LA50600 Week11a (April 30)

- Effects of Non-Maxwellian distribution function on Landau damping in electrostatic PIC simulation.
- Particle-in-Cell (PIC) in C.
- Take a look at each item of the particle code. Run.
- Some C syntax: module (global variables), complex variables.
As an introduction: Particle Codes are frequently used for the kinetic simulation

- Particle codes evolve plasma dynamics self-consistently by alternately “pushing” charged particles and “solving” the Maxwell’s equations.
- The initial value approach can incorporate interesting nonlinear dynamics and wave particle interactions (retains velocity space information).

\[
\begin{align*}
F &= q (E + v \times B) \\
\Delta t
\end{align*}
\]

(Left) Flow-chart of Particle Codes (PIC). (Right) Charge deposition
With the kinetic simulation we can incorporate velocity space dynamics

- In kinetic simulation the master equation is Boltzmann and Vlasov equation: $f(x,v,t)$
  \[
  \frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \frac{e}{m} (E + v \times B) \cdot \frac{\partial f}{\partial v} = C(f).
  \]
  combined with Maxwell's equation $\nabla \cdot E = \rho/\epsilon_0$, $\nabla \cdot B = 0$, $\nabla \times E = -\frac{\partial B}{\partial t}$, and $\nabla \times B = \mu_0 j$.
- Wave particle interaction, or Landau damping is incorporated.
- Magnetic mirror or trapped particle effects are incorporated.
- In high temperature plasma, one can ignore r.h.s. collision operator: Boltzmann $\rightarrow$ Vlasov.
We start from Vlasov simulation targeting plasma oscillation and Landau damping

- Plasma oscillation occurs due to small inertia of electrons (whether plasma have finite temperature or not).
- In the presence of finite thermal motions, the wave has finite phase velocity and Landau damping can take place.
A dispersion relation of an electrostatic plasma is given

- Coupling a Vlasov equation

\[ \frac{\partial f_s}{\partial t} + v \cdot \frac{\partial f_s}{\partial x} + \frac{eE}{m} \frac{\partial f_s}{\partial v} = 0. \]

and Poisson equation

\[ \frac{\partial E}{\partial x} = \frac{e}{\epsilon_0} \int dv f_s, \]

we obtain

\[ 1 + \frac{\omega_{pe}^2}{k^2} \int_{-\infty}^{\infty} \frac{\partial v f_0}{\omega/k - v} dv = 0. \]

where \( \omega_{pe} = \sqrt{n_0 e^2/m_e \epsilon_0} \).

- Dispersion relation is given by \(^a\)

\[ \omega = \omega_{pe} \left( 1 + \frac{3}{2} k^2 \lambda_{de}^2 \right) + i \frac{\pi \omega_{pe}^3}{2k^2} \partial_v f_0(v)|_{v=\omega_r/k} \]

where Debye Length: \( \lambda_e = \sqrt{\epsilon_0 T_e/n_0 e^2} \).

A method of characteristic is employed to solve Vlasov equation directly

- Equivalent to the lowest order symplectic integrator. We evolve the distribution function by tracing the characteristic curves in the phase space.

- The method takes three steps which are given by

\[
f^* (x,v) = f^n (x - v\Delta t/2, v)
\]

\[
f^{**} (x,v) = f^* (x, v + E(x)\Delta t)
\]

and finally,

\[
f^{n+1} (x,v) = f^{**} (x - v\Delta t/2, v)
\]

whose kinetic energy part and the potential energy part are time advanced alternatively (leap frog in PIC).

- This is not a finite element scheme. In the splitting scheme, if the reference points along the characteristic curves “\(x - v\Delta t/2\)” or “\(v + E(x)\Delta t\)” are exactly on the mesh points, the method is quite trivial. However, in general, the points of references are located in between mesh points of the \(x\) and \(v\) space. We thus need an interpolation technique.
Some of the Vlasov simulation details are given below

- We take an initial condition *initial kick*

\[ f(x, v, 0) = (1 + A \cos (ikx)) e^{-v^2/2} \]  

- Parameters employed are \( n_v = 128, n_x = 32 \), maximum velocity \( v_{\text{max}} = 10.0v_{\text{the}} \), and \( 0 \leq x/\lambda_e \leq 4\pi \). The frequency is within the range of \( \omega_{pe} \).

- Splitting scheme of Cheng and Knorr 1975 used to time advance Vlasov equation which takes advantage of characteristic curves. The method is symplectic and leap-frog equivalent.

- Both the iteration method and Fourier transform method are employed for the field solver.
Free streaming case with $E = 0$ is demonstrated

- Setting $E = 0$, we obtain

$$
\frac{\partial}{\partial t} f(x, v, t) + \frac{\partial}{\partial x} f(x, v, t) = 0. \tag{5}
$$

The analytical solution can be given by setting

$$
f(x, v, t) \sim \exp (-ikvt). \tag{6}
$$

For example, if we take an initial condition

$$
f(x, v, 0) = A \cos (kx)e^{-v^2/2} \tag{7}
$$

we obtain the analytical solution

$$
f(x, v, t) = A \cos (kx)e^{-v^2/2} \cos (kv t). \tag{8}
$$
We also take an initial condition

\[ f(x, v, 0) = (A \cos(ikx)) e^{-v^2/2} \]  

(9)

- Streams in positive direction in \( v > 0 \) while streams in negative direction in \( v < 0 \), needless to say.
Linear Landau damping is demonstrated in self-consistent simulation

- Diagnosed at fixed $x = \pi$. Recursive effect due to finite number of mesh points.
Self-consistent nonlinear simulation is shown

- (Left) Landau damping of electric field and (Right) Flattening of the distribution at $v = \omega/k$ (shown with fixed $x$)

- Let us see if we can produce the same with discrete particles.  

\[ \text{Similar to relation between the diffusion (Eulerian approach) to Monte-Carlo type (random walk) simulation.} \]
Non-Maxwellian taken as IC to see high energy electron effects

- A kappa distribution function we employed is given by

\[ f_v(v) \propto \left[ 1 + \frac{v^2}{2\kappa} \right]^{-\kappa-1}. \]  

(10)

Note that Maxwellian and kappa distribution function are related

\[ \lim_{\kappa \to \infty} f_v(v) = \exp\left(-\frac{v^2}{2}\right). \]  

(11)
**Landau damping rate increases and the real frequency decreases**

- A kappa distribution function we employed is given by

\[ f_v(v) \propto \left[ 1 + \frac{v^2}{2\kappa} \right]^{-\kappa-1}. \]  

(12)

Note that Maxwellian and kappa distribution function are related

\[ \lim_{\kappa \to \infty} f_v(v) = \exp(-v^2/2). \]  

(13)
**PIC simulation is yet another popular way of solving Vlasov equivalent**

- We solve equation of motion

\[
\begin{align*}
\dot{x} &= v \\
\dot{v} &= -(q/m)E
\end{align*}
\]

- The field solver part is the same as direct Vlasov
- Based on Monte-Carlo type sampling of discrete particles.
(Step 0) Initialization is done by random number generator

• For Landau damping we assume the zero-th order distribution to be Gaussian.

• Gaussian distribution can be generated a priori. The form below is frequently used for initial condition of velocity space distribution.

• Gaussian is given by a mapping function with a random number $0 \leq p \leq 0.5$,

$$t = \sqrt{\log \frac{1}{p^2}}$$

$$x_p = t - \frac{2.515517 + 0.802853t + 0.010328t^2}{1.0 + 1.432788t + 0.189269t^2 + 0.001308t^3}$$

^See section 26.2.23 of Abramowitz and Stegen (1970), for example
(Step 1) Particle pusher integrates ODE

- We use Leap-frog or the energy conserving symplectic method. A symplectic integrator advances kinetic energy and potential energy part separately.

- The pseudocode of Leap-frog, as a reminder

\[
\begin{align*}
x &\leftarrow x(0) \\
v &\leftarrow v(0) \\
\text{for } k = 1 \text{ to } n \text{ do } \\
&\quad x = x + 0.50 \cdot dt \cdot v \\
&\quad v = v - dt \cdot E(x) \\
&\quad x = x + 0.50 \cdot dt \cdot v \\
\text{end for}
\end{align*}
\]
(Step 2) Let us consider two dimensional interpolation

- Note that particle deposition and the interpolation are different processes, but uses almost the same algorithm.

- Let us take 2D interpolation for example.

- Remind 1D linear interpolation: say \( a = x - x_i \) and \( b = x_{i+1} - x \), the interpolated value is given by

\[
f(x) = \frac{bf(x_i) + af(x_{i+1})}{a + b}
\]

Note that this corresponds to the process of getting E-field on the particle position (from the previous page).

- Similarly, 2D linear interpolation: now \( a = x - x_i \) and \( b = x_{i+1} - x \), and \( c = y - y_i \) and \( d = y_{i+1} - y \), the interpolated value is given by

\[
F(x, y) = \frac{bdF(x_i, y_i) + adF(x_{i+1}, y_i) + bcF(x_i, y_{i+1}) + acF(x_{i+1}, y_{i+1})}{(a + b)(c + d)}
\]
(Step 3) Field solver gives $E$ field to complete the cycle

- In a periodic system, we can use Fourier transform to solve the Poisson equation. Defining Fourier transform of the charge density by

$$\hat{\rho}(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \rho(x, t) dx,$$

$$\rho(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \hat{\rho}(k, t) dk,$$

The Poisson equation in Fourier space is simply given by

$$\hat{E}(k, t) = \frac{1}{ik} \hat{\rho}(k, t)$$

then inverse Fourier transform to

$$E(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \hat{E}(k, t) dk.$$

- Fourier transform is for a general use in the nonlinear system.
- For linear system all we need is a component Fourier series $k$. The other
modes are filtered out. We can use Fourier series expansion

$$\rho(x, t) = A_k e^{ik\pi x/L} + B_k e^{-ik\pi x/L}$$

with $2L$ being the length of periodicity, and

$$A_k = \frac{1}{2L} \int_0^{2L} e^{-ik\pi x/L} \rho(x, t) dx,$$
$$B_k = \frac{1}{2L} \int_0^{2L} e^{ik\pi x/L} \rho(x, t) dx.$$ 

and thus

$$E(x, t) = \frac{-iL}{k\pi} A_k e^{ik\pi x/L} + \frac{iL}{k\pi} B_k e^{-ik\pi x/L}.$$
A simplest fourier expansion using trapezoid integral rule:

\[ f(x) = A_k \cos (kx) + B_k \sin (kx) \]

with \(-\pi < x < \pi \) being the domain of periodicity, and

\[ A_k = \frac{1}{\pi} \int_{-\pi}^{\pi} \cos (kx)f(x)dx, \]

\[ B_k = \frac{1}{\pi} \int_{-\pi}^{\pi} \sin (kx)f(x)dx. \]
\( \delta f \) method changes PDF to ODE by method of characteristics

- Since \( \delta f / f_0 \sim \delta n / n_0 \), this method reduces the unfavorable artificial collision.
- The linearized Vlasov (gyrokinetic) equation is given by
  \[
  \dot{\delta f} = -v_E \cdot \nabla f_0 - (q/m)E_\parallel \partial_{v_\parallel} f_0
  \]
  We now introduce weight function \( \delta f / g \) (\( g \) is a numerically loaded distribution function).
- In GK simulation, guiding center equation is solved:
  \[
  \dot{\mathbf{X}} = v_\parallel \frac{\mathbf{B}^*}{B^*_\parallel} + \frac{1}{qB^*}\mathbf{b} \times (\mu \nabla B - q\mathbf{E}^*)
  \]
  \[
  \dot{v}_\parallel = -\frac{\mathbf{B}^*}{mB^*_\parallel} \cdot (\mu \nabla B - q\mathbf{E}^*)
  \]
- On top, the weight equation is solved along the particle orbit.
  \[
  \dot{w} = -v_E \cdot \frac{\nabla f_0}{g} - (q/m)E_\parallel \frac{\partial_{v_\parallel} f_0}{g}
  \]

\(^a\)Gyro-average and delta-f orthogonal issue.
A concept of $\delta f$ method is introduced

- We split $f = f_0 + \delta f$:

- The $\delta f$ method is more than the perturbation method, however.
\( \delta f \) method changes PDF to ODE by method of characteristics

- Since \( \delta f / f_0 \sim \delta n / n_0 \), this method reduces the unfavorable artificial collision.
- Then the linearized Vlasov equation is given by

\[
\dot{\delta f} = -\mathbf{v} \cdot \nabla f_0 - (q/m)E \partial_v f_0
\]

We now introduce weight function \( w = \delta f / g \) (\( g \) is a numerically loaded distribution function).

- In delta-f simulation, equation of motions is solved first: (model here limited to electrostatic ones but can easily extend to general cases)

\[
\dot{x} = v \\
\dot{v} = -(q/m)E
\]

- On top, the weight equation is solved along the particle orbit.

\[
w = -(q/m)E \frac{\partial_v f_0}{g}
\]
• In full f

\[ n(x, t) = \int_{-\infty}^{\infty} f(x, v, t) dv. \]

• In the \( \delta - f \) method:

\[ \delta n(x, t) = \int_{-\infty}^{\infty} \delta f(x, v, t) dv. \]

which has much smaller density variation and thus the artificial collision in PIC can be reduced.
About the mid-term exam on May 3rd

• Numerical differentiation and numerical integral.
• ODE solving schemes Euler, Improved Euler, (no need for 4th order Runge-Kutta).
• Random number generator and Monte-Carlo simulation.
• Gaussian elimination, Jacobi, and Gauss-Seidel methods.

• See the home page, exam1 and exam2 (only RNG part is relevant) of 2011 is posted.
Summary and discussions

- Some exercise with PIC. Effects of non-Maxwellian.
- Particle-in-Cell (PIC) in C.
- PDE (Diffusion, Wave, Poisson, and KdV) starts May 7th (Monday) and continues until the end of the semester.