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SPRING COLLEGE ON PLASMA PHYSICS

(25 May - 19 June 1987)

COMPUTER SIMULATION TECHNIQUES IN PLASMA PHYSICS

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Computer Simulation Techniques in Plasma Physics

Trieste Spring College in Plasma Physics
(May 25 - June 19, 1987)

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Lecture I

1.) Introductory Concepts

- as computers developed 1950's → particle simulation of plasmas began. Object was to gain insight into physics of a plasma.

- physical system where force law known between individual bodies but how the collection of bodies move not known

- problem with plasma is that due to long range of Coulomb force, net force on a charge in a collisionless plasma determined by multiple, long-range interactions rather than short-range binary-type encounters.

- in particle simulation follow system on <u>microscopic</u> scale → <u>macroscopic</u> quantities constructed and are statistically signifigant if enough particles chosen.

- from simulation

  → test theories and ideas when experiment not possible

  → idealized or gedanken experiment which can be used to gain intuition and learn general behavior of systems.

  → <u>unlike</u> real experiments we can diagnose plasma behavior in detail without perturbing it and results are exactly reproducible given same initial conditions.

  → <u>like</u> a real experiment a great deal of data to assimilate and understand

- for evaluation of long range force

$$m_i \ddot{\underset{\sim}{r}}_i = q_i \sum_j \underset{\sim}{E}_j(\underset{\sim}{r}_i)$$

$$= (2\pi)^{1-n/2} q_i \sum_j{}' \frac{q_j(\underset{\sim}{r}_i - \underset{\sim}{r}_j)}{|\underset{\sim}{r}_i - \underset{\sim}{r}_j|^n}$$

N particles $\Rightarrow$ # operations $\propto N^2$

Let $\quad N_{op} \sim 10N^2$ / time step

$N = 10^5$ particles

10^{-7} sec = 1 arithmetic op.

$\Rightarrow \quad 10^4$ sec / time step to evaluate force.

1000 - 10,000 steps gives

<u>1 month - 1 yr. / run !</u>

2. Finite-size Particle model

- in discrete plasma model, uninterested in detailed particle motion but gross coll-ective motions involving many degrees of freedom.

- 2 approaches
  - → Vlasov equation $f(x,v,t)$
    → system with ∞ degrees of freedom. If f simple, can be described by a few parameters ⇒ one can follow development. If f complex large # of parameters and finite computer constraint. Smoothing in f helps but one never knows physical conseq. Like collisions in discrete mod but numerical in nature.

$$\partial f/\partial t + v\,\partial f/\partial x - \frac{|e|}{m} E\,\partial f/\partial v = 0$$

$$\underline{\nabla} \cdot \underline{E} = -4\pi |e| \left(\int f\,dv - n_0 \right)$$

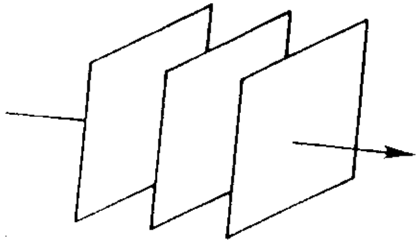
→ particle approach (most direct and fundamental way) → automatically limit information computer must handle to that which is required to specify particle motion. If enhanced collision effect can be sufficiently reduced then natural and physically motivated method for such limitations.

Gross plasma behavior does not somehow depend in a critical way on detailed motion of all particles.

$$\#\text{parameters} < \#\text{particles}$$

A method has been devised for keeping essential information and eliminating grea[t] mass of details — particle-in-cell method which acheives this by using finite # of particles and cells.

1D $E(x) = \dfrac{2\pi q(x-x_i)}{|x-x_i|}$



1D x, v_x

$1\tfrac{1}{2}$D x, v_x, v_y

$1\tfrac{2}{2}$D x, v_x, v_y, v_z

2D $E(\underset{\sim}{r}) = \dfrac{2q(\underset{\sim}{r}-\underset{\sim}{r}_i)}{|\underset{\sim}{r}-\underset{\sim}{r}_i|^2}$

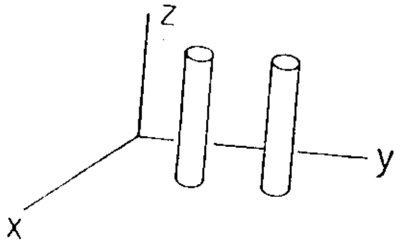
2D x, v_x

y, v_y

$2\tfrac{1}{2}$D x, v_x

y, v_x

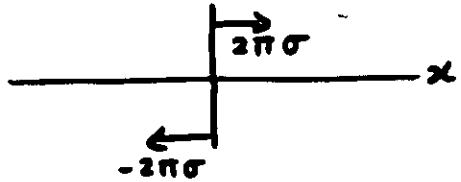
v_z



3D $E(\underset{\sim}{r}) = \dfrac{q(\underset{\sim}{r}-\underset{\sim}{r}_i)}{|\underset{\sim}{r}-\underset{\sim}{r}_i|^3}$

- electrostatic sheet model (1958–'66)

Poisson equation integrated directl[y]



$$\nabla\cdot E = 4\pi\rho \rightarrow E(x) = E(0) + \int_0^x \rho(x)$$

$$\rho(x) = \sigma_i\,\delta(x-x_i)$$

$$\therefore\ E(x) = E(0) + \sum_{x_i<x} \sigma_i = \text{const.}$$

At $x = x_i \Rightarrow E$ jumps by $-4\pi\sigma$

and when particles cross F changes.

$$m\ddot{x}_i = -\sigma E$$

$$x(t) = x(0) + v(0)t + \frac{1}{2}\frac{F}{m}t^2$$

- uniform ion background

$$E(x) = E(0) + 4\pi\bar{n}\sigma x - 4\pi\sum_{x_i<x}\sigma$$

$$\therefore\ x(t) = \frac{F}{m\omega_p^2} + \left[x(0) - \frac{F}{m\omega_p^2}\right]\cos(\omega_p t) + \frac{\dot{x}(0)}{\omega_p}\sin($$

- finite-size particles (1966-'68)

  → discont$^{\underline{s}}$ jumps in forces at short range must be smoothed out. This is collisional-type phenomena in particle codes.

  → Four contributions

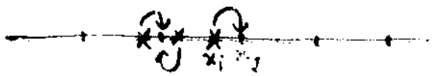
  R. Hockney (1966) (NGP)

  C. Birdsall + D. Fuss (1968) (CIC

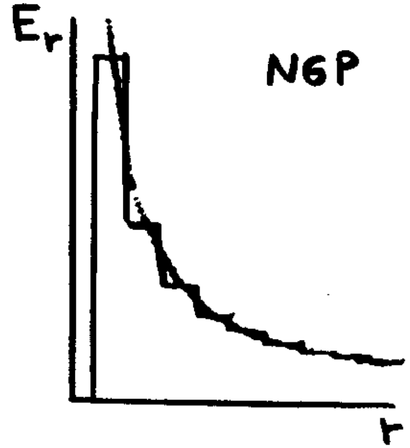
  R. morse + C. Nielsen (PIC

  J. Dawson (1968) (k-spa

- Nearest grid point (NGP)



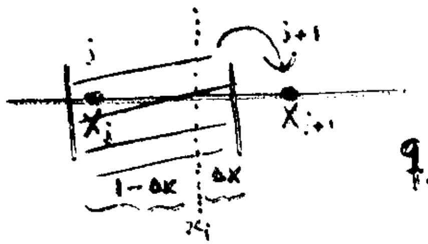
  - charge of particle assigned to nearest grid point. Equivalent to creating super-particle at each grid point. All particles nearest to same grid point don't interact



NGP $\rho(i) = q$

- Cloud in cell (CIC)

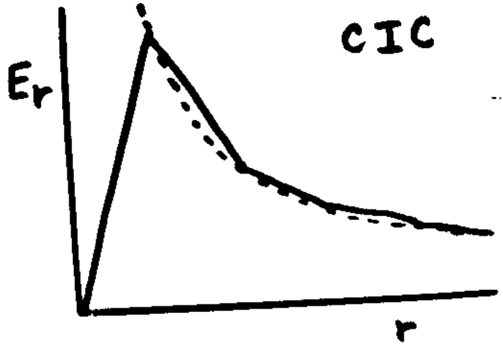
  assign particle charge to more than one grid point by linear interpolation from particle position

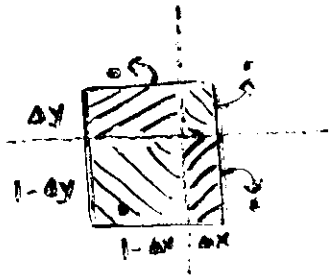


$$q_j = q_c \frac{\Delta x - (x_i - X_j)}{\Delta x}$$

$$q_{j+1} = q_c \frac{x_i - X_j}{\Delta x}$$

CIC

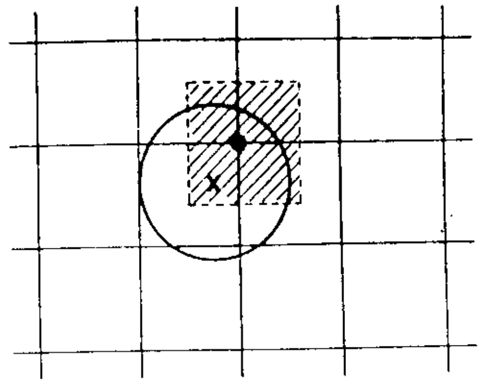




CIC - 2D
(Area weighting)

particle charge assigned four nearest grid points, bilinearly.

Finite-Size Particle-mesh model

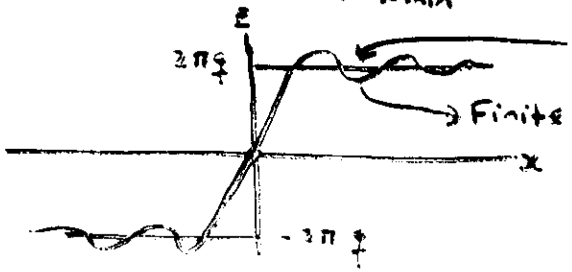


- k-space (Dawson, 1968)

consider gridless model again

Take E-field due to particle given by finite Fourier sum

$$\underset{\sim}{E}(r) = 4\pi q \sum_{k=k_{min}}^{k_{max}} \frac{i\underline{k}}{k^2} e^{i\underline{k}\cdot(\underline{r}-\underline{r}_i)}$$



Now physically motivate dropping E-fields for wavelengths shorter than those considered important for collisionless behavior.

$$k_{max} \sim \lambda_D^{-1}$$

$$k_{min} \sim L^{-1}$$

Collision time τ_c given by $\omega_{pe}\tau_c \simeq N_D$

If modes not collective for $k\lambda_D > 1$

collective modes $\approx (L/\lambda_D)^n$

n = # dimensions

$\omega_{pe}\tau_e \sim 1000$ and for 1000 mod.

$\Rightarrow N \sim 10^6$ particles.

To get finite sum to be more like exact result

$$\underset{\sim}{E}(\underset{\sim}{x}) = 4\pi q \sum_{k_{min}}^{k_{max}} \frac{i\underline{k}}{k^2} S(k)\, e^{i\underline{k}\cdot(\underline{x}-\underline{x}_i)}$$

Ask – what $S(k)$ will do this?

$k_{max} \to \infty \Rightarrow$ field produced by Gaussian

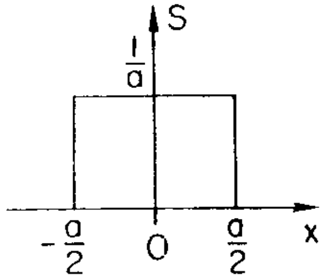
$$\rho(x) \propto q\, e^{-(x-x_i)^2/2a^2}$$

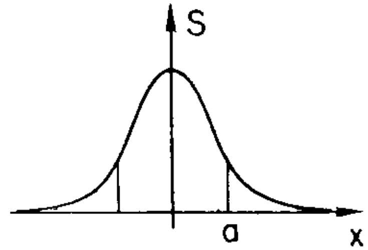
$\equiv$ field due to finite-size particle of dimension a.

For $k_{max}^2 a^2$ large $\Rightarrow$ all terms in sum for $k > k_{max}$ small and reduces oscillation in E-field.

• force of interaction between particles with charge density

$$\rho(x) = \frac{-q}{\sqrt{2\pi a}}\, e^{-(x-x_i)^2/2a^2}$$





F_{ij} = force on particle i due to j

$$= \int_{-\infty}^{\infty} E_j(x)\, \rho_i(x)\, dx$$

$$= \frac{2q^2 i}{\sqrt{2\pi a}} \int dk\, dx\, \frac{e^{ik(x_j - x) - \frac{a^2k^2}{2} - \frac{(x-x_i)^2}{2a^2}}}{k}$$

$$= F_0 \sum_{k=k_{min}}^{k_{max}} e^{-a^2k^2} \frac{\sin(k(x_j - x_i))}{k}$$

Force on i^{th} particle due to all other particles

$$F_i = m\ddot{x}_i = \sum_{k_{min}}^{k_{max}} \frac{A e^{-a^2k^2}}{k} \left\{ \sin(k x_i) \sum_j \cos(k x_j) - \cos(k x_i) \sum_j \sin(k x_j) \right\}$$

- Summation

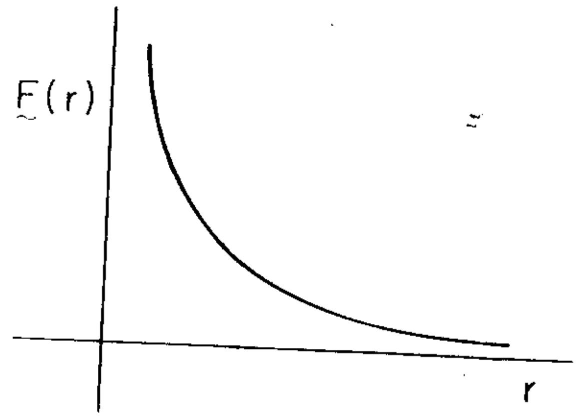
  If we think of simulation as dealing with finite-size particles from start, various mathematical smoothing techniques understood physically.

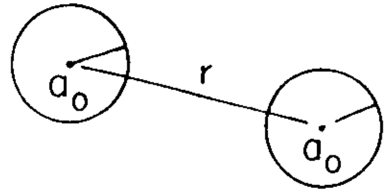
$$\frac{\partial f}{\partial t} + \underset{\sim}{v} \cdot \frac{\partial f}{\partial \underset{\sim}{x}} + \underset{\sim}{a} \cdot \frac{\partial f}{\partial \underset{\sim}{x}} = 0$$

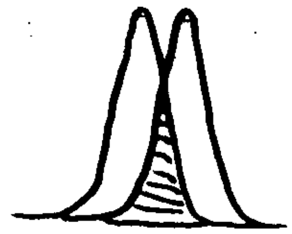
$$\underset{\sim}{a} = \frac{q}{m} \int d^3 r' \, S(\underset{\sim}{r} - \underset{\sim}{r}') \left[\underset{\sim}{E}(\underset{\sim}{r}') + \frac{\underset{\sim}{v} \times \underset{\sim}{B}(\underset{\sim}{r}')}{c} \right]$$

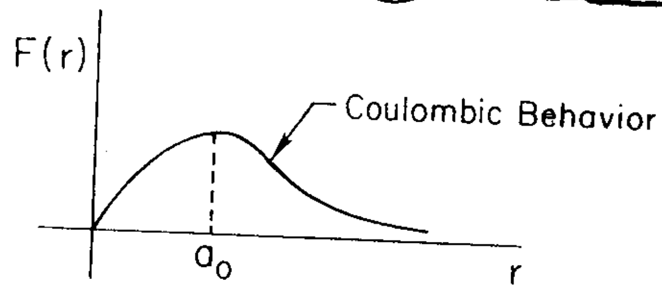
$$\underset{\sim}{\nabla} \cdot \underset{\sim}{E} = 4\pi \int \rho_p (\underset{\sim}{r}') \, S(\underset{\sim}{r} - \underset{\sim}{r}') \, d^3 r'$$

$$\rightarrow \quad \underset{\sim}{E}(\underset{\sim}{k}) = -\frac{i \underset{\sim}{k}}{k^2} S(\underset{\sim}{k}) \; 4\pi \rho_p (\underset{\sim}{k})$$









$$a_0 \approx \lambda_0$$

$$\rho(r - r_i) = q S(r - r_i), \quad \int S(r) d^n r = 1$$

- Gaussian [redacted] shaped particles

$$\rho(x) = \frac{q}{\sqrt{2\pi}\,a} \sum_j e^{-(x-x_j)^2/2a^2}$$

$$\rho(k) = \underbrace{q\, e^{-a^2k^2/2}}_{\text{part from k-space interpretation}} \underbrace{\sum_j e^{-ikx_j}}_{\text{part from NGP and CIC interpretation}}$$

$$x_j = n_j\delta + \Delta x_j = x_g + \Delta x_j$$

$$\Rightarrow \rho(k) = q\, e^{-a^2k^2/2} \sum_j e^{-ikn_j\delta} \underbrace{\sum_l \frac{1}{l!}(-ik\Delta x_j)^l}_{\text{multipole moment of each extended charge w.r.t. nearest grid location}}$$

- expand to dipole order

$$\rho(k) \doteq q\, e^{-a^2k^2/2} \sum_j e^{-ikx_g}(\underbrace{1}_{\text{NGP}} - \underbrace{ik\Delta x_j}_{\text{Dipole expansion}})$$

$$= q\, e^{-a^2k^2/2} \sum_j \left[e^{-ikx_g} + \frac{\Delta x_j}{2} e^{-ik(x_g+1)} - \frac{\Delta x_j}{2} e^{-ik(x_g-1)} \right]$$

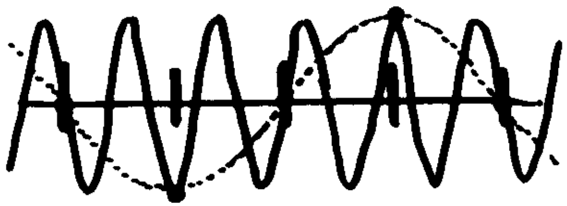
$\therefore$ Charge assignment

$$\left.\begin{aligned} 1 &\rightarrow x_g \\ \frac{\Delta x_j}{2} &\rightarrow x_{g+1} \\ -\frac{\Delta x_j}{2} &\rightarrow x_{g-1} \end{aligned}\right\} \text{Subtracted Dipole scheme.}$$

- Same with force

$$F(x_i) = \int S(x) \left[E(x+x_g) + (x_i - x_g)\cdot\nabla E(x+x_g) \right.$$

• using grid → aliasing can occur



• aliasing → sampling of cont$^{\underline{s}}$ data at discrete points

• If $\lambda <$ grid spacing ⇒ when density is evaluated it appears to have a longer wavelength.

• system periodic in wavenumber space

$$k' = k + 2n\pi/\Delta x \quad , \quad k < 2\pi/\Delta x$$

• with finite size particles

$$n(x) = \int n_p(x')\, S(x-x')\, dx'$$

$S \downarrow e^{-x^2/2a^2}$

$n_p \downarrow = n_0 + n_1 \sin(kx)$

$$\rightarrow n(x) = n_0 + n_1 e^{-a^2k^2/2} \sin(kx)$$

∴ $ka \sim 1$ short λ aliases remov

• what have we gained?

<u>pair by pair</u> $\quad \tau_{comp} \propto N^2$

<u>Finite size particle</u>

gridless → $\tau_{comp} \propto \alpha N M + \beta N M$

N = particle #

M = mode # ↔ grid points

$M < N$

N ↳ represents f

M ↳ represents x

gridded → $\tau_{comp} \propto \alpha N + \beta M^2$

FFT → $\tau_{comp} \propto \alpha N + \beta M \ln(M)$

Computation cycle