Particle-in-cell simulations
for pedestrians

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Introduction

Relevant scales in space: gyration

$$\Omega_L = \frac{eB}{mc} = (20\ \mathrm{Hz}) B_{\mu G} \frac{m_e}{m_x}$$

$$r_L = \frac{v}{\Omega_L} = \left(10^9 \mathrm{cm}\right) \frac{p_x}{m_e c B_{\mu G}}$$

Introduction

Relevant scales in space: plasma oscillations

$$\omega_p = (60\ \mathrm{kHz})\sqrt{n_e \frac{m_e}{m_x}}$$

$$\lambda_s = \frac{c}{\omega_p} = 5\ \mathrm{km}$$

Introduction

Compare Coulomb scattering frequency
and plasma frequency

→ collective plasma interactions dominate in space

→ we do not a priori know the distribution function

Introduction

How to describe matter in space?

Always: Maxwell‘s equation

Hydrodynamics needs knowledge of the EoS

Kinetic model solves for distribution function

Introduction

Kinetic descriptions:

Boltzmann equation

$$f_c = \frac{\partial f}{\partial t} + \dot{\vec{x}}\,\frac{\partial f}{\partial \vec{x}} + \dot{\vec{p}}\,\frac{\partial f}{\partial \vec{p}}$$

Solve equation of motion of many particles

→ Particle-in-cell simulations

Particle-in-cell

Solve equation of motion for each particle

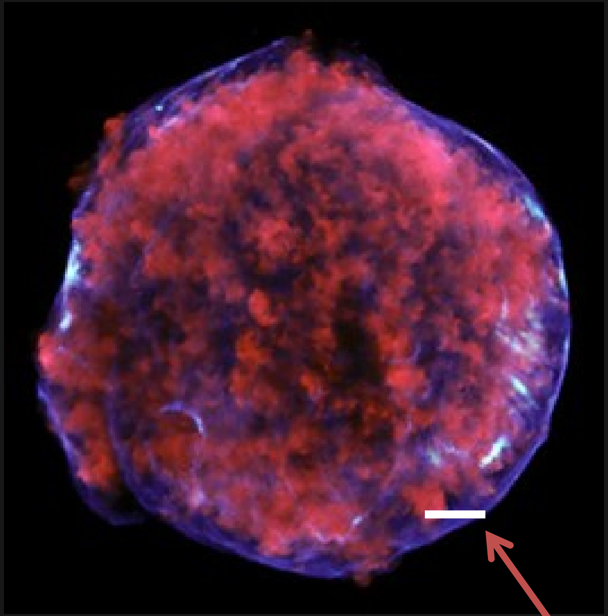
Derive the distribution function $f = \sum \delta(x - x_i)\delta(p - p_i)$

Solve Maxwell‘s equations on a grid

Interpolate information between grid points and particles

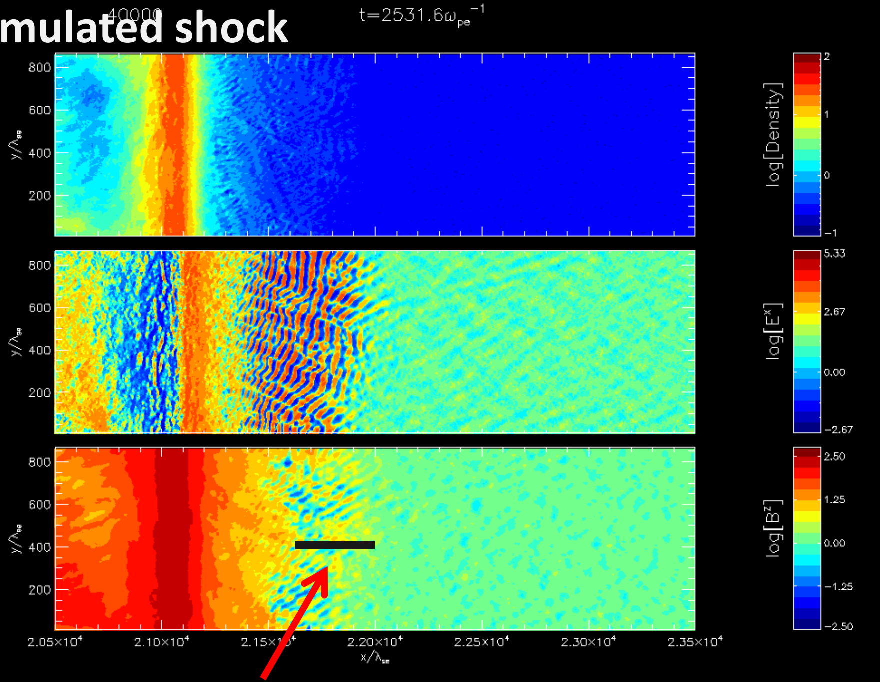
The challenge

Supernova remnant



1 light-year

Simulated shock



1 light-millisecond

The challenge

We use fluid methods for gas on large scales

We use kinetic methods for gas on very small scales

We always use kinetic methods fo energetic particles

The challenge

PIC simulations must resolve the electron skin length

- Can model shocks and plasma instabilities
- but not the big picture

Grid scale $\Delta << \lambda_s$ ➔ Need length exceeding $10^4\Delta$ per direction

Suppose 100 particles per cell ➔ at least 10^{10} particles in 2D

➔ At least TB-scale RAM needed ➔ massive parallelization

The How-to

Start with a solution to Maxwell‘s equation

→ You only need to update the fields

$$\delta B \propto \nabla x E + j \qquad \Rightarrow \nabla \delta B = \nabla j = \frac{\partial n_e}{\partial t} = \nabla \frac{\partial E}{\partial t} = 0$$

Keeping all particles and having number continuity implies we only solve time-derivative equations.

The How-to

Field update $\delta E = \delta t \ \nabla x B$

How to solve this equation?

Explicitly using a staggered grid

B and E displaced by a half timestep

B and E also spatially displaced by half a grid cell

The How-to

Consider $\frac{\partial X}{\partial t} = Y(t)$ and solve for discrete t_i

Taylor-expand *Y(t)* around $t_{i+0.5}$ and integrate.

$$X(i+1) = X(i) + \delta t\, Y(i+0.5) + \mathcal{O}(\delta t^2)$$

Automatically second-order accurate.
Implicit methods are better, but much more expensive.

The How-to

Consider $\frac{\partial}{\partial x} X(x,t) = \frac{\partial}{\partial t} Y(x,t)$ and solve for discrete x_i

and assume $X, Y \propto \exp(ikx - i\omega t)$

You find

$$\frac{\tilde{X}}{\Delta} \sin\left(\frac{k\Delta}{2}\right) = -\frac{\tilde{Y}}{\delta t} \sin\left(\frac{\omega \delta t}{2}\right)$$

The How-to

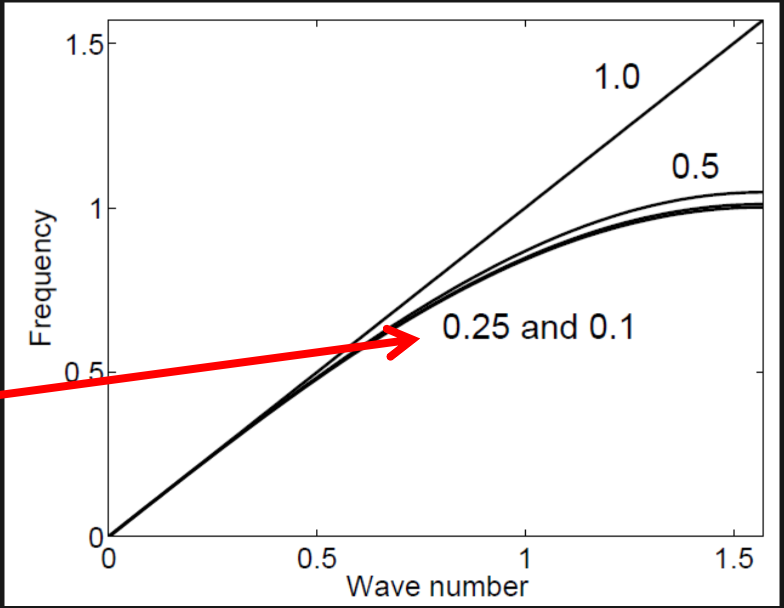
Amplication to electromagnetic waves

Dispersion relation in vacuum

Phase speed below *c*

CFL Parameter $\frac{c\,\delta t}{\Delta}$

Grid Cherenkov instability



The How-to

We use a finite number of particles per cell

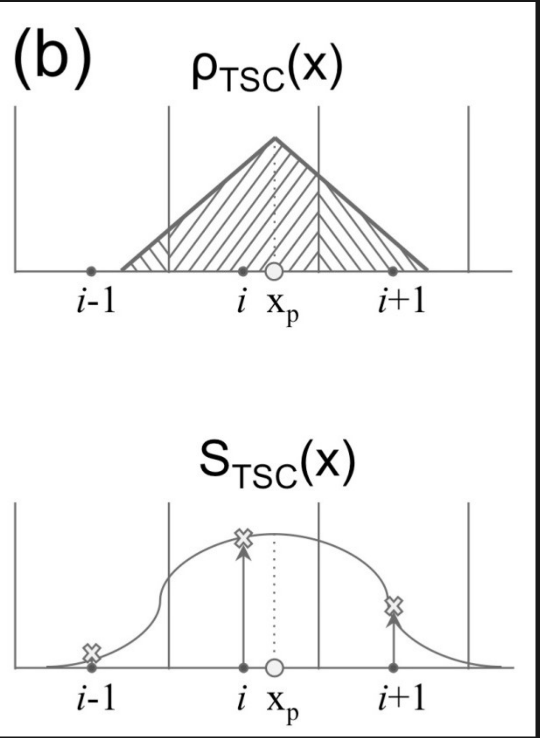
- Residual collisions
- Spurious heating
- Missing resonances

Residual collisions

If particles were point-like
→ electrostatic potential ~ 1/r

Treat particles as extended structures

- Suppresses binary collisions
- Provides interpolation to grid



Residual collisions

Scattering involves fluctuations in the density of particles, *n*

Consider a box of size R at distance R left and right of trajectory

Deflection by density fluctuation $\sqrt{nR^3}$

Mean free path for scattering $\lambda \propto n$

Optimization needed between low collisionality and expense

Residual collisions

Electric field fluctuations over shape size, *R*

$$E \propto \frac{q\sqrt{nR^3}}{R^2} \propto \frac{1}{\sqrt{nR}}$$

Equipartition of field noise with temperature

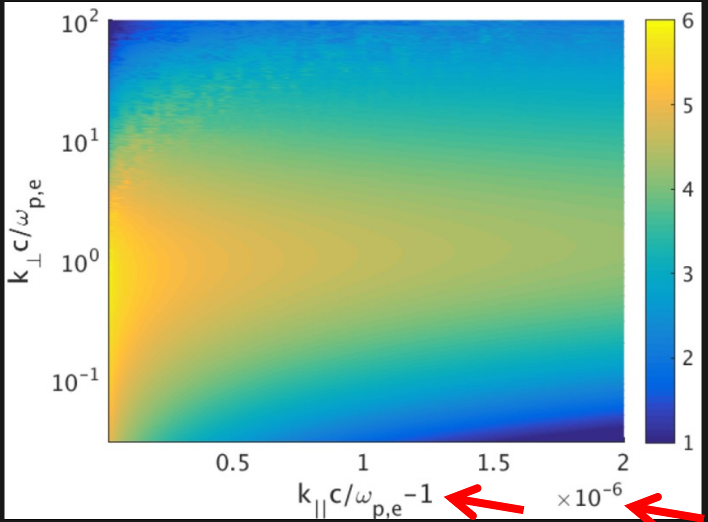
$$U_{ES} \propto \frac{1}{nR} \propto kT$$

Cold plasma requires many simulated particles

Missing resonances

Plasma instabilities may involve narrow resonances

Growth rate real parameters



TeV pair beams in intergalactic space

Longitudinal electrostatic mode

Velocity resonance

Missing resonances

- We must have particles in the resonance band → large *n*
- Our grid must carry the frequency/wavenumber

Grid of N cells of size Δ

→ $\delta k = 2\pi/N\Delta$ must be smaller than Δk of resonance
AND resonance must be covered by the grid, $\delta k/k > 2/N$

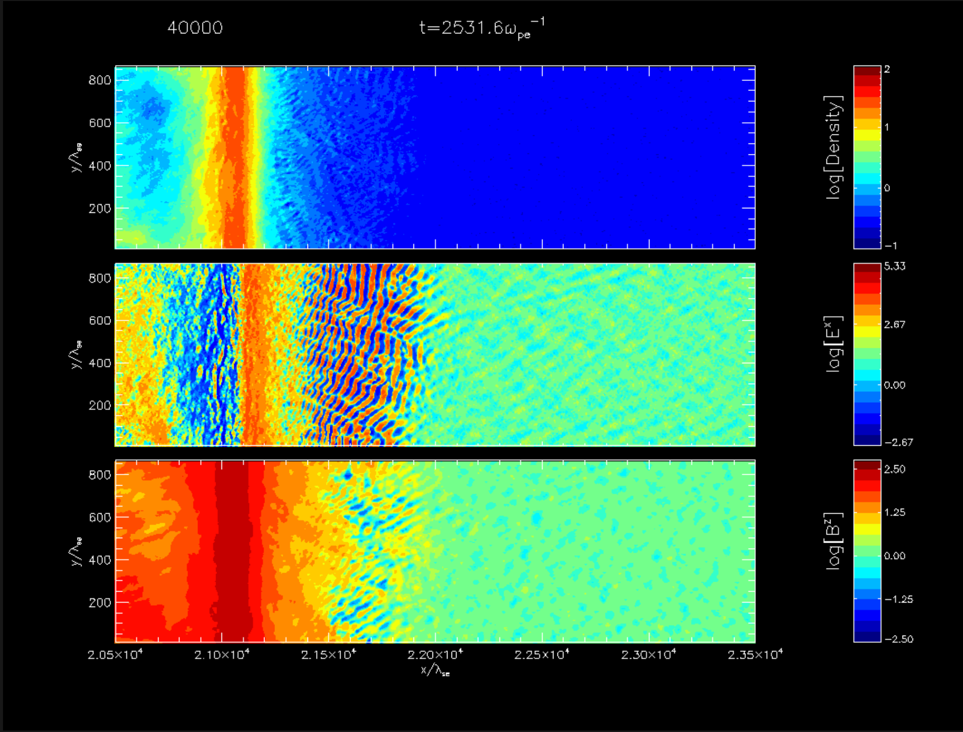
Lower and upper limit on δk!

The How-to: scales

Collisionless shock:
Thickness given by ion gyration

$$L = \frac{v_{sh}}{\Omega_i} = \frac{c v_{sh}}{v_A \omega_{pi}} = M_A \lambda_s \sqrt{\frac{m_i}{m_e}}$$

Too many grid cells?
-> Reduce mass ratio
and resolution



Summary

PIC simulations are an ab-initio tool to study kinetic processes

Particularly useful for collisionless media in space

Besides the Vlasov equation the only means to obtain the distribution function

Limited range of scales even for modified parameters (e.g. mass ratio)

Technically and computationally very demanding