Numerical properties of simulation plasmas

- Linear Properties
- Fluctuation-Dissipation Theorem
- Numerical Noise
- Time Step Restrictions
- Grid Spacing Restrictions
- Initial loading: Quiet Start - Fobanacci numbers
- Implicit Schemes

Normal Modes in a One-Dimensional Plasma

$$\delta f = -\frac{q}{T}\left[1 + \frac{\omega/k}{v-\omega/k} + i\pi\frac{\omega}{k}\delta(v-\omega/k)\right]\phi F_0$$ -- weakly damped modes

- Cold plasma limit, $|\omega/k| \gg v_{t\alpha}$

$$\omega \approx \omega_{pe}\sqrt{1+3k^2\lambda_{De}^2}\left[\pm 1 - i\sqrt{\frac{\pi}{8}}\frac{\exp(-1/2k^2\lambda_{De}^2)}{(k\lambda_{De})}\right]$$

$$\omega_{pe} \equiv \pm\sqrt{4\pi n_o e^2/m_e}$$ -- plasma waves contributed by electrons only

- Cold ions, $|\omega/kv_{ti}| >> 1$ and warm electrons, $|\omega/kv_{te}| << 1$

$$\omega \approx \frac{kc_s}{(1+k^2\lambda_{De}^2)^{1/2}}\left[\pm 1 - i\sqrt{\frac{\pi}{8}}\sqrt{\frac{m_e}{m_i}}\frac{1}{(1+k^2\lambda_{De}^2)^{3/2}}\right] \qquad c_s \equiv \sqrt{T_e/m_i}$$

-- ion acoustic waves contributed by both electrons and ions

- These are the damped normal modes based on the linear dispersion relation
- These oscillations can be observed in an one dimensional particle code.
- This is the first step in verifying the code: frequencies and damping rates of these normal modes.

Fluctuations in a Simulation Plasma

- Weakly damped modes are the long-lived normal modes of an equilibrium plasma. The level of their fluctuations can be obtained from the Fluctuation-Dissipation Theorem (FDT) through the linear dispersion relation. As such, its an invaluable tool for the particle pushers for diagnostic purposes -- one man's noise is another man's signal.

- FDT cannot tell us anything about a linearly unstable system. However, if we know the dispersion relation for a nonlinearly saturated system, we may be able compare the saturation level with the fluctuation (noise) level.

- It has always been a magic to me, even to this day. But, apparently, FDT has a solid theoretical base.

- For one-dimensional plasma in equilibrium,

$$\boxed{L|E(k,\omega)|^2/8\pi = -(T/\omega)Im(1/\epsilon)}$$ - FDT

$$\boxed{L|E(k)|^2/8\pi = (T/2)/(1+k^2\lambda_D^2)}$$ -- Total thermal fluctuation level

= *T/2* for long wavelength modes

Fluctuations in Weakly Damped Normal Modes [Klimontovich '67]

- From $$Im\frac{1}{\epsilon} = -\frac{\epsilon_I}{\epsilon_R^2+\epsilon_I^2} \quad , \qquad \text{and} \qquad \pi\delta(x) = lim_{\sigma\to 0}\sigma/(x^2+\sigma^2)$$

- FDT becomes $$L\frac{|E(k,\omega)|^2}{8\pi} = T\pi\delta(\omega_R\epsilon_R)$$

- Expanding around a normal mode, *Ω :* $\omega_R = \Omega + \Delta\omega_R$, $\epsilon_R(\Omega) = 0$

$$\omega_R\epsilon_R \approx \omega_R\ \epsilon_R|_\Omega + (\omega_R - \Omega)\left.\frac{\partial\omega_R\epsilon_R}{\partial\omega_R}\right|_\Omega$$

- Using $\delta(\sigma x) = \delta(x)/\sigma \longrightarrow \delta(\omega_R\epsilon_R) = \delta(\omega_R - \Omega)\Big/\frac{\partial\omega_R\epsilon_R}{\partial\omega_R}$.

- Integrating over frequency $\int d\omega/2\pi$, FDT becomes

$$L|E(k)|^2/8\pi = \sum_\Omega L|E(k,\Omega)|^2/8\pi = \frac{T}{2}\sum_\Omega 1\Big/\left|\frac{\partial\omega_R\epsilon_R}{\partial\omega_R}\right|_\Omega ,$$

- High frequency modes - plasma waves

$$L|E(k,\omega_{pe})|^2/8\pi = T/2$$

- Low frequency modes - ion acoustic waves

$$L|E(k,\omega_s)|^2/8\pi = (T/2)\frac{k^2\lambda_{De}^2}{1+k^2\lambda_{De}^2}$$

- Thus, all the fluctuation energy is in high frequency waves for long wave length modes.

Particle Noise in a Simulation Plasma

• The reason we are concerned about fluctuations in an equilibrium plasma is to estimate how many particles we have to use in the simulation.

• It can then be shown that

$$|e\Phi(k, w_{pe})/T_e|_{th} = \frac{1}{\sqrt{N} k \lambda_{De}} \qquad \text{plasma waves}$$

$$|e\Phi(k, w_s)/T_e|_{th} = \frac{1}{\sqrt{N}} \qquad \text{ion acoustic waves}$$

• N is the number of simulation particles in the wave, not in the Debye shielding volume.

• Noise resides mostly in high frequency space charge waves for long wavelength modes.

• Noise is much less in low frequency quasineutral waves -- good news for microinstabilities.

Fluctuations in Simulations with Finite Size Particles

[Many papers by Birdsall, Langdon and Okuda in '70's]

- Linear Dispersion Relation

$$\epsilon \equiv 1 + |S_k|^2[1 + \xi_e Z(\xi_e) + \tau + \tau\xi_i Z(\xi_i)]/(k\lambda_{De})^2 = 0$$

- Thermal fluctuations

$$L|E(k)|^2/8\pi = \frac{T/2}{1 + k^2\lambda_D^2 \exp(k^2a^2)}$$

- Finite size particles only affects short wavelength modes by reducing their fluctuation (noise) level .

- For long wavelength modes with $k^2\lambda_D^2 \ll 1$ and $k^2a^2 \ll 1$, physics is intact.

Time Step Restrictions in Particle Codes

- Plasma Dispersion Function [Dawson '61]

$$X_\alpha \equiv \xi_\alpha Z(\xi_\alpha) = -1 + (kv_{t\alpha})^2 \int_o^\infty t \exp\left[i\omega t - \frac{(kv_{t\alpha}t)^2}{2}\right] dt$$

- Let $t = q\Delta t$ and $\int_0^\infty dt \Rightarrow \sum_{q=o}^{\infty} \Delta t$

and substituting them into the above function for the electrons, we obtain a new form of the linear dispersion relation for an equilibrium plasmas

$$\epsilon \equiv 1 + (w_{pe}\Delta t)^2 \sum_{q=0}^{\infty} q \exp\left[i(\omega\Delta t)q - (k\lambda_{De})^2(\omega_{pe}\Delta t)^2 q^2/2\right] = 0$$

where the cold ion response is used.

- Langdon elegantly showed that Δt here is equivalent to the time step used in the leap-frog scheme [JCP '79]

- Limitations on the time step

$\omega_{pe}\Delta t \leq 1$ -- it's violation will cause numerical instability

$kv_{te}\Delta t \equiv (k\lambda_{De})(\omega_{pe}\Delta t) \leq 1$ -- it's violation will cause numerical inaccuracy only

Limitations on Grid Spacing in Particle Codes

- Finite difference for the potential

$$E(x) = [\Phi(x-\Delta x) - \Phi(x+\Delta x)]/2\Delta x$$

gives $$k \rightarrow k sin(k\Delta x)/(k\Delta x)$$

and $$k^2 \rightarrow k^2 \left[\frac{sin(k\Delta x/2)}{(k\Delta x/2)}\right]^2 \equiv k^2 W(k\Delta x/2)$$

- Dispersion relation for an equilibrium plasma including the finite time step and the finite grid spacing becomes

$$\epsilon \equiv 1 + (\omega_{pe}\Delta t)^2 |\tilde{S}_k|^2 \sum_{p=-\infty}^{\infty} (k_p/k) W^n(k_p \Delta x/2)$$
$$\times \sum_{q=0}^{\infty} q \exp[i(\omega\Delta t)q - (\omega_{pe}\Delta t)^2 (k_p \lambda_{De})^2 q^2/2] = 0$$

$k_p \equiv k - 2\pi p/\Delta x$, *n=2* NGP, *n=4* linear interpolation or SUDS

- Grid spacing limitation: $\Delta x \leq \lambda_{De}$ -- it's violation will cause numerical instability

- Suppression of plasma waves also alleviates this condition.

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Implications of the Numerical Restrictions on Particle Simulations

- After Langdon's JCP paper in '79 giving these restrictions:

$$\omega_{pe}\Delta t \leq 1\,,$$

$$k v_{te}\Delta t \equiv (k\lambda_{De})(\omega_{pe}\Delta t) \leq 1\,,$$

the implicit schemes were born in the early '80's.

- The reasoning behind is that we can let $\omega_{pe}\Delta t \gg 1$

and still keep the physics for $k^2\lambda_D^2 \ll 1$ intact, the inaccuracy for $k^2\lambda_D^2 >> 1$ is OK.

- So, let's get grid of plasma waves and the grid spacing restriction with implicit schemes.

- Development of the gyrokinetic scheme also in the early '80's

-- why not get rid of plasma oscillations and the grid spacing restrictions with an explicit simulation scheme?
-- how about using a reduced Vlasv-Poisson system based on gyrokinetic ordering?

- But, let us deal with the noise issue first.

The Direct Implicit Scheme

[Friedman, Langdon and Cohen, Comm. Plasma Phys. Control. Fusion **6**, 225 (1981)]

Leap-frog $v_{n+\frac{1}{2}} - v_{n-\frac{1}{2}} = \frac{q}{m} E_n \Delta t$ $\qquad x_{n+1} - x_n = v_{n+\frac{1}{2}} \Delta t$

Implicit $v_{n+\frac{1}{2}} - v_{n-\frac{1}{2}} + \frac{1}{2} v_{n-\frac{3}{2}} = \frac{1}{2} \frac{q}{m} E_{n+1} \Delta t$ $\qquad x_{n+1} - x_n = v_{n+\frac{1}{2}} \Delta t$

$x_{n+1} = x_{n+1}^{(0)} + \delta x$ zeroth order for free streaming

$\delta x = \beta (\Delta v)(\Delta t) \approx \beta \Delta t^2 (q/m) E_{n+1}$ $\qquad 0 < \beta \leq 1$ implicitness parameter

$$\rho_{n+1} = \rho_{n+1}^{(0)} + \delta x \frac{\partial}{\partial x} \rho_{n+1}^{(0)} \qquad \delta \rho = \delta x \frac{\partial}{\partial x} \rho_{n+1}^{(0)}$$

Let $\frac{\partial}{\partial x} [\chi E_{n+1}] = 4\pi \delta \rho$

$$\chi = 4\pi \beta \rho_{n+1}^{(0)} \frac{q}{m} \Delta t^2 = \beta \omega_p^2 \Delta t^2$$

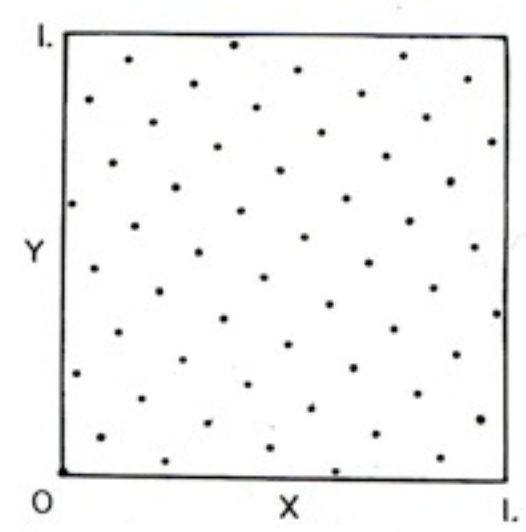
$$\boxed{\nabla \cdot [1 + \chi] \nabla \phi_{n+1} = -4\pi \rho_{n+1}^{(0)}}$$

Initial Loading of Particles

• Uniform loading in *x* and random loading of Gaussian in *v*,
-- too noisy

• Uniform loading in *x* and uniform loading of Gaussian in *v*
-- Beam - Beam instability

• Uniform loading in *x* and with non-random loading of Gaussian in *v* by staggering the particle velocities based on number theory for optimal set of points for Monte-Carlo simulation [Zaremba, "Applications of Number Theory to Numerical Analysis, Academic, New York (1972), pp. 39-119.]



-- For 2D

$$x_i^k = \frac{ig^k}{N} mod\ 1 \qquad (g^1, g^2) = (1, N_{Fibonancci})$$

$$N = \alpha_9 = 55$$
$$g^1 = 1$$
$$g^2 = \alpha_8 = 34$$

-- For higher dimensional problems: using tabulated numbers

• The question of mathematical accuracy in PIC must be regarded as a convergence problem in the frequency and wave number spectra, not from a single particle point of view.

• Initial loading should not have any effects in the long time PIC simulation.

Quiet Start

- Uniform loading in *x* and with non-random loading of Gaussian in *v* with Fobanacci numbers

$$x_i = \frac{2i-1}{2\alpha_m}$$

$$v_i = \sqrt{2}v_{th}erfc^{-1}(2y_i)$$

$$y_i = \alpha_{m-1}x_i$$

$$i = 1,\dots, N$$

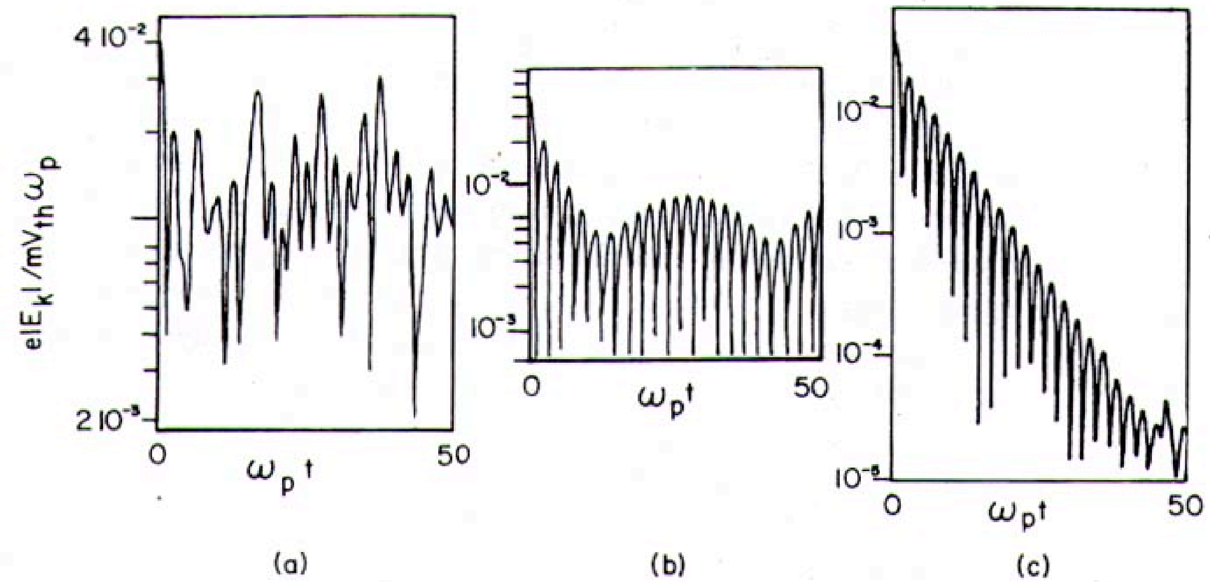


FIGURE 4 Fundamental electric field amplitude $|E_k|$ as a function of time for Landau damping example. (a) Random initialization with 17711 particles. (b) Nonrandom initialization with 17711 particles. (c) Result of a Vlasov simulation.

N = α_m is the number of particles

[J. Denavit and J. M. Walsh, Comments Plasma Phys. Cont. Fusion, 6, 209 (1981).]

- Steady state fluctuation level agrees with FDT

$$e|E_k|/mv_{th}\omega_p = k\lambda_D|\frac{e\phi}{T}| = \frac{1}{\sqrt{N}}$$

- Higher dimensional problems: bit-reverse scheme, Hemmersley numbers, and Zaremba numbers.

[J. Reynders, Ph.D. Thesis, Princeton University (1992).]

- Can we do better than that? Delta-f ?

1 (m =1)
2 (m =2)
3 (m =3)
5 (m =4)
8 (m =5)
13 (m =6)
21 (m =7)
34 (m =8)
55 (m =9)
89 (m =10)
144 (m =11)
233 (m =12)
377 (m =13)
610 (m =14)
987 (m =15)
1597 (m =16)
2584 (m =17)
4181 (m =18)
6765 (m =19)
10946 (m =20)
17711 (m =21)
28657 (m =22)
46368 (m =23)

Remarks

• The question of mathematical accuracy in PIC must be regarded as a convergence problem in the frequency and wave number spectra, not from a single particle point of view.

• Don't let computers do the thinking for you.

• Courant condition is relaxed in PIC.

• There are many attempts on the implicit schemes for particle codes as recent as last ICNP conference in Texas. But, they all suffer from the lack of energy conservation.

• Now, we will proceed to improve particle codes in terms of noise, time step, grid spacing and etc.
  -- perturbative particle particle simulation (δf)
  -- gyrokinetic particle simulation
  -- multiscale particle simulation