# **Kinetic Plasma Simulations**

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# Plasma: ionized gas (typically T>10<sup>4</sup>K), 4th state of matter

Examples: stars, sun, ISM, solar wind, Earth magnetosphere, fluorescent lights, lightning, thermonuclear fusion

Plasma physics: studies plasma behavior through experiment, theory and ... *simulation*!

Simulation needed to study collective and kinetic effects, especially in the nonlinear development.

Applications: reconnection, anomalous resistivity, instabilities, transport, heating, etc.

Characteristic time and length scales



When are collisions important?

 $L >> \lambda_D$ ,  $t >> \omega_P^{-1}$ ,  $\omega_c^{-1}$ We are interested in Number of particles in Debye cube

Plasma is collisionless if

Plasma Type	$n { m cm}^{-3}$	$T   \mathrm{eV}$	$\omega_{pe}~{\rm sec}^{-1}$	$\lambda_D$ cm	$n\lambda_D{}^3$	$\nu_{ei}\;{\rm sec}^{-1}$
Interstellar gas	1	1	$6 \times 10^4$	$7 \times 10^2$	$4 \times 10^8$	$7 \times 10^{-5}$
Gaseous nebula	$10^{3}$	1	$2 \times 10^{6}$	20	$8 \times 10^6$	$6\times 10^{-2}$
Solar Corona	$10^{9}$	$10^{2}$	$2 \times 10^9$	$2 \times 10^{-1}$	$8 \times 10^6$	60
Diffuse hot plasma	1012	$10^{2}$	$6 \times 10^{10}$	$7 \times 10^{-3}$	$4 \times 10^5$	40
Solar atmosphere, gas discharge	1014	1	$6 \times 10^{11}$	$7 \times 10^{-5}$	40	$2 \times 10^9$
Warm plasma	1014	10	$6 \times 10^{11}$	$2 \times 10^{-4}$	$8 \times 10^2$	107
Hot plasma	1014	$10^{2}$	$6 \times 10^{11}$	$7 \times 10^{-4}$	$4 \times 10^4$	$4 \times 10^{6}$
Thermonuclear plasma	10 <sup>15</sup>	104	$2 \times 10^{12}$	$2 \times 10^{-3}$	$8 \times 10^{6}$	$5 \times 10^4$
Theta pinch	10 <sup>16</sup>	$10^{2}$	$6\times 10^{12}$	$7 \times 10^{-5}$	$4 \times 10^3$	$3 \times 10^8$
Dense hot plasma	10 <sup>18</sup>	$10^{2}$	$6 \times 10^{13}$	$7 \times 10^{-6}$	$4 \times 10^2$	$2 \times 10^{10}$
Laser Plasma	$10^{20}$	$10^2$	$6 \times 10^{14}$	$7 \times 10^{-7}$	40	$2 \times 10^{12}$

Collisionless system has a very large number of particles in Debye sphere

 $\mathbf{N}_{\mathrm{D}} \equiv \mathbf{n} \lambda_{\mathrm{D}}^{3}$ 

 $L \gg \lambda_D$ ,  $N_D \gg 1$ 

 $ec{j}(ec{x}) = \sum_i q_j ec{v}_j \delta(ec{x} - ec{x}_j)$ 

Collisionless plasma can be described by Vlasov-Maxwell system of equations for distribution function f(x,v,t):

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} + \frac{q}{m} \left( \vec{E} + \frac{\vec{v} \times \vec{B}}{c} \right) \cdot \frac{\partial f}{\partial \vec{v}} = 0 \qquad \qquad \frac{d\vec{v}_j}{dt} = \frac{q_j}{m_j} (\vec{E} + \frac{\vec{v}_j \times \vec{B}}{c}) \\ \nabla \cdot \vec{E} = 4\pi \int qf d^3 \vec{v}, \qquad \qquad \qquad \frac{d\vec{x}}{dt} = \vec{v} \\ \nabla \times \vec{B} = \frac{1}{c} \frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c} \int qf \vec{v} d^3 \vec{v}, \qquad \qquad \nabla \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t} \\ \nabla \cdot \vec{B} = 0, \quad \nabla \times \vec{E} = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t}. \qquad \qquad \nabla \times \vec{B} = \frac{4\pi \vec{j}}{c} + \frac{1}{c} \frac{\partial \vec{E}}{\partial t} \\ \text{Direct solution is 6D -- very expensive Can solve along characteristics -- particles} \qquad \qquad \rho(\vec{x}) = \sum_{j} q_j \delta(\vec{x} - \vec{x}_j) \\ \end{array}$$

Ca Delta functions cause collisions -- smooth them

particle method!

### PIC Approach to Vlasov Equation (VE)

- 6D-VE not practical on a grid
- (Re-)introduce N<sub>p</sub> computational particles for discretizing f<sub>1</sub>(**r**, **p**, t)
- Macroscopic force (F) becomes again granular (stochastic noise)

$$\delta \mathbf{F}^s \rightarrow \sqrt{1/N_p}$$

Particle equations of motion (EQM):

$$\frac{d\mathbf{r}_p}{dt} = \frac{\mathbf{p}_p}{m}, \quad \frac{d\mathbf{p}_p}{dt} = \mathbf{F}_p$$

VE characteristics: f<sub>1</sub> = const.
 Particle strength (charge) const.



 Reduce operation count by computing forces on a grid

### **PIC Approach to Vlasov Equation**



### Finite-size particles Coulomb force between point charges



short range force is responsible for collision effects

long range force is responsible for collective effects

FIG. 1. Coulomb force law between particles in two and three dimensions.

Since one simulation particle represents many point particles (Q=Nq), the short range force is over-estimated. So, finite-size particles are used.

### The force law between finite-size particles



FIG. 4. Square and Gaussian charge shapes—two shapes often used for finite-sized particles.

FIG. 2. Force law between finite-size particles in two dimensions for various sized particles. A Gaussian-shaped chargedensity profile was used.

### How PIC works

### **Simulation Flow-Chart**



### How PIC works

## A bit of history:

In late 1950s John Dawson began 1D electrostatic "charge-sheet" experiments at Priceton, later @ UCLA.

1965 Hockney, Buneman -- introduced grids and direct Poisson solve

1970-s theory of electrostatic PIC developed (Langdon) First electromagnetic codes

1980s-90s 3D EM PIC takes off "PIC bibles" come out in 1988 and 1990 Always in step with Moore's law





Key names: J. Dawson, O. Buneman B. Langdon, C. Birdsall.



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Timescales of the system >> light crossing time; magnetic fields static.



# Four Major Criteria to Choose an Algorithm for Integration of Equations of Motion

•**Convergence** – Which means that the numerical solution converges to the exact solution of the differential equation in the limits as  $\Delta t$  and  $\Delta x$  tend to zero.

•Accuracy – Which means the truncation error associated with approximating derivatives with differences.

•**Stability** – If total errors (including truncation error and round-off error) grows in time, then the scheme is unstable.

•Efficiency – This is a critical consideration since whatever scheme we choose will be used for each particle at each time step.

### Other Criteria to Choose an Algorithm for Integration of Equations of Motion

•**Dissipation** – The dissipation of some physical quantities caused by the truncation error associated with approximating derivatives with differences.

•**Conservation** – The deviation of the conservation law caused by the truncation error associated with approximating derivatives with differences.

### Integration of Equations of Motion

The conventional wisdom is that the simple second order leapfrog achieves the best balance between accuracy, stability and efficiency.



### Integration of Equations of Motion

For an electrostatic case, if  $\omega_p \Delta t \leq 2$ , the leap frog scheme is stable.



Figure 3. Angular frequency  $\omega_r$  and numerical growth rate  $\omega_i$  for the leapfrog scheme. Phase error is the difference between the numerical and exact frequency  $\omega_0$ .

### Charge Assignment and Force Interpolation

Once we introduce the grid we can no longer view the particles as point particles, this leads naturally to the idea of a finite sized particle.



### Charge Assignment and Force Evaluation by Cloud-in-Cell in 1D

To ensure momentum conservation, the same interpolation scheme is used to compute the force on a particle as was used to perform the assignment of the particles charge to the mesh.



### Filtering Action of Shape Functions



### Integration of Field Equations

Here we solve the 1D form of Poisson's equation, then computes the electric field. *L* is the length of the system of interest.



In this case, differencing acts to dampen high  $k_l$  modes.

### Aliasing

The spurious fluctuations which appear as a result of the loss of displacement invariance, manifest themselves in *k*-space as non-physical mode couplings, known as 'aliasing'.



The extra contributions (from |n| > 0) to inside the principal zone are called aliases.

## Aliasing

- The spurious fluctuations of high frequency causes the noise and error in the main lobe, which might make the numerical system to be unstable.
- The high-*k* components of S(k) is determined by the smoothness of S(x); The high-*k* component of  $n_c(k)$  is determined by the smoothness of  $n_c(x)$ , i.e. the number of particles.
- The major noise exists in the particle-in-cell method mainly comes from the aliasing effect. Two methods for reducing the aliasing effect:
  - 1. Increase the particle number.
  - 2. Increase the order of the shape function.

# Noise Reduction in PIC

- The granularity of a particle representation inevitably introduces short-scale fluctuations into the force field, and the mean amplitude of these fluctuations is proportional to  $\sqrt{n}$ , where *n* is the particle number density.
- The ratio of the mean amplitudes of the fluctuations to the slowly varying component varies as  $\frac{1}{\sqrt{n}}$ , the effect of these fluctuations is greatly enhanced because our numerical model typically uses far fewer particles than are present in reality.
- We do not need to reduce the fluctuation amplitudes to their correct values, but merely to levels at which they no longer dominate the forces on the particles, or influence the particles significantly during the course of our simulation.

If Debye length is unresolved on the grid (<1cell), aliasing will heat up the plasma until Debye length is resolved -- num. heating

Effects of particle shape factor on plasma dispersion





Extensions to 2D:

Usually, area weighting scheme is used for charge deposition and force interpolation

But -- can use other shape factors as well! Particles don't have to be squares!!!

but the alternative is 6D Vlasov... PIC issues.

- Particle discretization error
- •Smoothing error (finite size particles)
- Statistical noise (granular force)
- •Grid aliasing (grid assignment)
- Deterioration of quadrature in time integration
- •Short-range forces (collisions) neglected



### PIC codes

# Summary for Restrictions of simulation parameters

Value of time step

1. Courant condition (rectangular coordinate)

$$dt < 1 / \sqrt{\frac{1}{dx_1^2} + \frac{1}{dx_2^2}}$$
  $c = 1$   
 $\omega_{pe} = 1$ 

2.  $\omega_{\rm max} dt < 0.25$ 

 $\bot$  The maximum frequency of system

$$3. \quad v_{\max} dt < \min(dx_1, dx_2)$$

particle move one time step < 1 cell (grid size)



# Summary for Restrictions of simulation parameters

Resolution

1.Cell (grid) size

 $dx < \frac{\lambda}{m}$   $m \approx 6 \sim 12$   $\lambda = \frac{2 \pi}{k_{\max}}$ 

2.Particles per cell per species : 4-9

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$$\begin{split} E^{n+1/2} &= E^{n-1/2} + \varDelta t [c(\boldsymbol{\nabla}\times B^n) - 4\pi J^n] \\ B^{n+1} &= B^n - c\varDelta t \boldsymbol{\nabla}\times E^{n+1/2} \;. \end{split}$$





Fields defined on the Yee mesh. Currents, not shown, are co-located with the corresponding electric field components. Exploded view shows an integration surface.

Fields are decentered both in time and in space Finite-difference Time-Domain Maxwell solver on Yee (1966) mesh: robust and very simple. Second order in space and time. Decentering conserves div B to machine precision

## Integration of Field Equations

The new set of field variables encapsulate the mesh metrics.  $\widetilde{E} = \int E \bullet dl \quad \widetilde{D} = \int D \bullet dS$  $\widetilde{H} = \int H \bullet dl \quad \widetilde{B} = \int B \bullet dS$  $\widetilde{I} = \int J \bullet dS$ 

$$E^{n+1/2} = E^{n-1/2} + \Delta t [c(\boldsymbol{\nabla} \times B^n) - 4\pi J^n]$$
$$B^{n+1} = B^n - c\Delta t \boldsymbol{\nabla} \times E^{n+1/2} .$$



Fields defined on the Yee mesh. Currents, not shown, are co-located with the corresponding electric field components. Exploded view shows an integration surface.



Vacuum dispersion curve for leapfrog difference scheme for wave equation.

Numerical dispersion is anisotropic (best along grid diagonal) Phase error for short wavelengths Causes numerical Cherenkov radiation (when relativistic particles move faster than numerical speed of light)

# Integration of Equations of Motion

Newton–Lorentz equations of motion



## Integration of Equations of Motion

Boris Scheme\*  $u_{t-\Delta t/2} = u^{-} - \frac{qE}{m} \frac{\Delta t}{2}$  $u_{t+\Delta t/2} = u^{+} + \frac{qE}{m} \frac{\Delta t}{2}$  $\frac{u^+ - u^-}{\Lambda t} = \frac{q}{2m}(u^+ + u^-) \times B$  $u^+$ u'x s u' /u⁻ x t<sup>t</sup> U<sup>-</sup>

(Explicit Scheme)



with

$$\mathbf{t}' = \frac{q\Delta t}{2\gamma^t m} \mathbf{B}^t$$

 $\theta = 2 \arctan(t') = 2 \arctan(qB\Delta t/2\gamma m)$ 

\* Boris J P 1970 Relativistic plasma simulation—optimization of a hybrid code *Proc. 4th Conf. on Numerical Simulation of Plasmas (Washington, DC)* pp 3–67.

Can overstep magnetic rotation without stability issues.

Charge and current deposition  $\partial E/\partial t = c(\nabla \times B) - 4\pi J$ ,

 $\partial B/\partial t = -c(\boldsymbol{\nabla} \times E) \;,$ 

Should we solve an elliptic equation in addition to hyperbolic Ampere's and Faraday's laws?

Turns out we can avoid solving Poisson equation if charge is conserved.

Take divergence of Ampere's law:

What to do about the Poisson equation?

$$\frac{\partial \nabla \cdot E}{\partial t} = c \nabla \cdot (\nabla \times B) - 4\pi \nabla \cdot J$$
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot J$$

If charge is conserved, Poisson equation is just an initial condition. Like divB=0, if Poisson is true at t=0, it will remain satisfied.

#### Charge and current deposition

Charge-conservative current deposition method If just use volume-weighting, charge is not conserved.

Villasenor & Buneman (92):

Count what is the "volume current" through appropriate faces.

Also, need to know if the particle crosses four or 7 boundaries (2d).



### Weighting Charge to the Grids



### Weighting Current to the Grids

 $I_{1,j+\frac{1}{2},k} = \sum_{i} \frac{q_i}{\Delta t} \Delta w_1 (1 - \overline{w}_2)$  $I_{1,j+\frac{1}{2},k+1} = \sum_{i} \frac{q_i}{\Delta t} \Delta w_1 \overline{w}_2$  $I_{2,j,k+\frac{1}{2}} = \sum_{i} \frac{q_i}{\Delta t} \Delta w_2 (1 - \overline{w}_1)$  $I_{2,j+1,k+\frac{1}{2}} = \sum_{i} \frac{q_i}{\Delta t} \Delta w_2 \overline{w}_1$  $w = x_i - X_{jk}$ 



 $x_i$ : refers to the position of the  $i_{th}$  particle  $X_{jk}$ : the position of the nearest lower mesh node

$$\bar{w} = \frac{w^{t+\Delta t} + w^t}{2}$$

#### Charge and current deposition



Current deposition can take as much time as the mover (sometimes more). More optimized deposits exist (Umeda 2003).

Charge conservation makes the whole Maxwell solver local and hyperbolic (like nature intended!). Static fields can be established dynamically.

#### **Special sauce**

Particle shape should be smoothed to reduce noise. We use current filtering after deposition to reduce high frequency aliases.

Higher order FDTD schemes (4th spatial order) work better at reducing unphysical Cherenkov instability.

#### **Boundary conditions**

Periodic is simple -- just copy ghost zones and loop particles. Should not forget particle charge on the other side of the grid!

Conducting BCs: set E field parallel to boundary to 0. Boundary has to lie along the grid.

Outgoing BCs: match an outgoing wave to E, B fields at boundary (Lindman 1975).

### **Boundary conditions**

Perfectly matched layer (Berenger 1994) -- works like absorbing material with different conductivity for E and B fields)

Moving window: simulation can fly at c to follow a fast beam. Outgoing plasma requires no conditions.

Injection: particles can be injected from boundary, or created in pairs throughout the domain. We implemented moving injectors and expanding domains for shock problems.

#### Parallelization

We use domain decomposition with ghost zones that are communicated via MPI. In 3D we decompose in slabs in y-z plane, so all x-s are on each processor (useful for shocks).

### Public codes

### http://ptsg.eecs.berkeley.edu/



Our most recent, popular and well kept up codes are on bounded plasma, plasma device codes XPDP1, XPDC1, XPDS1, and XPDP2. The P, C, and S mean planar, cylindrical, or spherical bounding electrodes; the 1 means 1d 3v and the 2 means 2d 3v. These are electrostatic, may have an applied magnetic field, use many particles (like hundreds to millions), particle-in-cell (PIC), and allow for collisions between the charged particles (electrons and ions, + or -) and the background neutrals (PCC-MCC). The electrodes are connected by an external series R, L, C, source circuit, solved by Kirchhoff's laws simultaneously with the internal plasma solution (Poisson's equation), The source may be V(t) or I(t), may include a ramp-up (in time). XPDP2 is planar in x, periodic in y or fully bounded in (x,y), driven by one or two sources.(For detailed information, click here)

## Not so public codes

XOOPIC (2D RPIC, free unix version, Mac and Windows are paid through Tech-X); OOPIC-PRO
VORPAL (1,2,3D RPIC, hybrid, sold by Tech-X)
TRISTAN (public serial version), 3D RPIC (also have 2D), plans for release "real soon now"™
OSIRIS (UCLA) 3D RPIC, mainly used for plasma accelerator research

LSP -- commercial PIC and hybrid code, used at PPPL

VLPL -- laser-plasma code

Reconnection research code (UMD, UDelaware)

Every national lab has PIC codes.

All are tuned for different problems, and sometimes use different formulations (e.g. vector potential vs fields, etc). Direct comparison is rarely done.

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