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Basic Plasma Physics and PIC Simulation

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I. Basic Plasma Physics

1. What is a plasma ?

- It is often said that plasma is the 4th state of matter.
 - solid, liquid, gas \rightarrow plasma
- The word “plasma” comes from the Greek “πλάσμα, -ατοζ, το” which means something molded or fabricated.
- Plasma was called for the first time by Langmuir and Tonks, in 1929.

Definition of plasma

- *A plasma is a quasineutral gas of charged (and neutral) particles which exhibit collective behavior.* by F.F. Chen
 - Collective ?
- Important physical parameter of plasma
 - Debye length λ_D
 - Plasma frequency ω_{pe}

Plasma parameter (1)

$$\lambda_D \ll L$$

The physical dimension of the system (L) is very large compared to Debye length.

$$n\lambda_D^3 \gg 1 \quad \longleftrightarrow \quad \frac{e^2}{r_0} \ll T \quad r_0 \text{ is the distance between particles}$$

The number of particles inside a Debye sphere needs to be very large.

Coulomb potential energy is much less than thermal energy (particle kinetic energy).

Plasma parameter (2)

$$\omega_{pe} > \nu_{en}$$

Collision frequency between electrons and neutral particles (ν_{en}) is smaller than the electron plasma frequency.

Basic equations

$$m_j \frac{d(\gamma_j \mathbf{v}_j)}{dt} = q_j \left(\mathbf{E} + \frac{\mathbf{v}_j}{c} \times \mathbf{B} \right)$$

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v}_j$$

$$\gamma_j = 1 / \sqrt{1 - \mathbf{v}_j^2 / c^2}$$

$$\begin{cases} \mathbf{j}(\mathbf{x}, t) = \sum_j q_j \mathbf{v}_j(t) \delta[\mathbf{x} - \mathbf{x}_j(t)] \\ \rho(\mathbf{x}, t) = \sum_j q_j \delta[\mathbf{x} - \mathbf{x}_j(t)] \end{cases}$$

$$\frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \frac{4\pi}{c} \mathbf{j}$$

$$\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\nabla \cdot \mathbf{E} = 4\pi \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

2. Single particle motion

- Let us consider particle motions in the given electromagnetic field.
 - Cyclotron motion
 - $\mathbf{E} \times \mathbf{B}$ drift
 - Drift due to external force
 - Gradient B drift
 - Curvature drift

Cyclotron motion (1)

$$m_j \frac{d\mathbf{v}_j}{dt} = q_j \left(\frac{\mathbf{v}_j}{c} \times \mathbf{B} \right)$$

$$\mathbf{B} = (0, 0, B)$$

$$\frac{dv_{jx}}{dt} = - \left(\frac{q_j B}{m_j c} \right)^2 v_{jx}$$

$$\frac{dv_{jx}}{dt} = \frac{q_j B}{m_j c} v_{jy}$$

$$\frac{dv_{jy}}{dt} = - \frac{q_j B}{m_j c} v_{jx}$$

$$\frac{dv_{jz}}{dt} = 0$$

$$v_{jx} = v_{\perp} \sin \omega_{cj} t$$

$$v_{jy} = v_{\perp} \cos \omega_{cj} t$$

$$v_{jz} = v_{\parallel}$$

$$\omega_{cj} = \frac{q_j B}{m_j c}$$

Cyclotron motion (2)

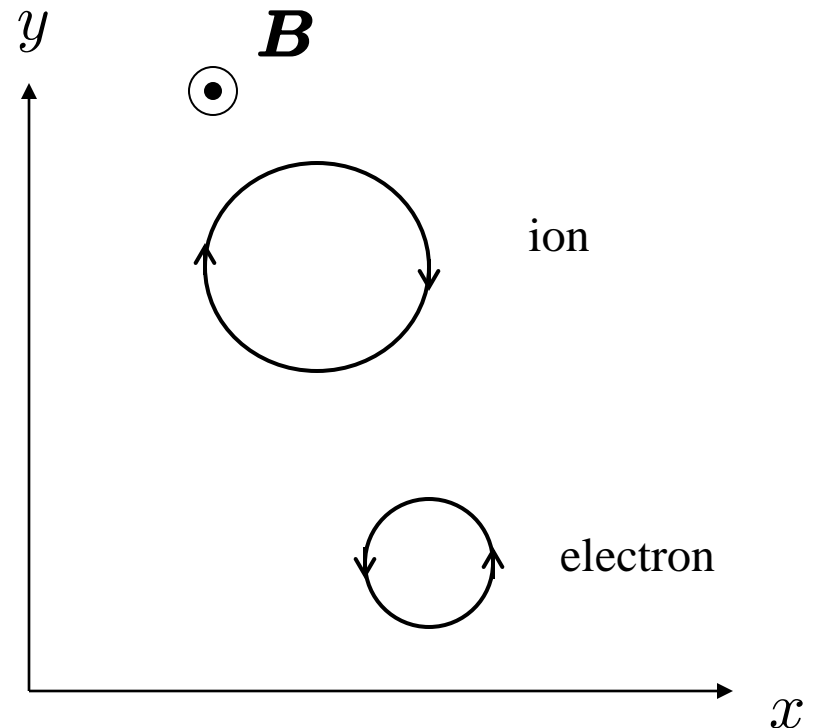
$$x_j = -\rho_L \cos \omega_{cj} t$$

$$y_j = \rho_L \sin \omega_{cj} t$$

$$z_j = v_{//} t$$

$$\omega_{cj} = \frac{q_j B}{m_j c} \quad \begin{array}{l} \text{Cyclotron frequency} \\ \text{(gyro frequency)} \end{array}$$

$$\rho_L = \frac{v_{\perp}}{\omega_{cj}} \quad \begin{array}{l} \text{Larmor radius} \\ \text{(gyro radius)} \end{array}$$



$\mathbf{E} \times \mathbf{B}$ drift

$$m_j \frac{d\mathbf{v}_j}{dt} = q_j \left(\mathbf{E} + \frac{\mathbf{v}_j}{c} \times \mathbf{B} \right)$$

$$\mathbf{E} = (0, E, 0), \mathbf{B} = (0, 0, B)$$

$$\frac{dv_{jx}}{dt} = \frac{q_j B}{m_j c} v_{jy}$$

$$\frac{dv_{jy}}{dt} = \frac{q_j}{m_j} E - \frac{q_j B}{m_j c} v_{jx}$$

$$\frac{dv_{jz}}{dt} = 0$$

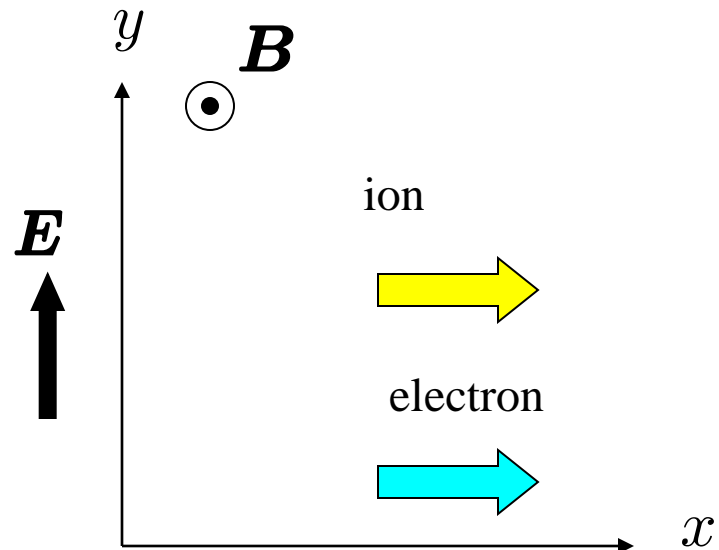
$$v_{jx} = \boxed{c \frac{E}{B}} + v_{\perp} \sin \omega_{cj} t$$

$\mathbf{E} \times \mathbf{B}$ drift

$$v_{jy} = v_{\perp} \cos \omega_{cj} t$$

$$v_{jz} = v_{//}$$

$$\mathbf{v}_{Ej} = c \frac{\mathbf{E} \times \mathbf{B}}{B^2}$$



Drift due to external force

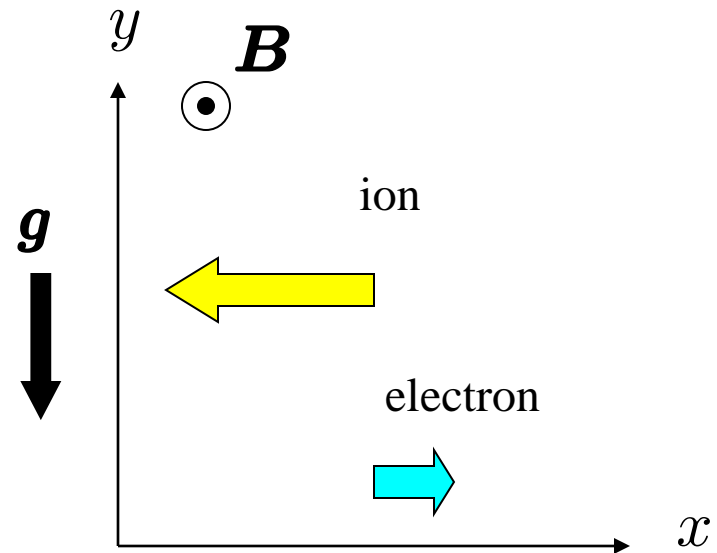
$$m_j \frac{d\mathbf{v}_j}{dt} = \mathbf{F} + q_j \left(\frac{\mathbf{v}_j}{c} \times \mathbf{B} \right)$$

$$\mathbf{v}_{Fj} = \frac{c}{q_j} \frac{\mathbf{F} \times \mathbf{B}}{B^2}$$

For example, $\mathbf{F} = m_j \mathbf{g}$

$$\mathbf{v}_{Fj} = \frac{m_j c}{q_j} \frac{\mathbf{g} \times \mathbf{B}}{B^2}$$

Gravitational drift



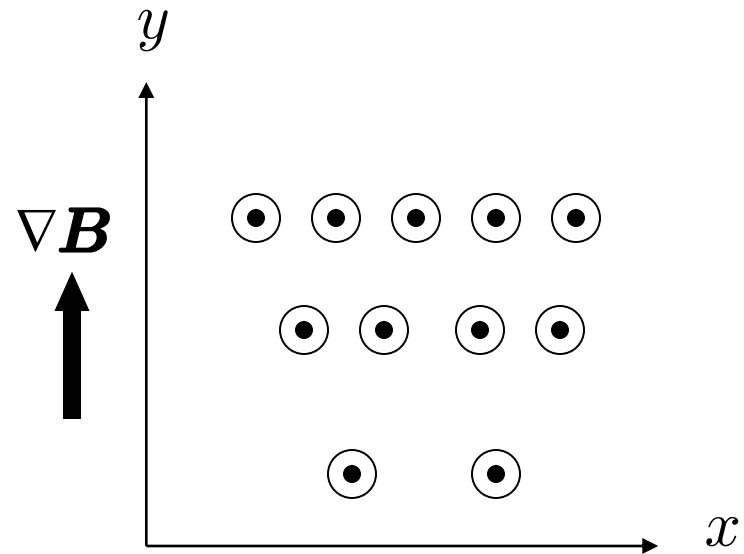
Gradient B drift (1)

$$m_j \frac{d\mathbf{v}_j}{dt} = q_j \left(\frac{\mathbf{v}_j}{c} \times \mathbf{B} \right) = \mathbf{F}$$

$$\mathbf{B} = (0, 0, B(y))$$

$$\mathbf{B} = \mathbf{B}_0 + (\mathbf{r} \cdot \nabla) \mathbf{B} + \dots$$

$$B(y) = B(0) + y \frac{\partial B}{\partial y} + \dots$$



$$F_y = -q_j \frac{v_{jx}}{c} B(y)$$

$$= -q_j \frac{v_{\perp}}{c} \sin \omega_{cj} t \left[B(0) + \rho_L \sin \omega_{cj} t \frac{\partial B}{\partial y} \right]$$

Gradient B drift (2)

$$\begin{aligned}\langle F_y \rangle &= -q_j \frac{v_\perp}{c} \langle \sin \omega_{cj} t \rangle B(0) \\ &\quad - \frac{q_j \omega_{cj} \rho_L^2}{c} \langle \sin^2 \omega_{cj} t \rangle \frac{\partial B}{\partial y}\end{aligned}$$

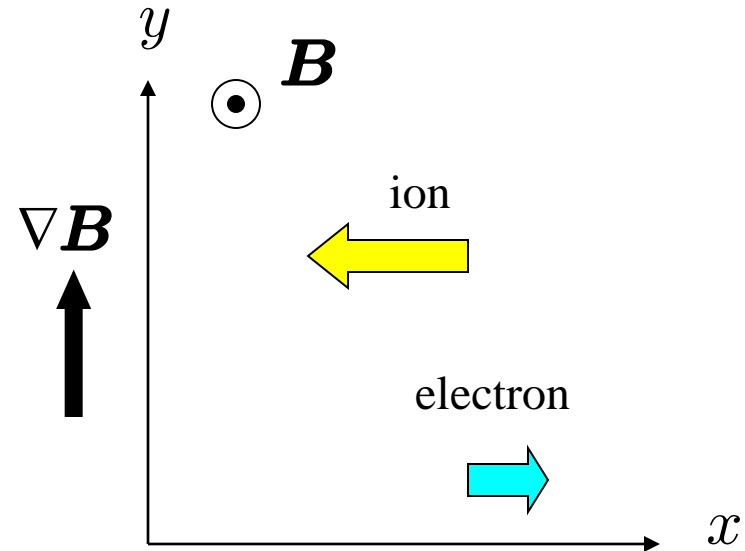
$$= -\frac{q_j \omega_{cj} \rho_L^2}{2c} \frac{\partial B}{\partial y}$$

$$\langle \mathbf{F} \rangle = -\frac{q_j \omega_{cj} \rho_L^2}{2c} \nabla B$$

$$\mathbf{v}_{Fj} = \frac{c}{q_j} \frac{\mathbf{F} \times \mathbf{B}}{B^2}$$

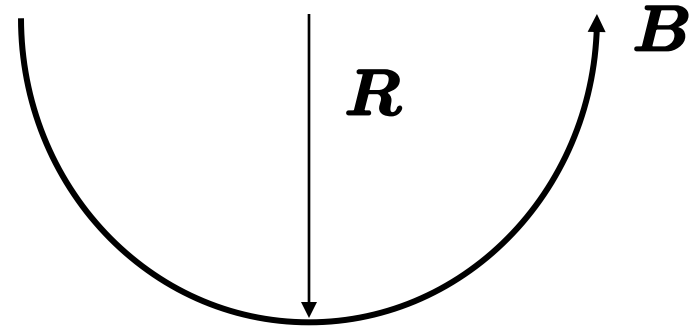
Gradient B drift

$$\mathbf{v}_{\nabla B j} = \frac{\omega_{cj} \rho_L^2}{2} \frac{\mathbf{B} \times \nabla B}{B^2}$$



Curvature drift

Curved magnetic field line with a constant radius of curvature R



We consider the motion along the field line. The particle experience a centrifugal force \mathbf{F}_c from curvature.

$$\mathbf{F}_c = \frac{m_j v_{||}^2}{R^2} \mathbf{R}$$

$$\mathbf{v}_{Fj} = \frac{c}{q_j} \frac{\mathbf{F} \times \mathbf{B}}{B^2}$$

Curvature drift

$$\mathbf{v}_{Rj} = \frac{v_{j||}^2}{\omega_{cj} R^2} \frac{\mathbf{R} \times \mathbf{B}}{B}$$

3. Collective behavior

- Debye shielding
- Plasma oscillation

Debye shielding (1)

The charged particles in a plasma arrange themselves so as to effectively shield electrostatic fields within a distance of the order of the Debye length.

Boltzmann distribution

$$n_e = n_0 \exp[e\phi/T_e] \approx n_0(1 + e\phi/T_e)$$

$$n_i = n_0 \exp[-e\phi/T_i] \approx n_0(1 - e\phi/T_i)$$

Poisson equation

$$\nabla^2\phi = -4\pi[e(n_i - n_e) + q\delta(r)]$$

for $r > 0$

$$\nabla^2\phi = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\phi}{dr} \right) = \left(\frac{4\pi n_0 e^2}{T_e} + \frac{4\pi n_0 e^2}{T_i} \right) \phi$$

Debye shielding (2)

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\varphi}{dr} \right) = \frac{1}{\lambda_D^2} \varphi$$

$$\varphi = f/r$$

$$\frac{d^2 f}{dr^2} = \frac{1}{\lambda_D^2} f$$

$$f = A \exp \left[-\frac{r}{\lambda_D} \right] + B \exp \left[\frac{r}{\lambda_D} \right]$$

$$\varphi = \frac{A}{r} \exp \left[-\frac{r}{\lambda_D} \right] + \frac{B}{r} \exp \left[\frac{r}{\lambda_D} \right]$$

$$r \rightarrow \infty, \varphi \rightarrow 0 \quad r \rightarrow 0, \nabla^2 \varphi = -4\pi q \delta(r), \therefore \varphi \rightarrow q/r$$

$$B = 0 \quad A = q$$

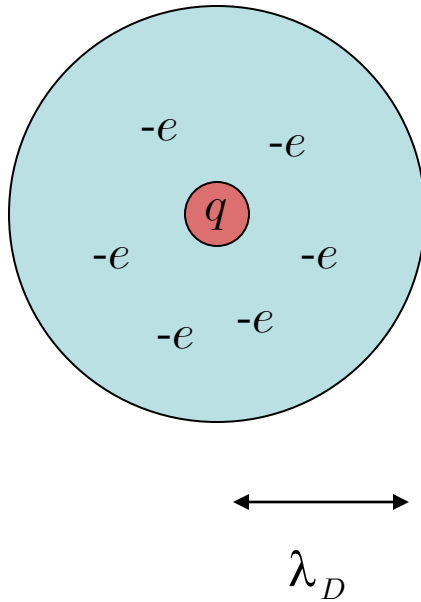
$$\varphi = \frac{q}{r} \exp \left[-\frac{r}{\lambda_D} \right]$$

$$\lambda_{De} = \sqrt{\frac{T_e}{4\pi n_0 e^2}}$$

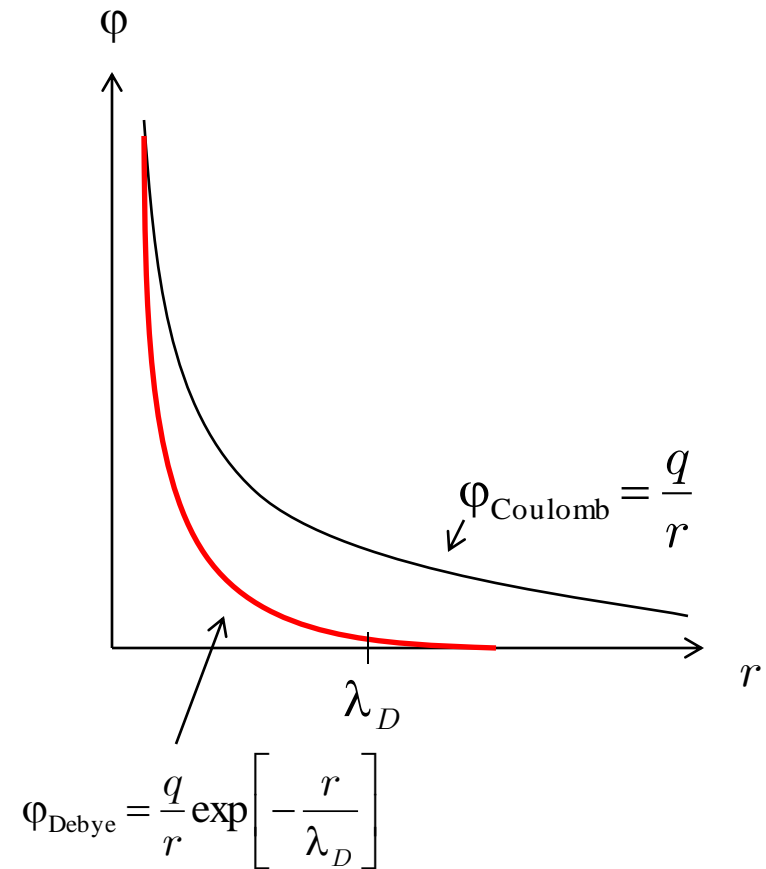
$$\lambda_{Di} = \sqrt{\frac{T_i}{4\pi n_0 e^2}}$$

$$\frac{1}{\lambda_D^2} = \frac{1}{\lambda_{De}^2} + \frac{1}{\lambda_{Di}^2}$$

Debye shielding (3)



Electrostatic field is shielded within a distance $\sim \lambda_D$.

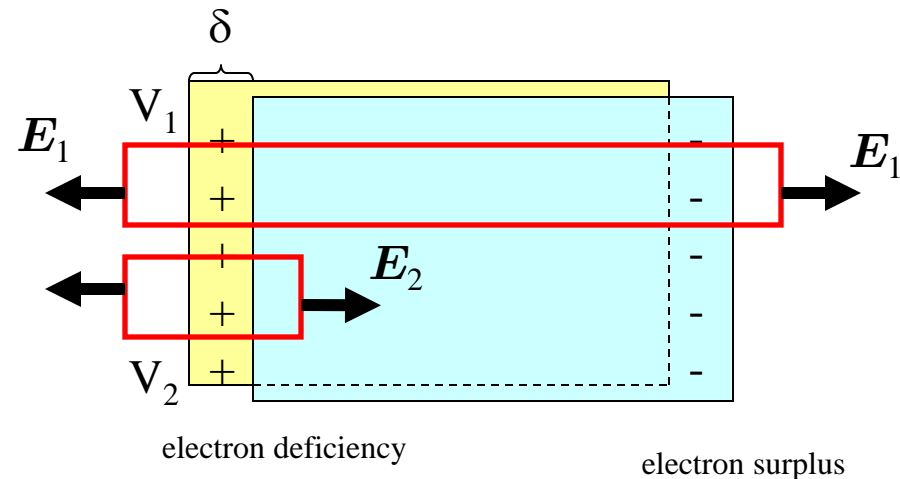


Plasma oscillation (1)

When electrons are instantaneously disturbed from equilibrium condition, resulting internal field tends to restore the original charge neutrality. Because of inertia, electrons overshoot and oscillate around the equilibrium positions.

$$\nabla \cdot \mathbf{E} = 4\pi\rho$$

$$\int \mathbf{E} \cdot \mathbf{n} dS = 4\pi \int \rho dV$$



For volume V_1

$$E_1 S_1 = 0$$

$$E_1 = 0$$

For volume V_2

$$E_1 S_1 + E_2 S_2 = 4\pi e n_0 \delta S_2$$

$$E_2 = 4\pi e n_0 \delta$$

Plasma oscillation (2)

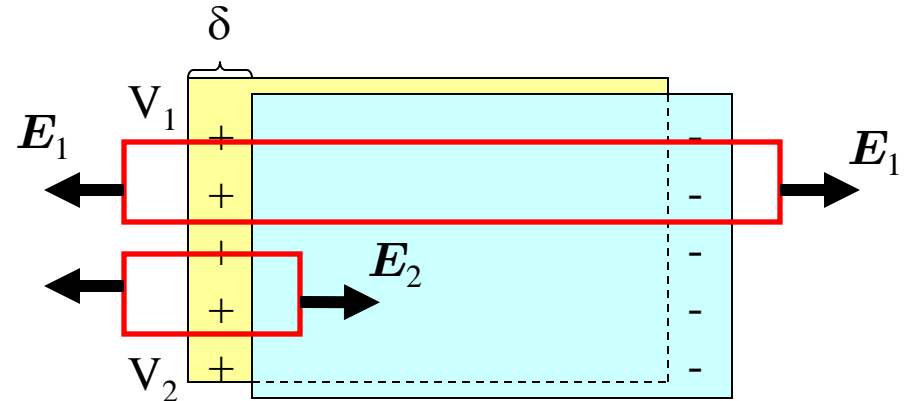
$$m \frac{d^2 \delta}{dt^2} = -e E_2$$

$$\frac{d^2 \delta}{dt^2} = -\frac{4\pi n_0 e^2}{m} \delta$$

$$\delta = \delta_0 \exp[-i\omega_{pe} t]$$

$$\omega_{pe} = \sqrt{\frac{4\pi n_0 e^2}{m}}$$

Electron plasma
frequency



References

- F. F. Chen: *Introduction to Plasma Physics and Controlled Fusion (second edition)*, Plenum press, 1984.
- J. A. Bittencourt: *Fundamental of Plasma Physics (third edition)*, Springer, 2004.
- N. A. Krall and A. W. Trivelpiece: *Principles of Plasma Physics*, McGRAW-HILL, 1973.

II. PIC simulation

4. Simulation method

- What is PIC simulation ?
- Basic equations and Normalization
- Super-particle and Finite-sized-particle
- Spatial grid
- Time step
- Cycle of PIC simulation
- Simulation stability

What is PIC simulation ?

- PIC (Particle-In-Cell) simulation is one of particle simulations.
 - Equations of motion for many particles
 - Maxwell equations for electromagnetic fields
- The name “PIC” represents a method how particle charges are assigned to the grid points (cell points) and field quantities are assigned to particles.

Basic equations

Equations of motion

$$m_j \frac{d(\gamma_j \mathbf{v}_j)}{dt} = q_j \left(\mathbf{E} + \frac{\mathbf{v}_j}{c} \times \mathbf{B} \right)$$

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v}_j$$

$$\gamma_j = 1 / \sqrt{1 - \mathbf{v}_j^2 / c^2}$$

j is particle name

$$\begin{cases} \mathbf{j}(\mathbf{x}, t) = \sum_j q_j \mathbf{v}_j(t) \delta[\mathbf{x} - \mathbf{x}_j(t)] \\ \rho(\mathbf{x}, t) = \sum_j q_j \delta[\mathbf{x} - \mathbf{x}_j(t)] \end{cases}$$

Maxwell equations

$$\frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \frac{4\pi}{c} \mathbf{j}$$

$$\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\nabla \cdot \mathbf{E} = 4\pi \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

Normalization

- In simulation, dimensionless quantities are usually used.

$$m = \tilde{m} m_e, q = \tilde{q} e, t = \tilde{t} / \omega_{ce}, v = \tilde{v} c$$

$$x = \tilde{x} c / \omega_{ce}, E = \tilde{E} \frac{m_e c \omega_{ce}}{e}, B = \tilde{B} \frac{m_e c \omega_{ce}}{e}$$

Super-particle (1)

- In real typical plasmas, number density is 10^8 - 10^{14}cm^{-3} , system size is 1m – over 1000km.
- It is impossible to calculate so many particles.
- Super-particle: one super-particle contains N real particles.
 - Charge: $q^{\text{sp}}=Nq$
 - Mass: $M^{\text{sp}}=Nm$

As a result, number density n/N , temperature NT

Super-particle (2)

■ Plasma parameters do not depend on N .

$$\lambda_{De}^{\text{SP}} = \sqrt{\frac{NT_e}{4\pi(n_0/N)(Ne)^2}} = \sqrt{\frac{T_e}{4\pi n_0 e^2}} = \lambda_{De}$$

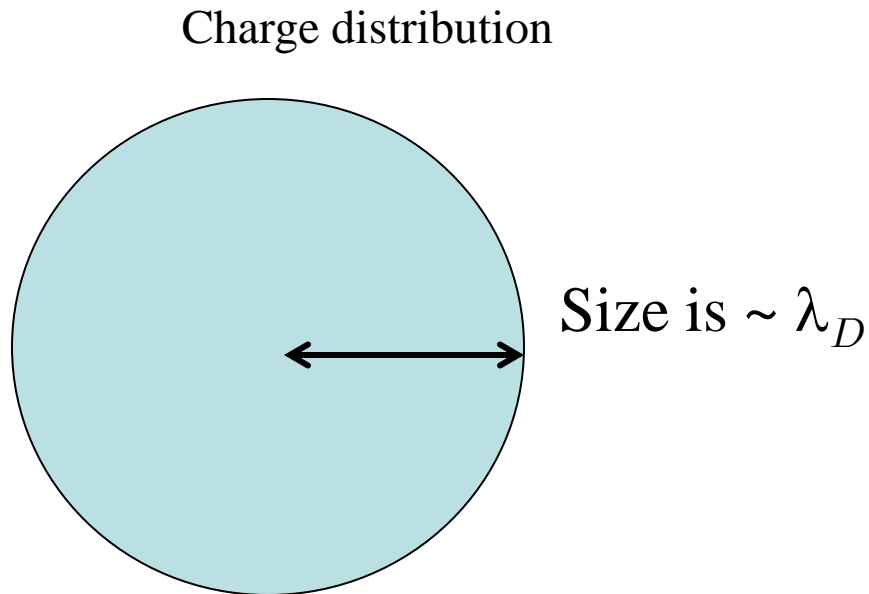
$$\omega_{pe}^{\text{SP}} = \sqrt{\frac{4\pi(n_0/N)(Ne)^2}{Nm}} = \sqrt{\frac{4\pi n_0 e^2}{m}} = \omega_{pe}$$

Cyclotron frequency is also not changed.

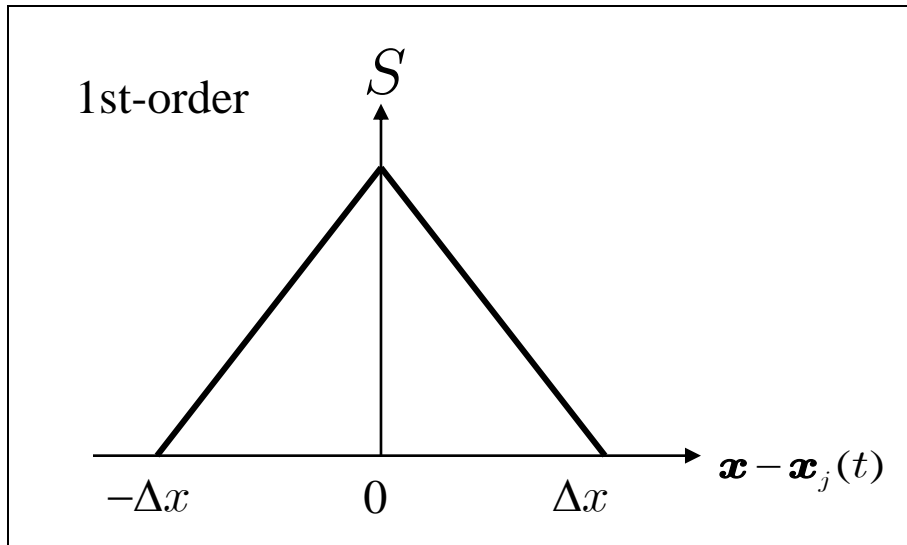
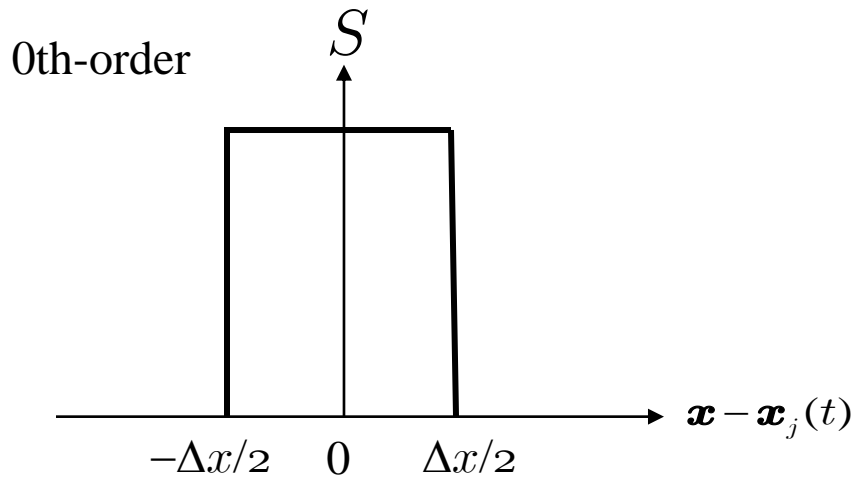
$$\omega_{ce}^{\text{SP}} = \frac{(Ne)B}{(Nm)c} = \frac{eB}{mc} = \omega_{ce}$$

Finite-sized-particle (1)

- Charge distributes in a finite-sized region.
- Mass is located only at the center.

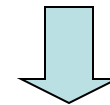


Finite-sized-particle (2)



Particle shape function S

$$\begin{cases} \mathbf{j}(\mathbf{x}, t) = \sum_j q_j \mathbf{v}_j(t) \delta[\mathbf{x} - \mathbf{x}_j(t)] \\ \rho(\mathbf{x}, t) = \sum_j q_j \delta[\mathbf{x} - \mathbf{x}_j(t)] \end{cases}$$



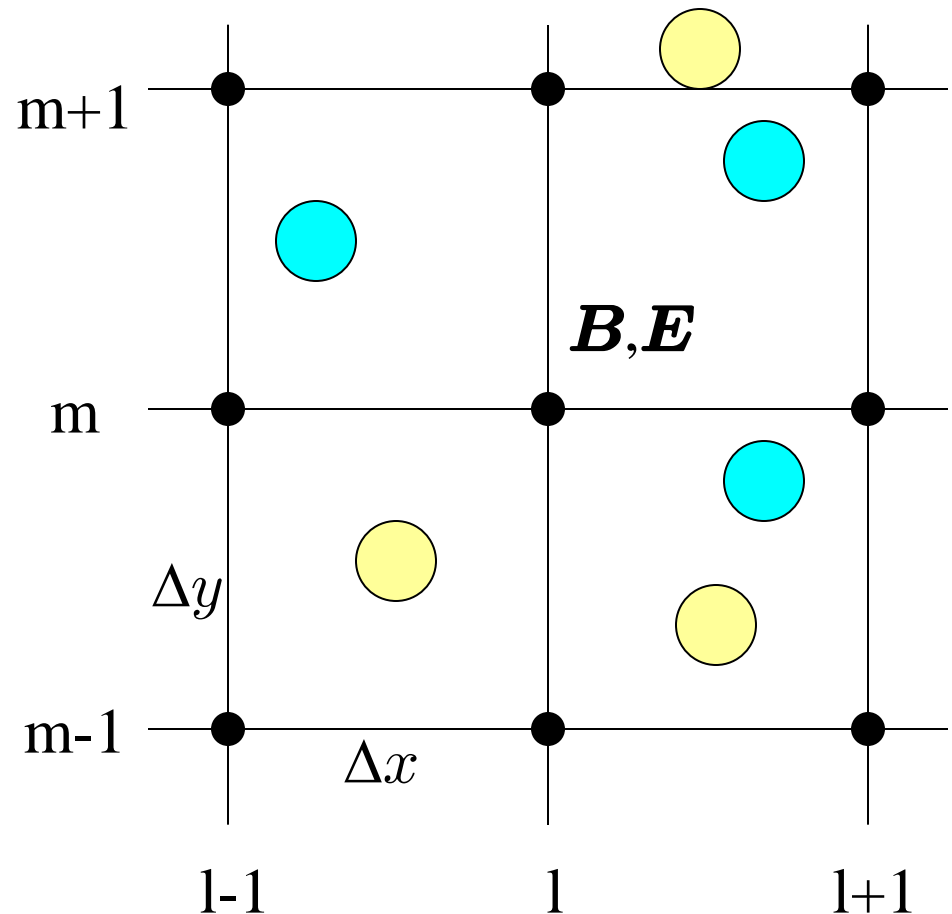
$$\begin{cases} \mathbf{j}(\mathbf{x}, t) = \sum_j q_j \mathbf{v}_j(t) S[\mathbf{x} - \mathbf{x}_j(t)] \\ \rho(\mathbf{x}, t) = \sum_j q_j S[\mathbf{x} - \mathbf{x}_j(t)] \end{cases}$$

Spatial grid

Field quantities can not be obtained at the continuous position (x, y, z) .

They are defined only on the grid points (l, m, n) .

On the other hand, particles positions \boldsymbol{x}_j are continuous.



$\Delta x, \Delta y, \Delta z$: grid spacing

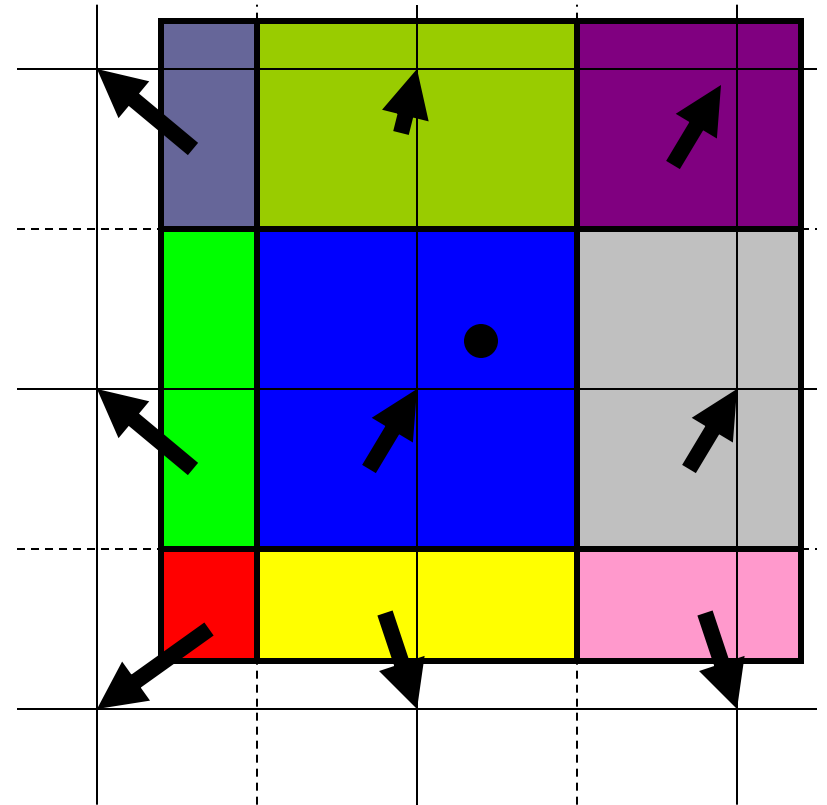
\mathbf{J} and ρ on the grid points

Current and charge densities on the grid point \mathbf{X}_{lmn}

$$\begin{cases} \mathbf{j}(\mathbf{X}_{lmn}) = \sum_j q_j \mathbf{v}_j S'[\mathbf{X}_{lmn} - \mathbf{x}_j] \\ \rho(\mathbf{X}_{lmn}) = \sum_j q_j S'[\mathbf{X}_{lmn} - \mathbf{x}_j] \end{cases}$$

$S'[\mathbf{X}_{lmn} - \mathbf{x}_j]$ is a weighting function.

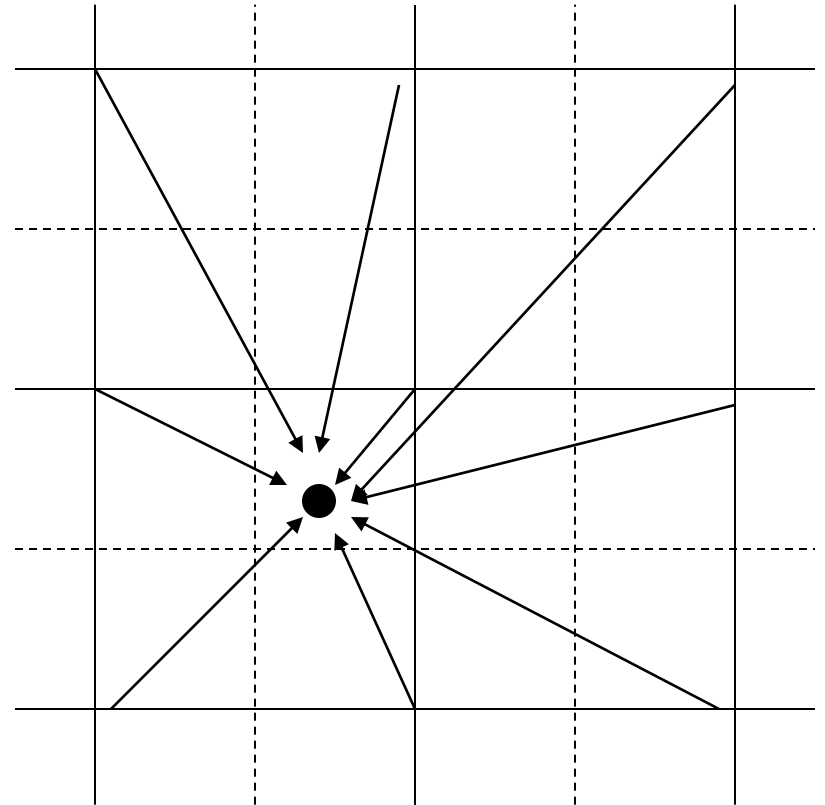
Weighting function S' is the average of shape function S over the grid (l, m, n) , and is different from shape function S .



E and ***B*** at the particle positions

Electric and magnetic fields
acting at particle position \mathbf{x}_j

$$\begin{cases} \mathbf{E}(\mathbf{x}_j) = \Delta x \Delta y \Delta z \sum_{lmn} \mathbf{E}(\mathbf{X}_{lmn}) S'[\mathbf{X}_{lmn} - \mathbf{x}_j] \\ \mathbf{B}(\mathbf{x}_j) = \Delta x \Delta y \Delta z \sum_{lmn} \mathbf{B}(\mathbf{X}_{lmn}) S'[\mathbf{X}_{lmn} - \mathbf{x}_j] \end{cases}$$



Space derivative

Differential equation \rightarrow Finite difference equation

$$\left(\frac{du}{dx}\right)_l = \frac{u_{l+1} - u_{l-1}}{2\Delta x} \quad \text{Centered difference}$$

Taylor expansion

$$u_{l+1} = u(x_l + \Delta x) = u_l + \left(\frac{du}{dx}\right)_l \Delta x + \frac{1}{2} \left(\frac{d^2u}{dx^2}\right)_l (\Delta x)^2 + O[(\Delta x)^3] \quad (1)$$

$$u_{l-1} = u(x_l - \Delta x) = u_l - \left(\frac{du}{dx}\right)_l \Delta x + \frac{1}{2} \left(\frac{d^2u}{dx^2}\right)_l (\Delta x)^2 + O[(\Delta x)^3] \quad (2)$$

$$(1) - (2) \quad u_{l+1} - u_{l-1} = 2 \left(\frac{du}{dx}\right)_l \Delta x + O[(\Delta x)^3]$$

$$\left(\frac{du}{dx}\right)_l = \frac{u_{l+1} - u_{l-1}}{2\Delta x} + O[(\Delta x)^2]$$

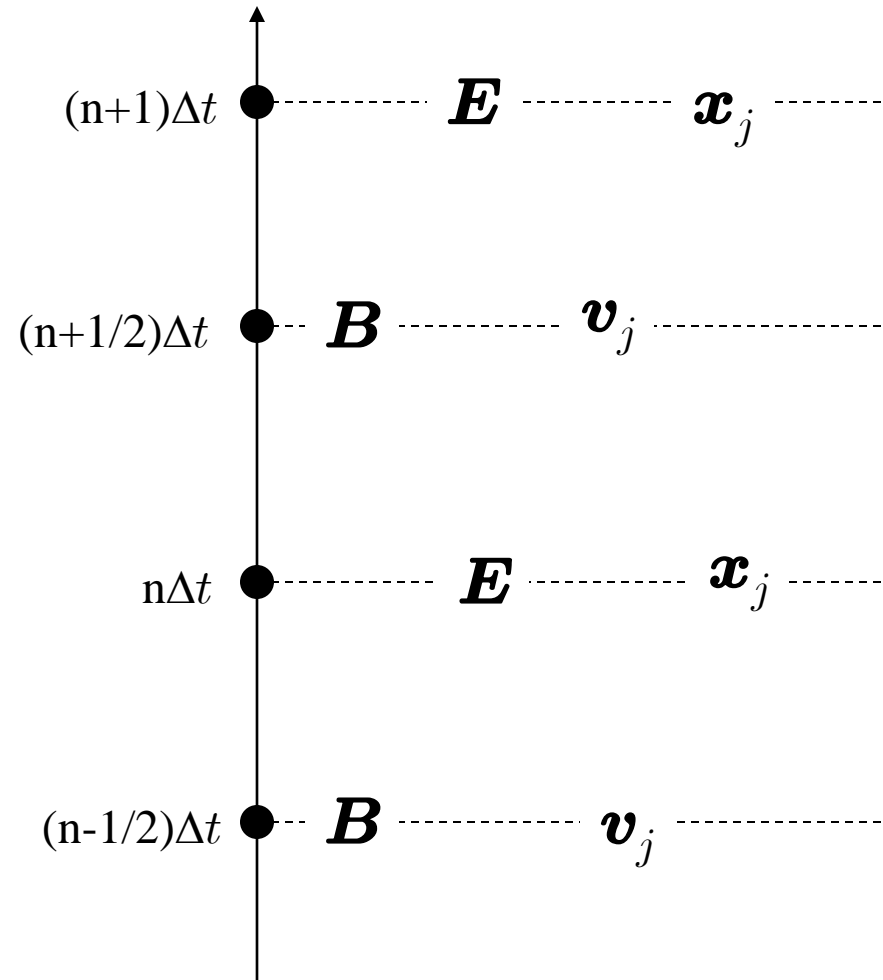
$$\left(\frac{du}{dx}\right)_l = \frac{u_{l+1} - u_l}{\Delta x} + O[\Delta x]$$

Time step (discrete)

All quantities can not be obtained at the continuous time t .

They are defined only at the discrete time $n\Delta t$ or $(n+1/2)\Delta t$.

Leap-Frog Method



Time integration

$$\frac{1}{c} \frac{\mathbf{B}^{(n+1/2)} - \mathbf{B}^{(n-1/2)}}{\Delta t} = -\nabla \times \mathbf{E}^{(n)}$$

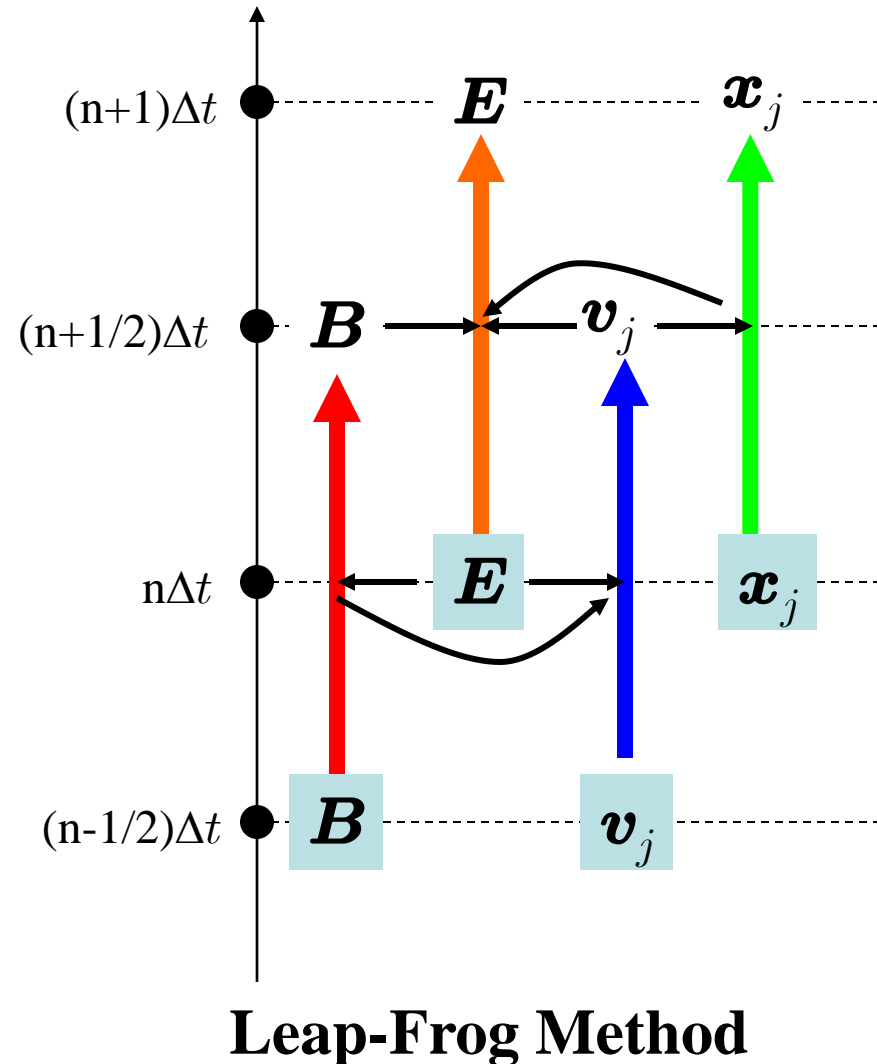
$$\frac{\mathbf{v}_j^{(n+1/2)} - \mathbf{v}_j^{(n-1/2)}}{\Delta t} = \frac{q_j}{m_j} \left(\mathbf{E}^{(n)} + \frac{\mathbf{v}_j^{(n+1/2)} + \mathbf{v}_j^{(n-1/2)}}{2c} \right)$$

$$\frac{\mathbf{x}_j^{(n+1)} - \mathbf{x}_j^{(n)}}{\Delta t} = \mathbf{v}_j^{(n+1/2)} \times \left[\frac{\mathbf{B}^{(n+1/2)} + \mathbf{B}^{(n-1/2)}}{2} \right] \mathbf{B}^{(n)}$$

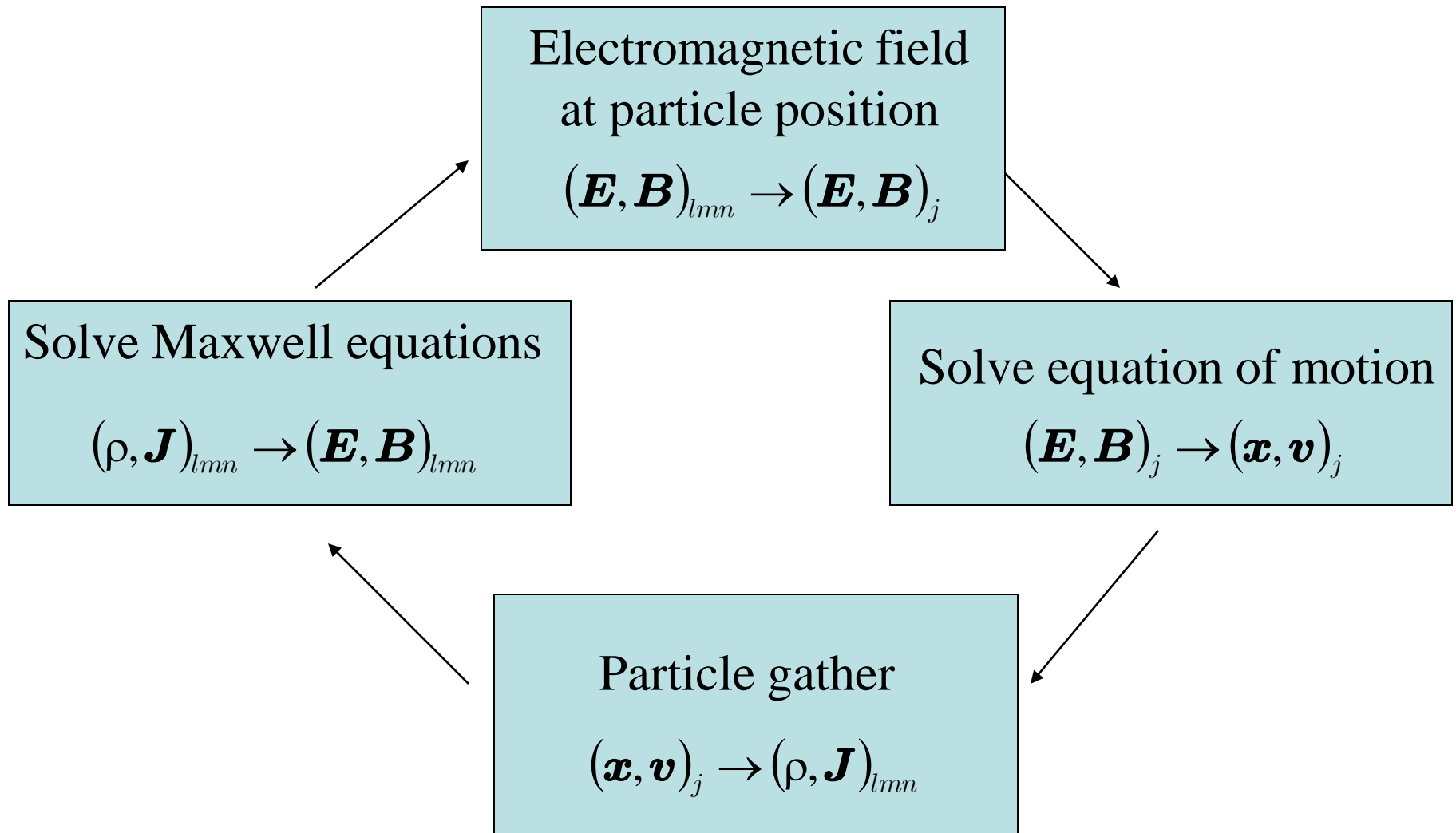
$$\frac{1}{c} \frac{\mathbf{E}^{(n+1)} - \mathbf{E}^{(n)}}{\Delta t} = \nabla \times \mathbf{B}^{(n+1/2)} - \frac{4\pi}{c} \mathbf{j}^{(n+1/2)}$$

$$\mathbf{j}^{(n+1/2)} = \sum_k q_k \mathbf{v}_k^{n+1/2} S[\mathbf{x} - \mathbf{x}_k^{(n+1/2)}]$$

$$\frac{\mathbf{x}_j^{(n+1/2)} - \mathbf{x}_j^{(n)}}{2\Delta t} = \mathbf{v}_j^{(n+1/2)}$$



Cycle of PIC simulation



Simulation stability

Grid spacing

$$\Delta x \leq \lambda_D$$

Time step width

$$\omega_{pe} \Delta t < 1$$

$$\omega_{ce} \Delta t < 1$$

Courant-Friedrichs-Lewy condition

$$\frac{\Delta x}{c \Delta t} > 1$$

References

- C. K. Birdsall and A. B. Langdon: *Plasma Physics via Computer Simulation*, IoP, 1991.

5. Application

■ Particle acceleration by magnetosonic shock waves

- hydrogen ion

- heavy ion

- electron

- relativistic fast ion

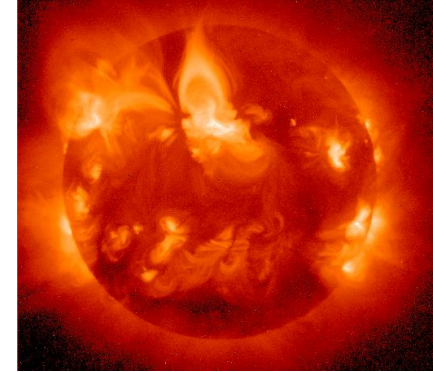
- positron

High-energy particles in the universe

■ Solar flare:

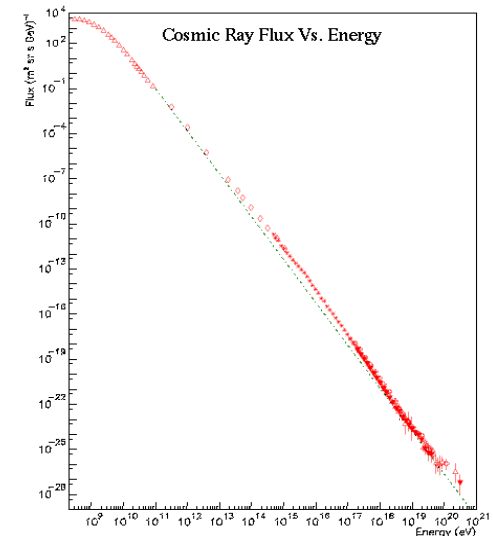
- Ion $10^9 \sim 10^{10}$ eV

- Electron $10^7 \sim 10^8$ eV



■ Cosmic ray:

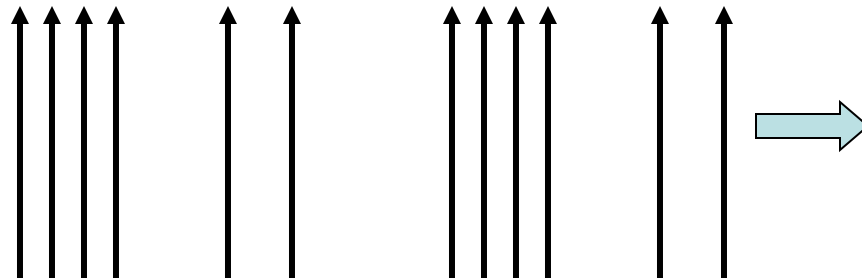
- Maximum 10^{20} eV



Researching acceleration mechanism of high-energy particles
with theory and computer simulations

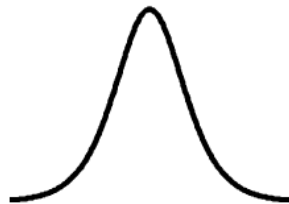
Magnetosonic wave

- Magnetosonic wave is a low-frequency electromagnetic wave propagating across the external magnetic field, causing compressions and rarefactions of magnetic pressure and plasma pressure.
 - Small-amplitude: linear sine wave
 - Large-amplitude: solitary wave, shock wave

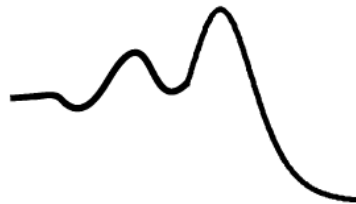


Magnetosonic shock wave

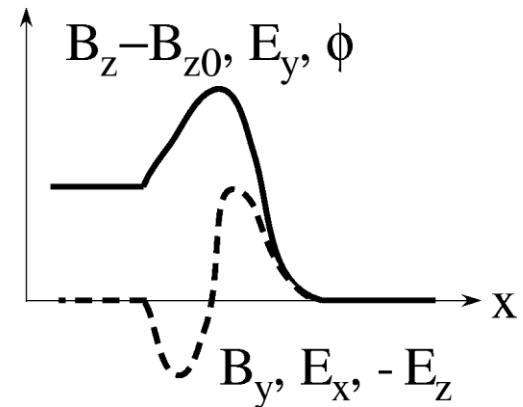
- Large-amplitude: a solitary wave is formed
- If there is dissipation, a solitary wave changes into a shock structure.



Solitary wave

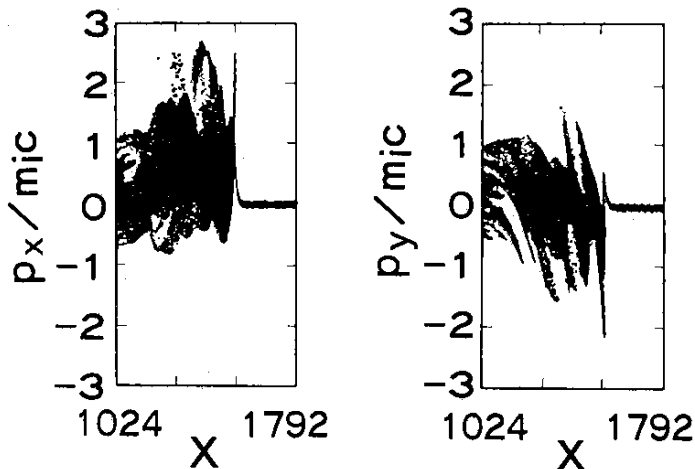
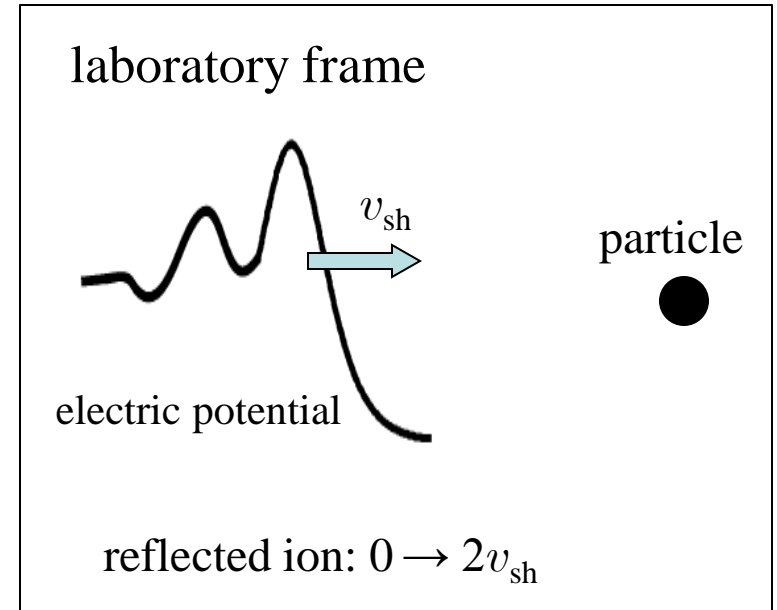
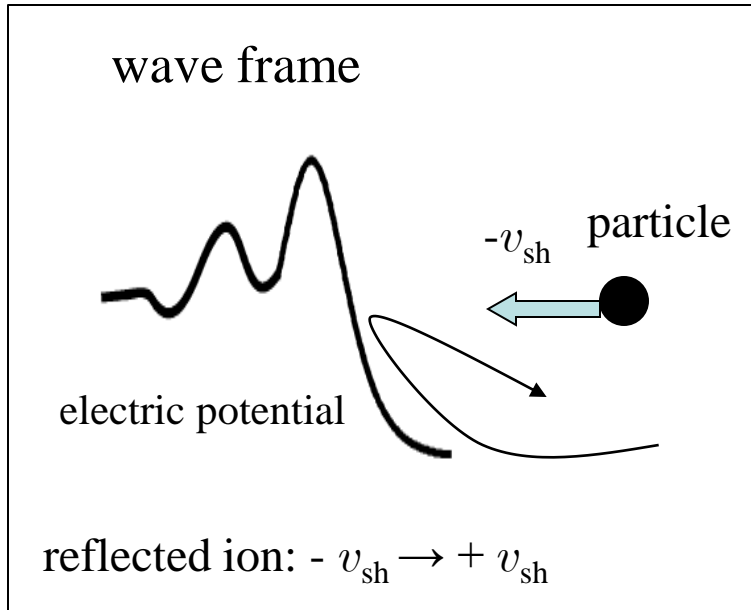


Shock wave



Electromagnetic field
structure of shock wave

Hydrogen ion acceleration

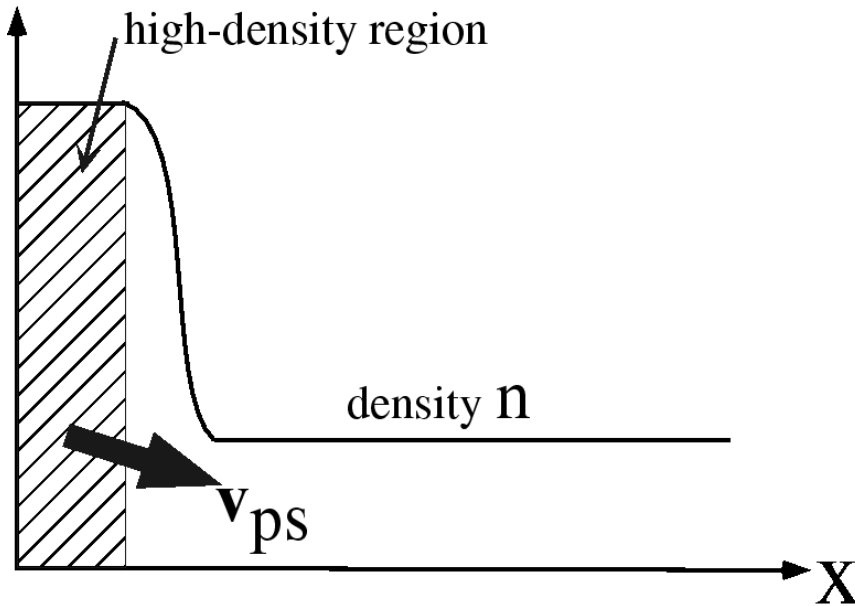


Shock waves can reflect some of the thermal hydrogen ions and accelerate them to high energies. These ions can have relativistic energies.

Enhanced acceleration of fast ions

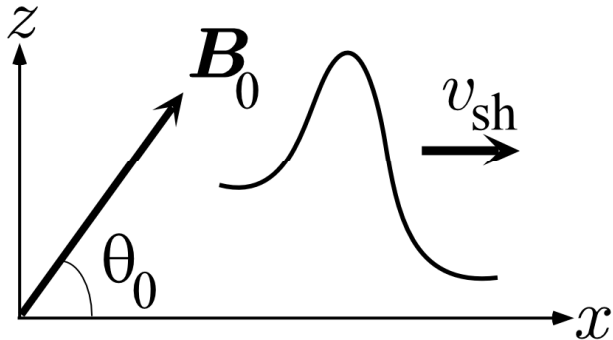
- Consider the case that when ions encounter a shock wave, they are already energetic (fast).
- Such nonthermal fast ions can be accelerated to much higher energies with a different mechanism.
- A part of such ions can suffer the acceleration process extremely many times.

How to excite shock wave

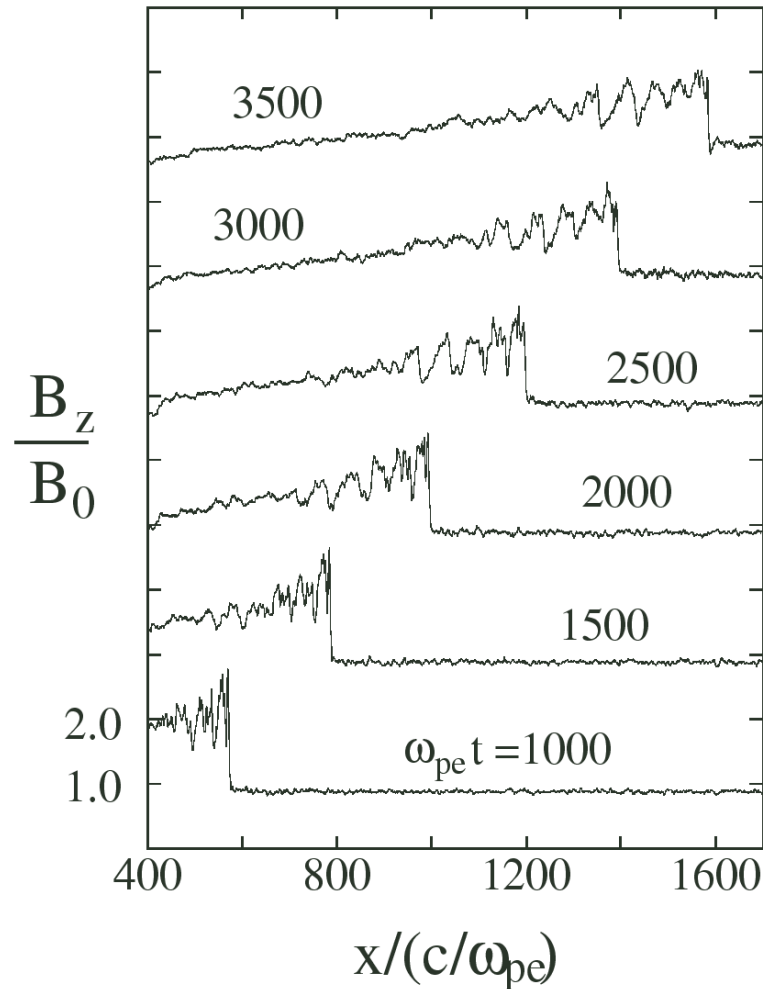


Particles in the shaded are initially have a shifted Maxwellian velocity distribution function. These particles act as a piston that pushes the neighboring particles and excite a shock wave.

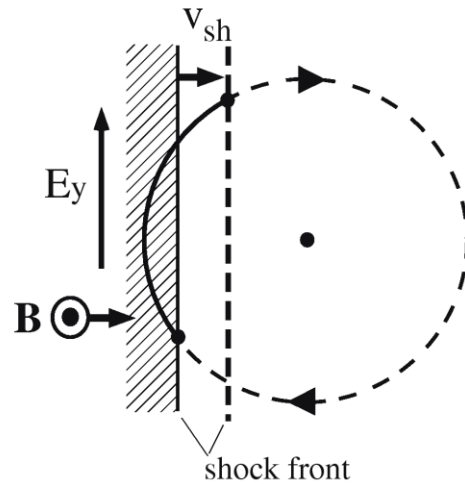
Propagation of a shock wave



Simulation result

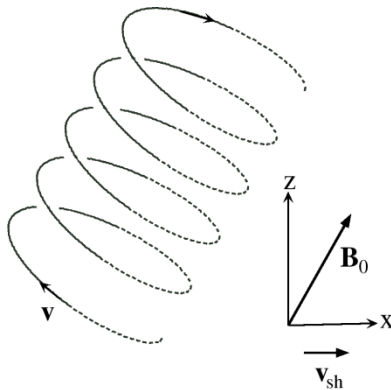


Acceleration mechanism of fast ions



While fast ions are in shock region, they gain energy from E_y .

If the time-averaged velocity v_x of the fast ion is nearly equal to v_{sh} , the fast ion can move with the shock wave for long period of time, and acceleration processes are repeated.



Unlimited acceleration?

Time-averaged velocity v_x

$$\langle v_x \rangle \cong v_{//} \cos \theta_0$$

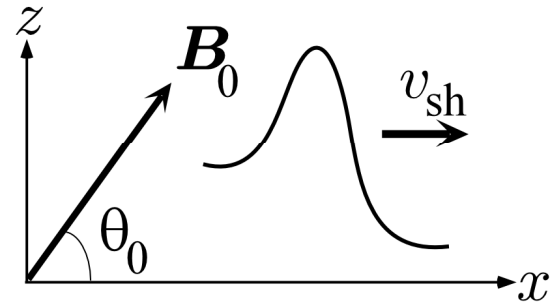
The condition that acceleration processes are repeated

$$\langle v_x \rangle \cong v_{//} \cos \theta_0 \cong v_{\text{sh}}$$

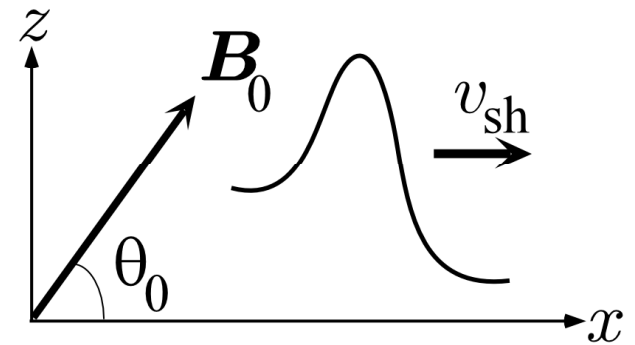
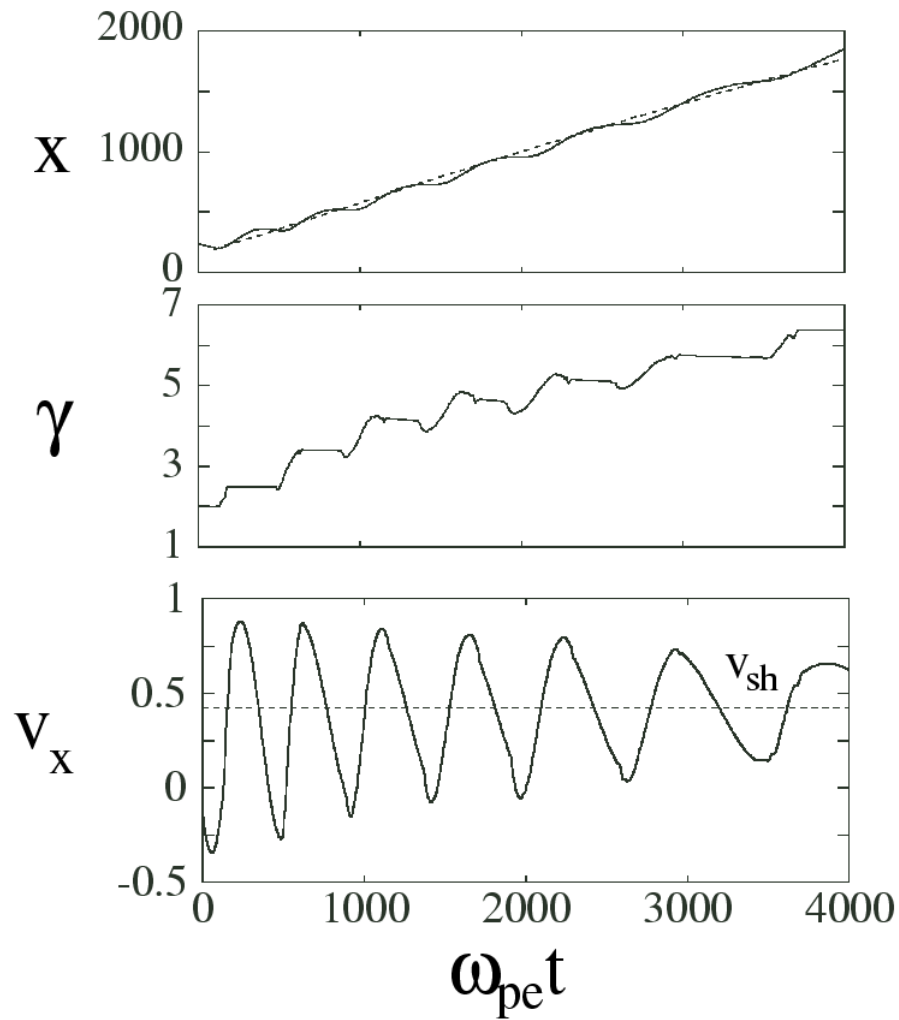
If shock speed is

$$v_{\text{sh}} \cong c \cos \theta_0$$

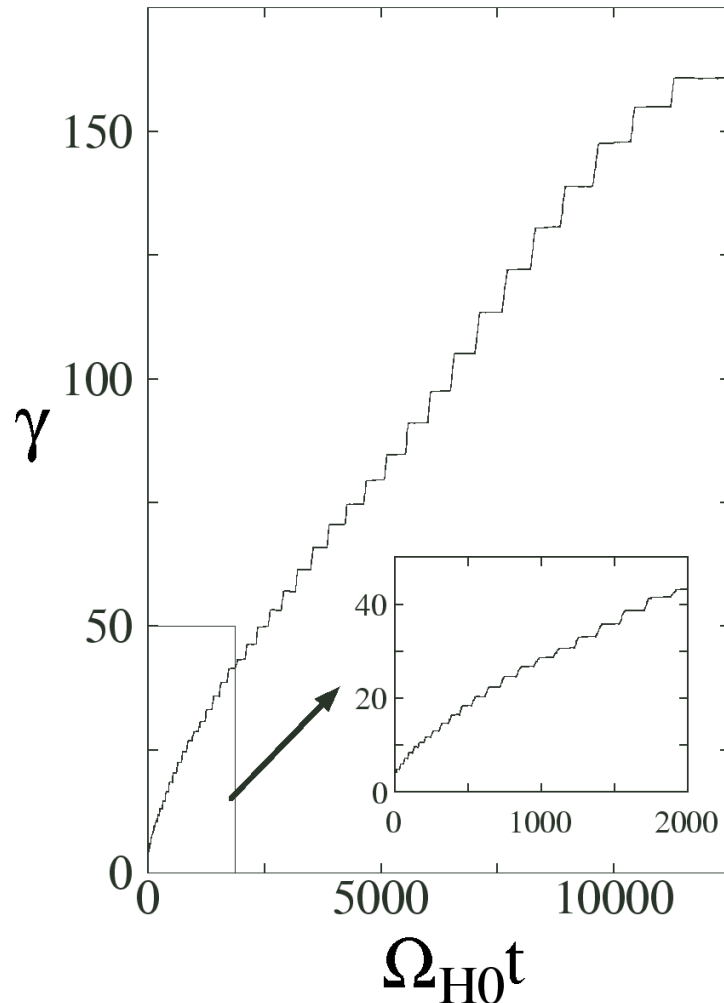
Due to the relativistic effect that $v_{//}$ can not exceed c , even though energy can increase indefinitely, particles can not outrun the shock wave and the acceleration process could repeat extremely long time.



PIC simulation results



(Test particle simulation)



The shock wave accelerated fast ions repeatedly.
This ion suffered energy jumps 42 times.
The Lorentz factor γ increased from $\gamma \sim 4$ to $\gamma \sim 160$.

References

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- S. Usami, H. Hasegawa, and Y. Ohsawa: Phys. Plasmas Vol.8, 2666-2672 (2001).
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