D\alpha} \equiv \sqrt{T_\alpha/4\pi n_0 e^2}$$

- Cold plasma response

$$\epsilon \equiv 1 + \frac{\omega_{pi}^2}{\Omega_i^2 - \omega^2}\frac{k_\perp^2}{k^2} + \frac{\omega_{pe}^2}{\Omega_e^2 - \omega^2}\frac{k_\perp^2}{k^2} - \frac{\omega_{pi}^2}{\omega^2}\frac{k_\parallel^2}{k^2} - \frac{\omega_{pe}^2}{\omega^2}\frac{k_\parallel^2}{k^2} = 0$$

$$\left\{\begin{array}{ll} \text{gives the lower hybrid waves,} & \omega_{LH}^2 = \omega_{pi}^2 + \Omega_i^2 \\ \text{and the upper hybrid waves,} & \boxed{\omega_{UH}^2 = \omega_{pe}^2 + \Omega_e^2} \end{array}\right\} \qquad \Omega_{UH}^2 \gg \Omega_{LH}^2$$

- Cold response with gyrating ions and drift kinetic electrons,

$$\epsilon \equiv 1 + \frac{\omega_{pi}^2}{\Omega_i^2 - \omega^2}\frac{k_\perp^2}{k^2} - \frac{\omega_{pe}^2}{\omega^2}\frac{k_\parallel^2}{k^2} = 0 \qquad \boxed{\omega_{LH}^2 = \omega_{pi}^2 + \Omega_i^2}$$ lower hybrid waves

- Cold response with drift kinetic electrons and ions (guiding center plasma)

$$\epsilon \equiv 1 - \frac{\omega_{pi}^2}{\omega^2}\frac{k_\parallel^2}{k^2} - \frac{\omega_{pe}^2}{\omega^2}\frac{k_\parallel^2}{k^2} = 0 \qquad \boxed{\omega^2 = \omega_{pe}^2\frac{k_\parallel^2}{k^2}}$$ modified plasma waves with $k_\parallel^2 \ll k^2$

- These are all space charge waves, which give rise to undesirably high level of numerical noise

The gyrokinetic PIC

[perhaps, the beginning of modern nonlinear gyrokinetics]

- For $\omega^2 \ll \Omega_i^2$

$$\epsilon \equiv 1 + \frac{\omega_{pi}^2}{\Omega_i^2 - \omega^2}\frac{k_\perp^2}{k^2} - \frac{\omega_{pe}^2}{\omega^2}\frac{k_\parallel^2}{k^2} = 0$$

becomes

$$\epsilon \equiv 1 + \frac{\omega_{pi}^2}{\Omega_i^2}\frac{k_\perp^2}{k^2} - \frac{\omega_{pe}^2}{\omega^2}\frac{k_\parallel^2}{k^2} = 0$$

- For $k_\perp^2 \gg k_\parallel^2$ and $\Omega_i^2 \gg \omega^2$, we obtain

$$\boxed{\omega_= \pm \sqrt{\frac{m_i}{m_e}}\frac{k_\parallel}{k_\perp}\Omega_i}$$

-- quasineutral waves, since the unity term is negligible

- How? [Lee, PF ’83; Lee, JCP ’87]