

# PIC Simulations 1

## Tutorial lecture

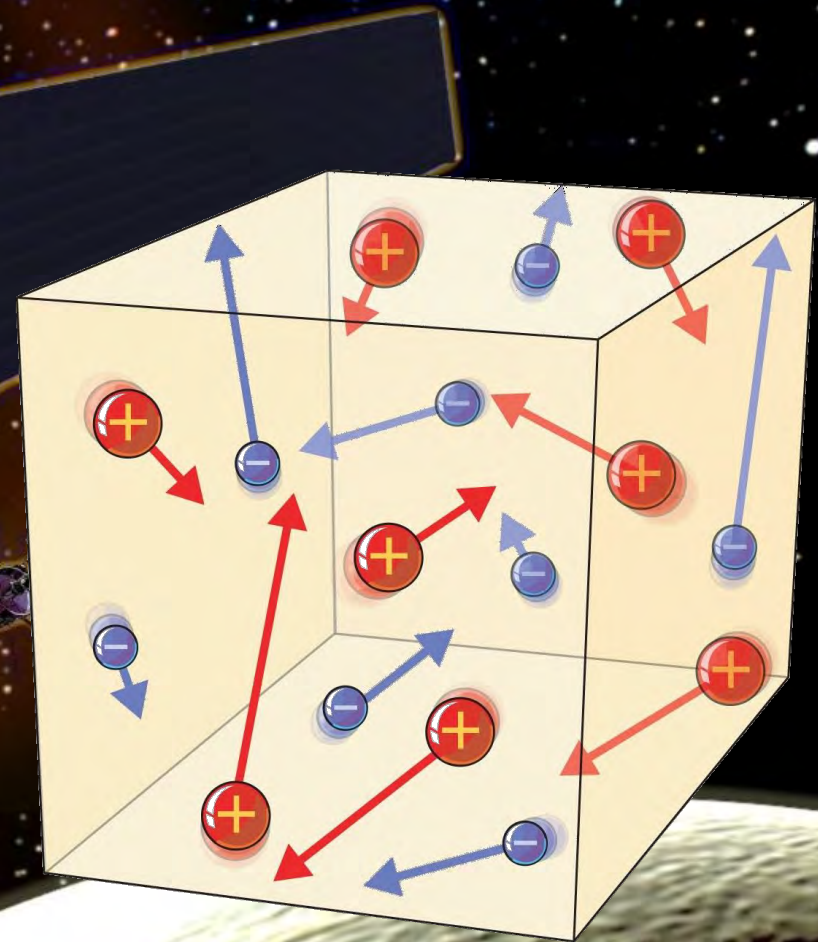
Yohei Miyake<sup>1\*</sup> and Yoshiharu Omura<sup>2</sup>

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# Space plasma

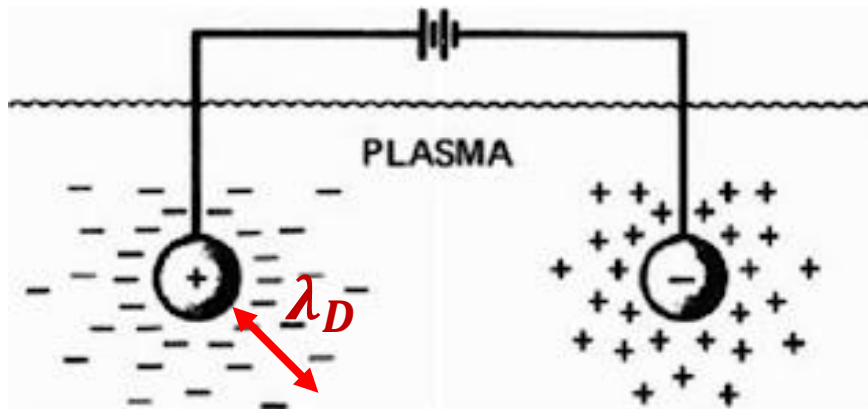
- 4th state of matter
- So hot: atoms split up into electrons & ions
- Quasi-neutral: same numbers of e & i
- Electrons & ions moving independently
- Dynamics influenced by electromagnetic forces
- Plasma current generates electromagnetic field
- Exhibiting “collective” behaviors



# Collective effects in shortest spatio-temporal scales

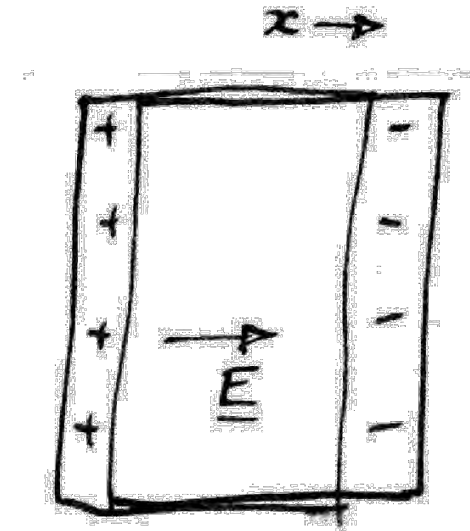
➤ Debye shielding

➤ Plasma oscillation



Debye length:

$$\lambda_D = \sqrt{\frac{\epsilon_0 k_B T_e}{n_e e^2}}$$



(electron) Plasma frequency:

$$\omega_{pe} = \sqrt{\frac{n_e e^2}{m_e \epsilon_0}}$$

Behavior as “plasma” manifests on spatio-temporal scales larger than these characteristic quantities.

# Criteria for plasmas

Criterion 1: System scales should be greater than  $\lambda_D$  in space and than  $\omega_{pe}^{-1}$  in time.

Criterion 2: Debye sphere should contain large number of particles.

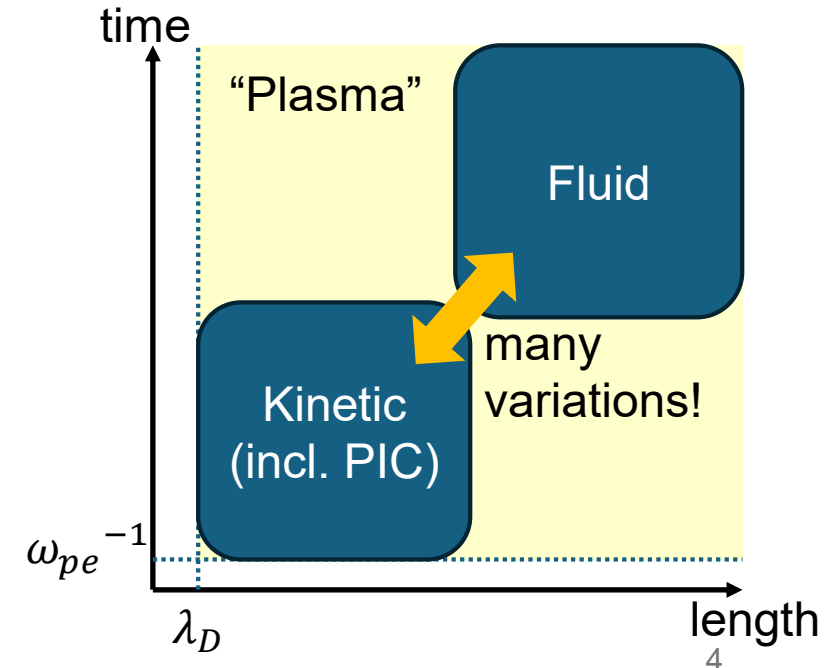
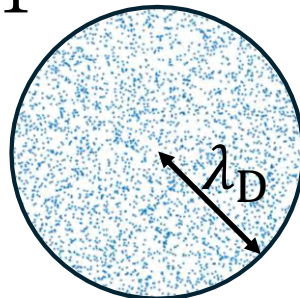
...coming from the condition that the potential energy by a nearest particle should be much smaller than the particle's kinetic energy (“weakly-coupled”).

Potential energy:  $\phi \sim \frac{e^2}{\epsilon_0 r} \sim \frac{e^2}{\epsilon_0} n^{\frac{1}{3}}$ , Kinetic energy:  $K = k_B T_e$

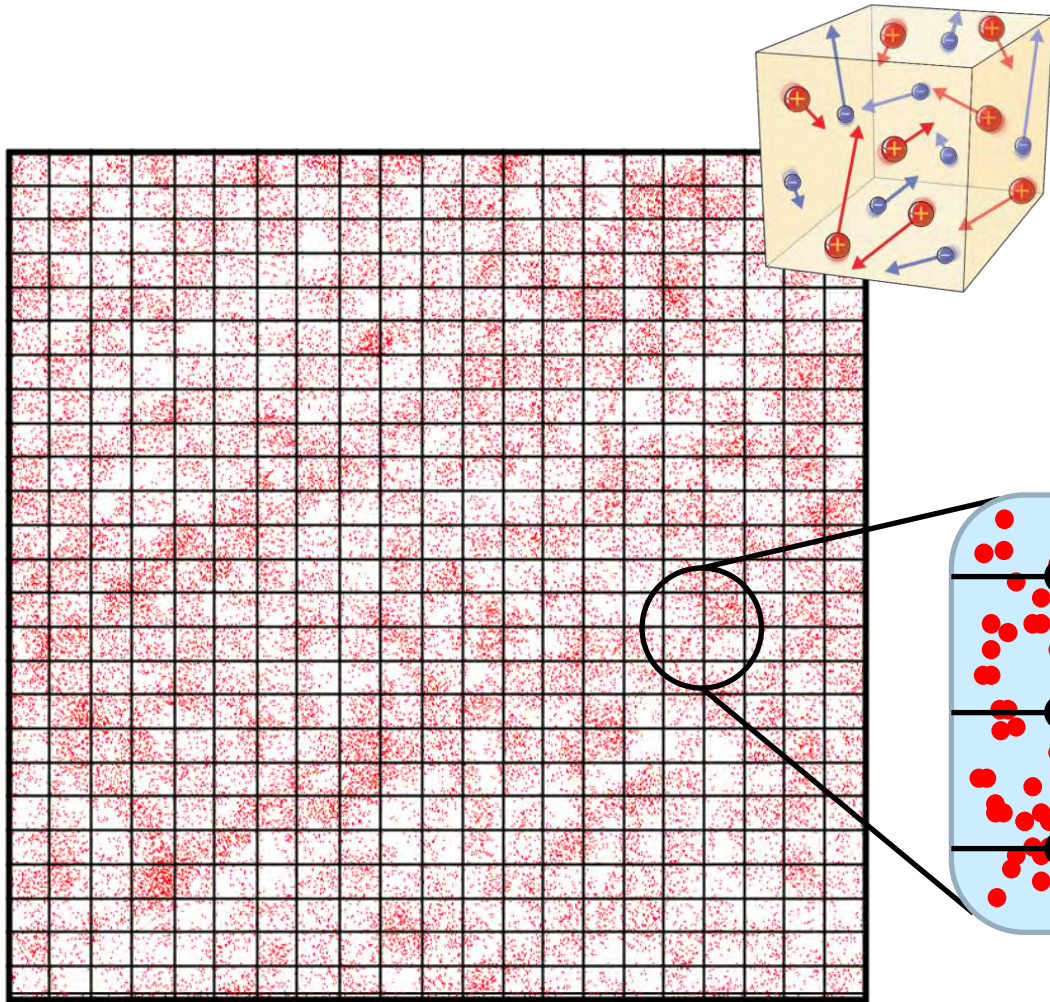
Weakly-coupled condition:  $k_B T_e \gg \frac{e^2}{\epsilon_0} n^{\frac{1}{3}}$  yields

$$n^{\frac{2}{3}} \left( \frac{\epsilon_0 k_B T_e}{n e^2} \right) = n^{\frac{2}{3}} \lambda_D^2 \gg 1$$

This also reads  $n \lambda_D^3 \gg 1$ ,  
where  $n$ : number density.



# Particle-in-Cell (PIC) simulations



Large number of discrete Lagrangian particles  
→ Newton's equations of motion

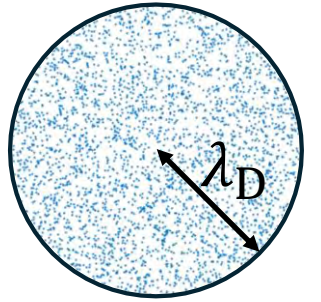
$$m \frac{d\mathbf{v}_j}{dt} = q_j (\mathbf{E}(\mathbf{x}_j) + \mathbf{v}_j \times \mathbf{B}(\mathbf{x}_j))$$
$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v}_j$$

EM-field (force)  
on Eulerian mesh (grid)  
→ Maxwell's equations

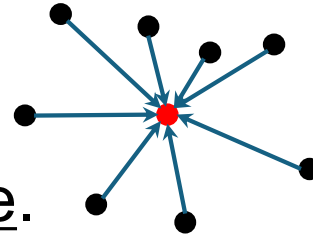
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$$

# Design of “plasma behavior” in PIC code

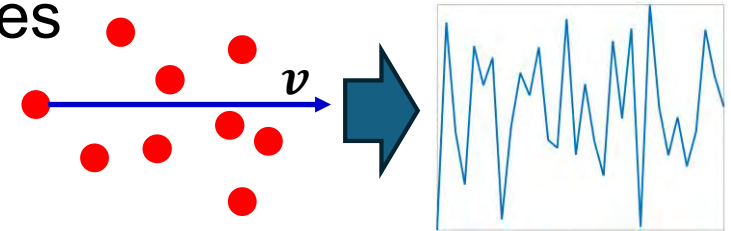
Plasma criterion 2: Debye sphere must contain large number of particles.  
...request us to solve huge particles  
→ Computationally too expensive!



Solution 1: use of a computational particle that combine many real-world particles into one.

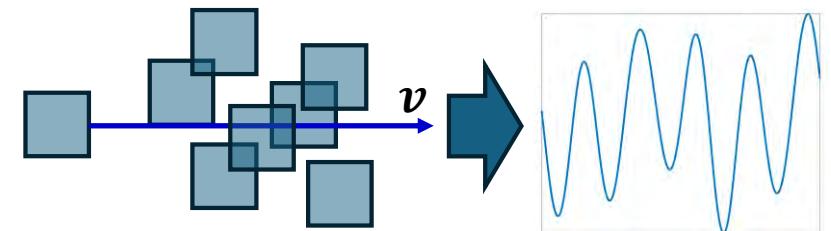


Caveat: a small number of particles with larger charge causes too large electrostatic interactions between the particles.

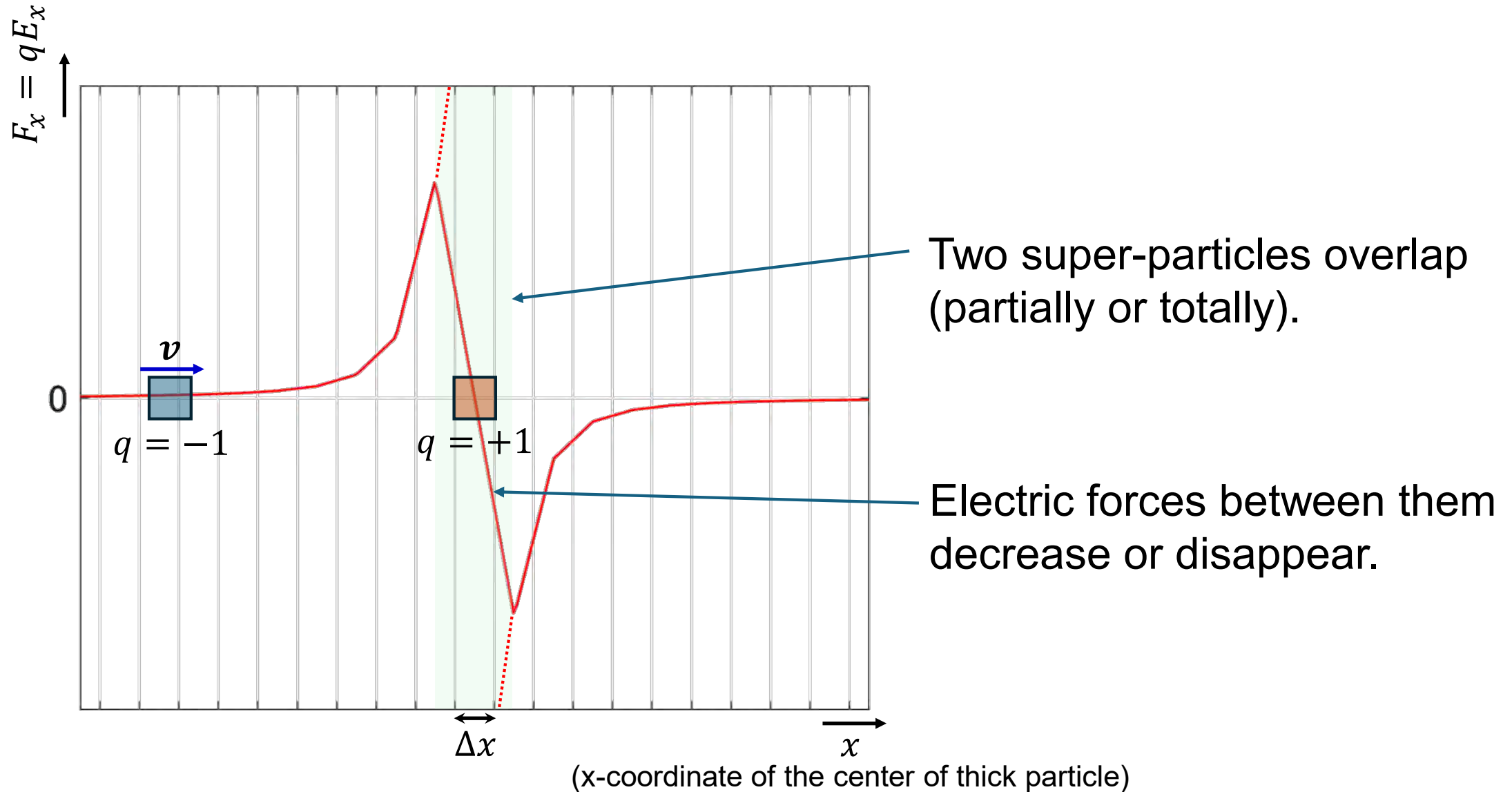


Solution 2:  
use of a “thick” particle or a “charge-cloud” particle,  
to reduce short-range inter-particle collisions.

This is often referred to as a “super-particle”.



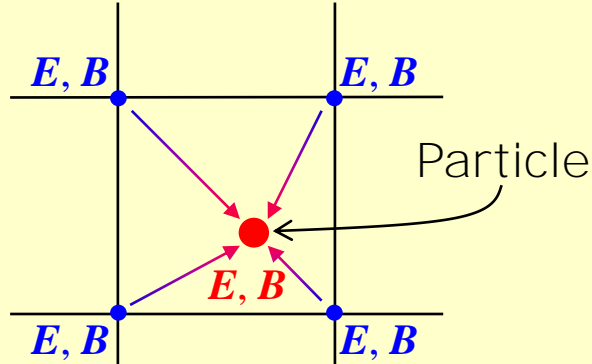
# Collisionless nature of super-particles



# Numerical procedures of PIC simulations

## Initialization

- Variable definition
- Memory allocation
- Particle initialization
- Field initialization



Field to Particle

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

$$\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J}$$

or

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \text{ in ES approx.}$$

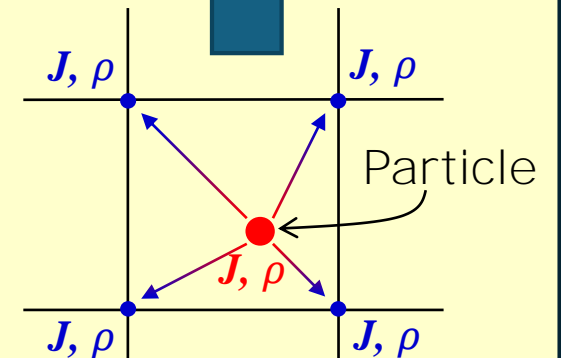
Update of EM-field

Main loop  
 $\Delta t$

$$\frac{d(m_i \mathbf{v}_i)}{dt} = q_i (\mathbf{E} + \mathbf{v}_i \times \mathbf{B})$$

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

Update of particle  
velocities/positions



Particle to Field

Job completion  
Diagnostics



# Maxwell's equations

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$$

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

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

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

where  $\epsilon_0 \mu_0 = \frac{1}{c^2}$

# Centered difference scheme

Define  $u_i = u(x_i)$ . Then, Taylor-expand  $u_{i+1/2}$  and  $u_{i-1/2}$  around  $x_i$ .

$$u((i + 1/2)\Delta x) = u_{i+1/2} = u_i + \frac{\Delta x}{2} \left( \frac{\partial u}{\partial x} \right)_i + \frac{1}{2!} \left( \frac{\Delta x}{2} \right)^2 \left( \frac{\partial^2 u}{\partial x^2} \right)_i + \frac{1}{3!} \left( \frac{\Delta x}{2} \right)^3 \left( \frac{\partial^3 u}{\partial x^3} \right)_i + \dots$$

$$u((i - 1/2)\Delta x) = u_{i-1/2} = u_i - \frac{\Delta x}{2} \left( \frac{\partial u}{\partial x} \right)_i + \frac{1}{2!} \left( \frac{\Delta x}{2} \right)^2 \left( \frac{\partial^2 u}{\partial x^2} \right)_i - \frac{1}{3!} \left( \frac{\Delta x}{2} \right)^3 \left( \frac{\partial^3 u}{\partial x^3} \right)_i + \dots$$

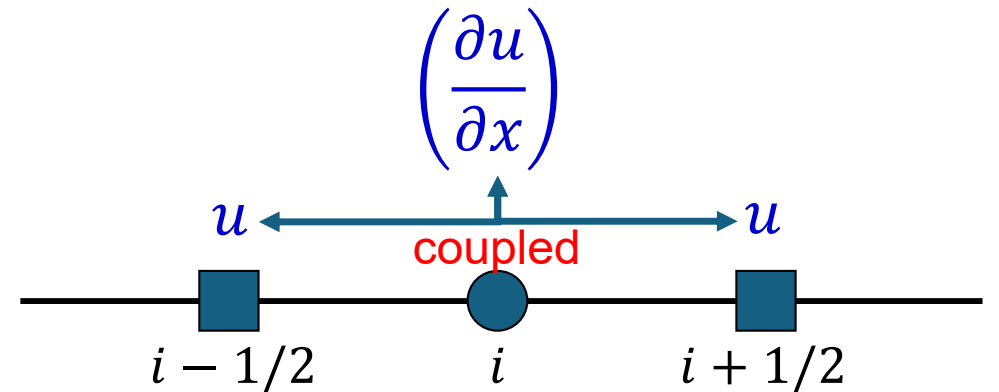
Subtraction of each other gives

where,  $\Delta x = x_i - x_{i-1}$ .

$$u_{i+1/2} - u_{i-1/2} = \Delta x \left( \frac{\partial u}{\partial x} \right)_i + \frac{2}{3!} \left( \frac{\Delta x}{2} \right)^3 \left( \frac{\partial^3 u}{\partial x^3} \right)_i + \dots$$

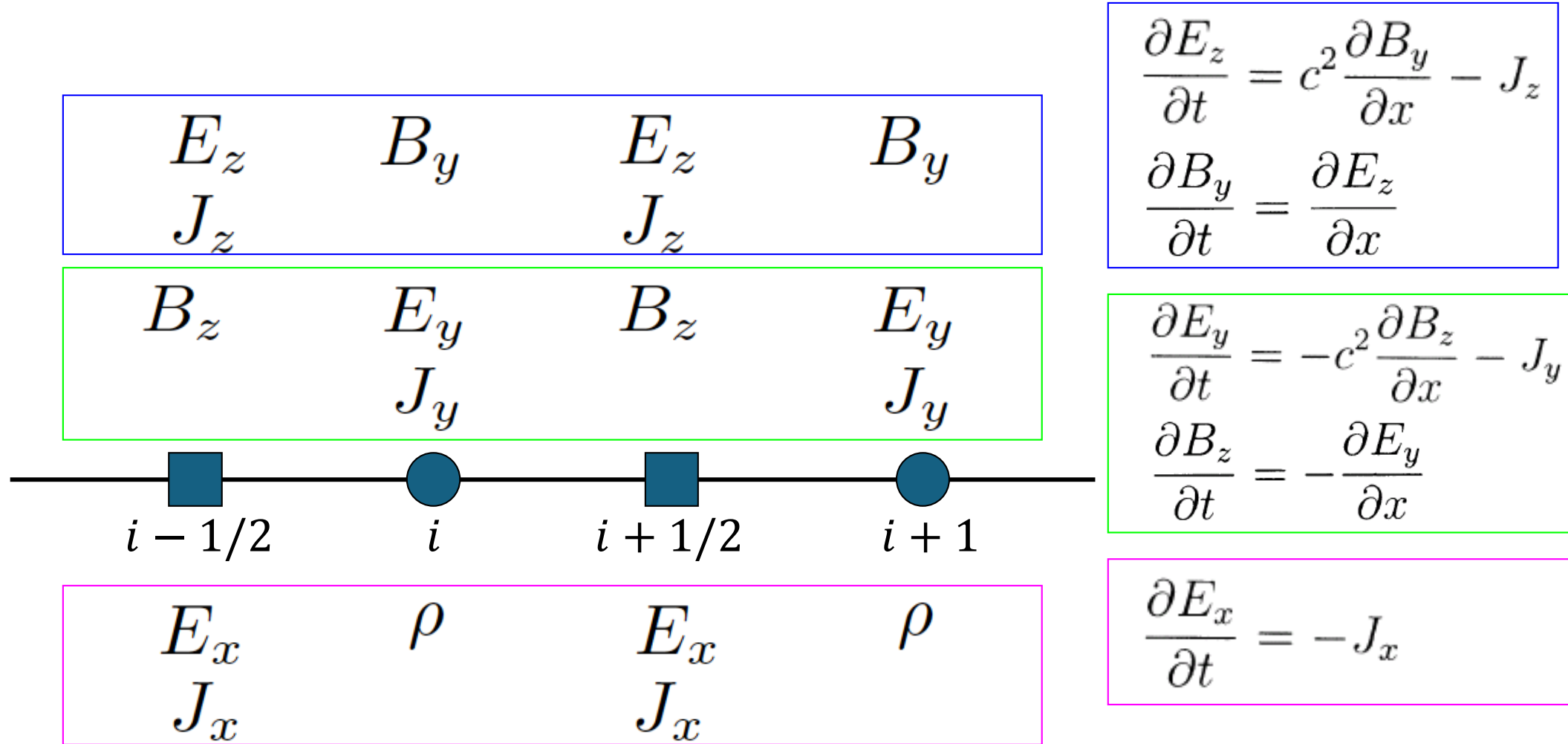
Centered difference expression

$$\begin{aligned} \left( \frac{\partial u}{\partial x} \right)_i &= \frac{u_{i+1/2} - u_{i-1/2}}{\Delta x} + O(\Delta x^2) \\ &\sim \frac{u_{i+1/2} - u_{i-1/2}}{\Delta x} \end{aligned}$$



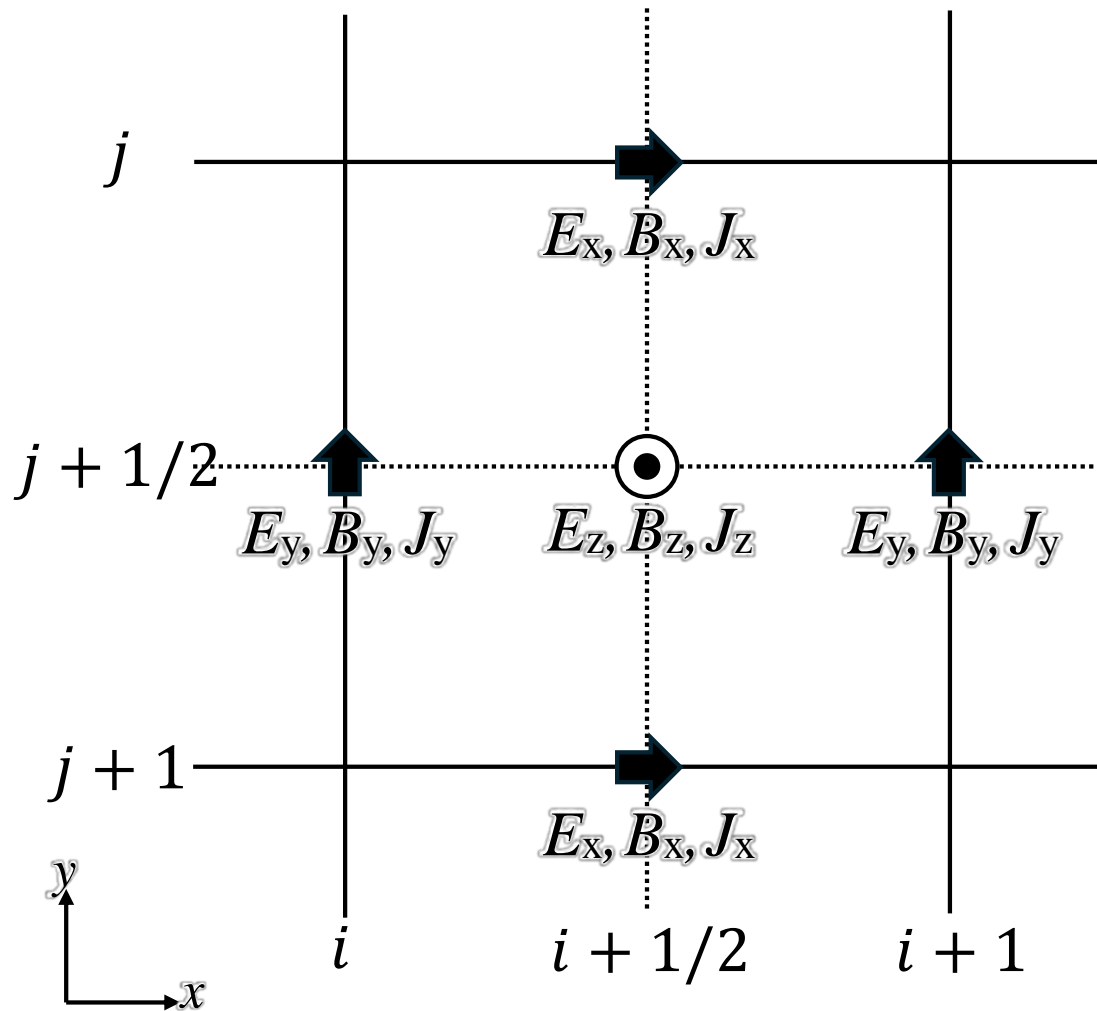
“Staggered” grid assignment

# Example of grid assignment (1D along x-axis)

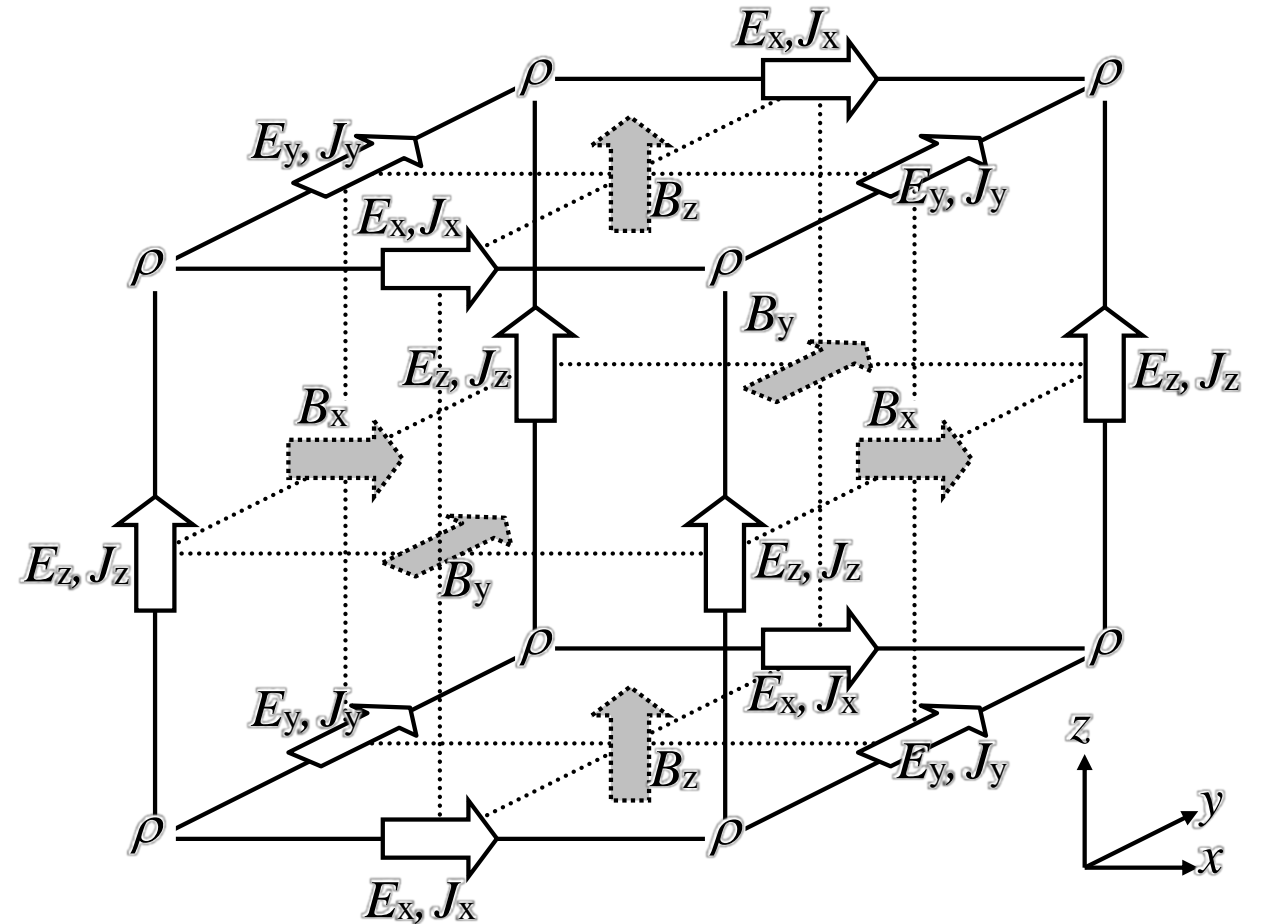


# Examples of grid assignment (2D & 3D)

➤ 2D



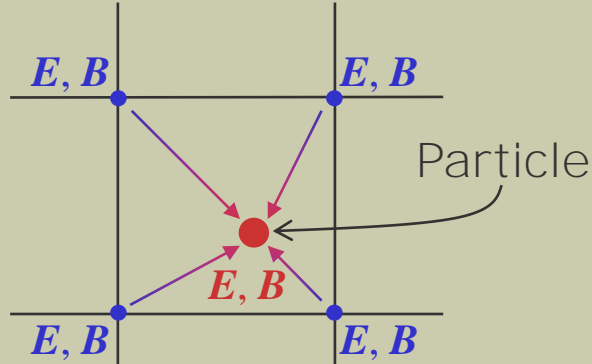
➤ 3D



# Numerical procedures of PIC simulations

## Initialization

- Variable definition
- Memory allocation
- Particle initialization
- Field initialization



Field to Particle

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J}$$

or

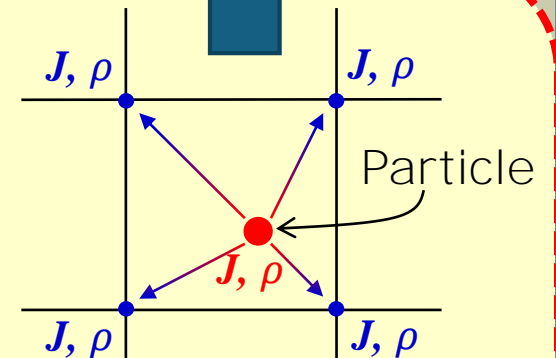
$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \text{ in ES approx.}$$

Update of EM-field

Main loop  
 $\Delta t$

$$\frac{d(m_i \mathbf{v}_i)}{dt} = q_i (\mathbf{E} + \mathbf{v}_i \times \mathbf{B})$$
$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

Update of particle  
velocities/positions



Particle to Field

Job completion  
Diagnostics

# Charge density

$$\rho_i = \frac{1}{\Delta x} \sum_j^{N_p} q_j W(x_j - X_i)$$

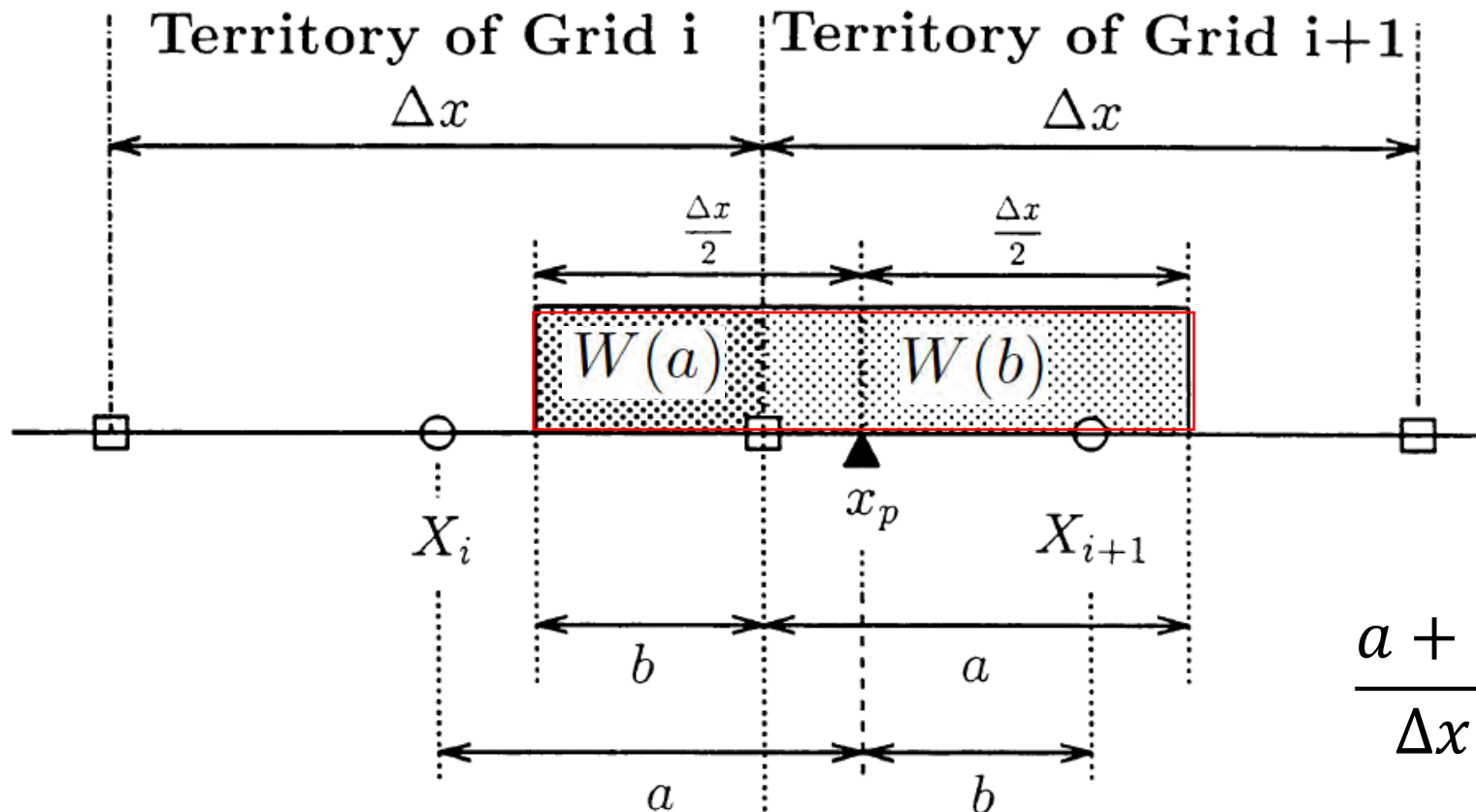
## Shape Function

$$W(x) = 1 - \frac{|x|}{\Delta x}, \quad |x| \leq \Delta x$$

$$= 0, \quad |x| > \Delta x$$

$N_p$ : Number of Particles

“thick particle”



$$\frac{a+b}{\Delta x} = 1$$

$$W(a) = \frac{b}{\Delta x}$$

$$W(b) = \frac{a}{\Delta x}$$

# Current density in 1D system along $x$ -axis

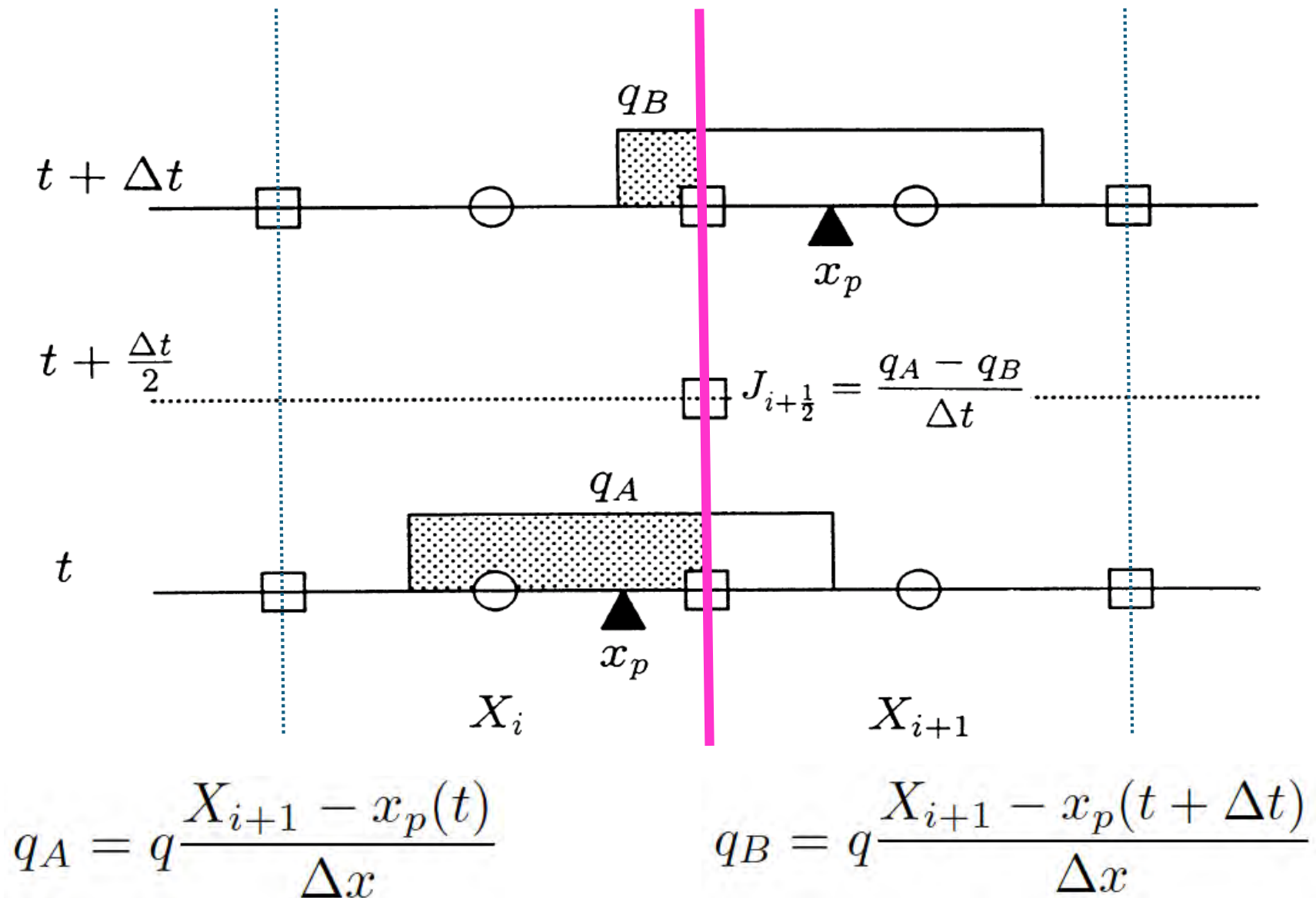
- $J_y, J_z$  components: area-weighting method (same as charge density)
- $J_x$  computed based on the area-weighting does **NOT satisfy** charge continuity equation:  $\frac{d\rho}{dt} = -\nabla \cdot \mathbf{J} = -\frac{\partial J_x}{\partial x} \dots (1)$   
→ cause an accumulative error in an electrostatic (ES) field.

## ◆ Solution 1: Correcting an ES field every time step

1. Define charge  $\rho_c$  associated with error in ES field :  $\rho_c = \rho - \nabla \cdot \mathbf{E}$
2. Solve Poisson's equation:  $\nabla^2 \phi_c = -\rho_c$  , for  $\phi_c$ : electric potential
3. Compute ES field correction:  $\mathbf{E}_c = -\nabla \phi_c$
4. Add  $\mathbf{E}_c$  to  $\mathbf{E}$ .

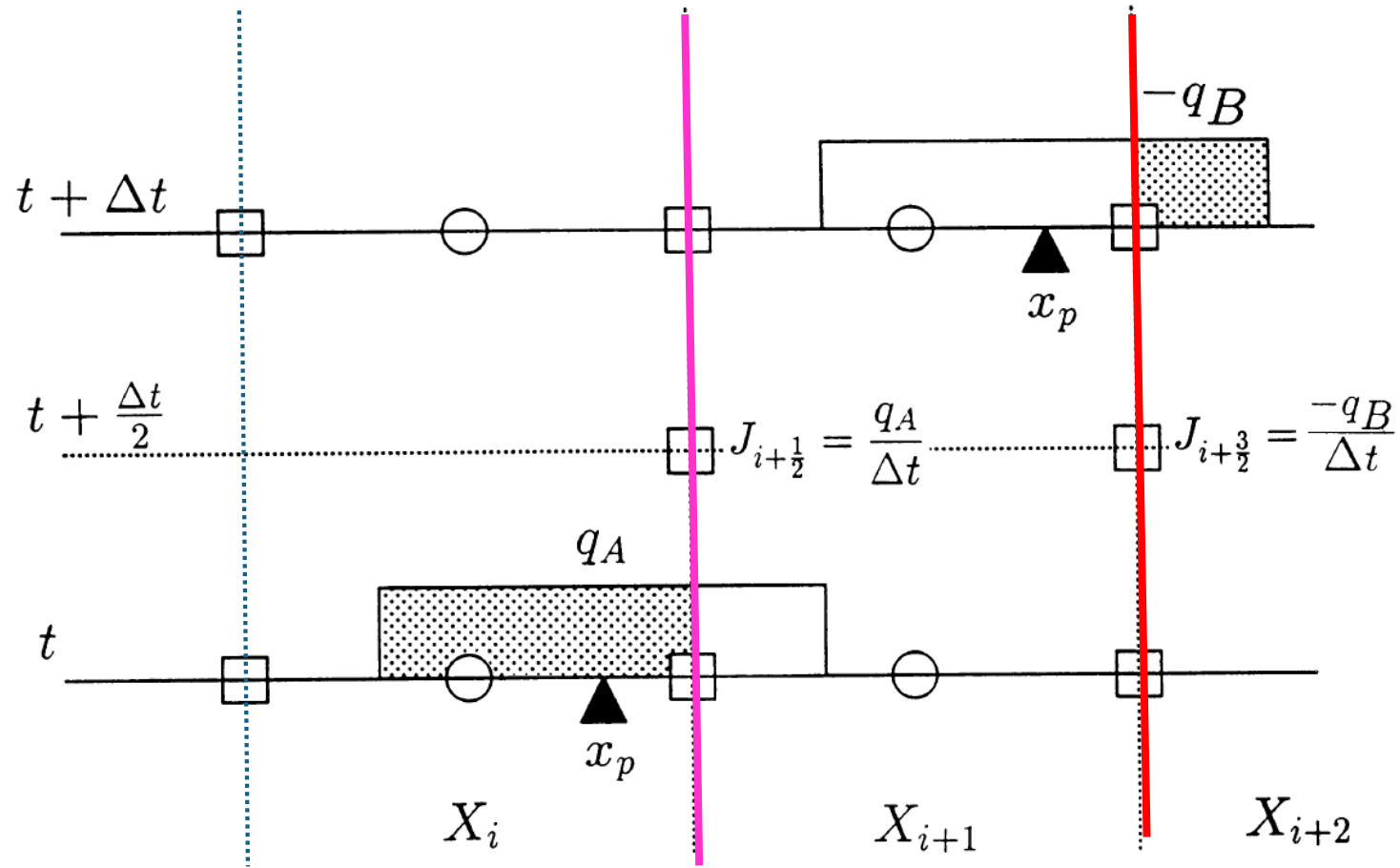
## ◆ Solution 2: Using a “Charge Conservation Method (CCM)” to compute current, which satisfies (1) in the machine accuracy.

# Charge conservation method in 1D ( $J_x$ ): case 1





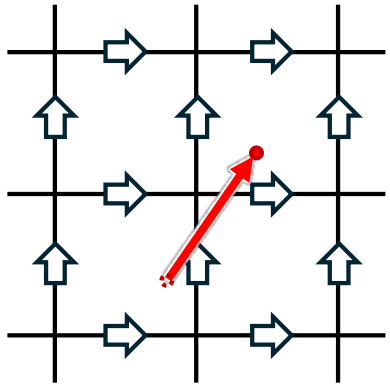
# Charge conservation method in 1D ( $J_x$ ): case 2



$$q_A = q \frac{X_{i+1} - x_p(t)}{\Delta x}$$

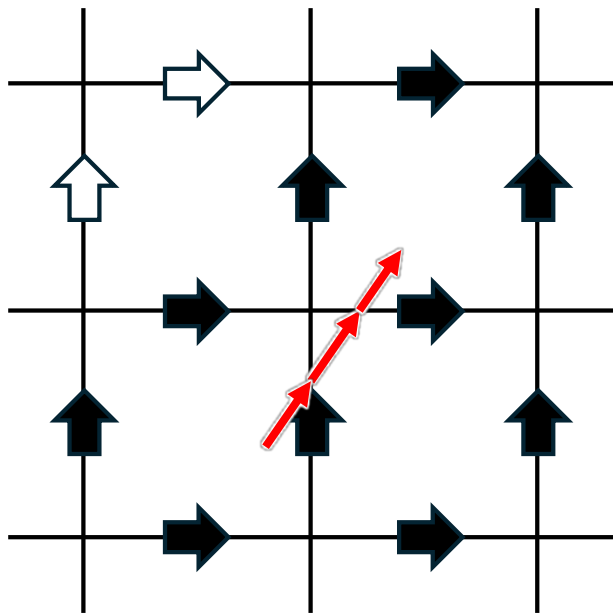
$$q_B = q \frac{X_{i+1} - x_p(t + \Delta t)}{\Delta x}$$

# Charge conservation methods in higher dimensions



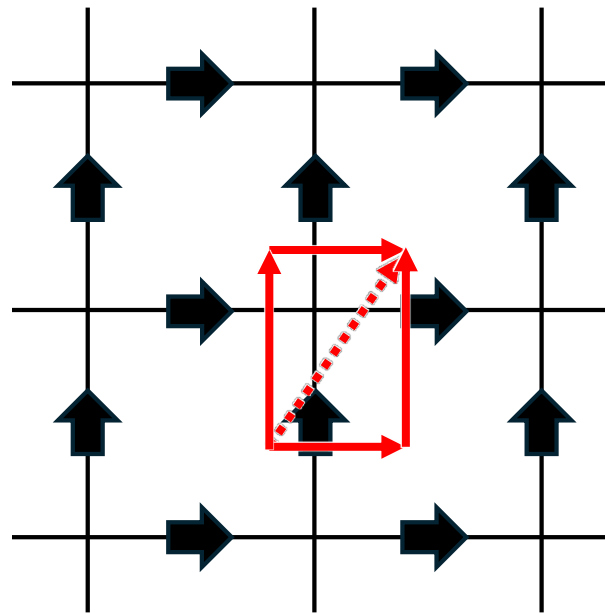
Trajectory decomposition needed in case the particle moves across cell edges; various approaches proposed.

Rigorous decomposition



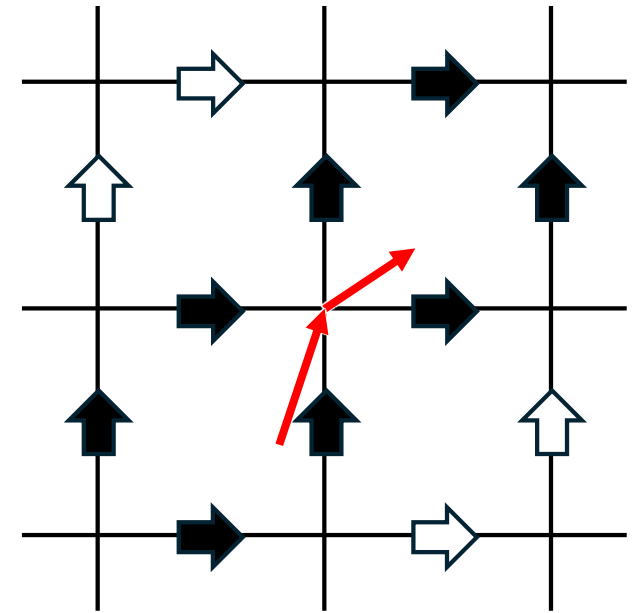
[Villasenor & Buneman, 1992]

Density decomposition



[Esirkepov, 2001]

Zig-zag decomposition

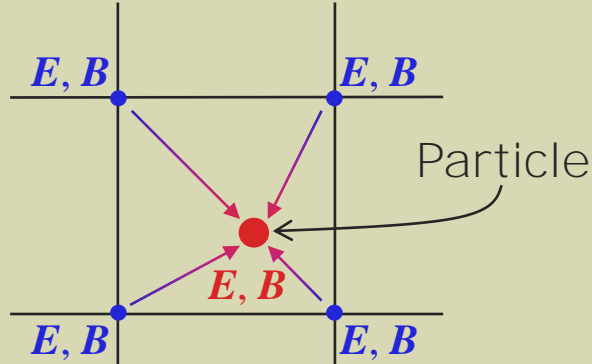


[Umeda+, 2003]

# Numerical procedures of PIC simulations

## Initialization

- Variable definition
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- Field initialization



Field to Particle

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

$$\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J}$$

or

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \text{ in ES approx.}$$

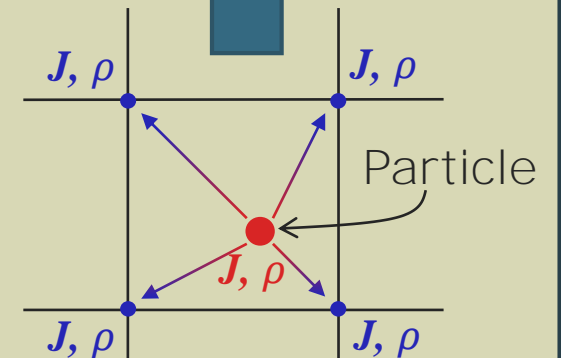
Update of EM-field

Main loop  
 $\Delta t$

$$\frac{d(m_i \mathbf{v}_i)}{dt} = q_i (\mathbf{E} + \mathbf{v}_i \times \mathbf{B})$$

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

Update of particle  
velocities/positions



Particle to Field

Job completion  
Diagnostics

# Update of velocity: Buneman-Boris method

$$\frac{\mathbf{v}^{t+\Delta t/2} - \mathbf{v}^{t-\Delta t/2}}{\Delta t} = \frac{q_s}{m_s} \left( \mathbf{E}^t + \frac{\mathbf{v}^{t+\Delta t/2} + \mathbf{v}^{t-\Delta t/2}}{2} \times \mathbf{B}^t \right)$$

$$\mathbf{v}^- = \mathbf{v}^{t-\Delta t/2} + \frac{q_s}{m_s} \mathbf{E}^t \frac{\Delta t}{2} \quad \mathbf{v}^+ = \mathbf{v}^{t+\Delta t/2} - \frac{q_s}{m_s} \mathbf{E}^t \frac{\Delta t}{2}$$

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{1}{2} \frac{q_s}{m_s} (\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}^t$$

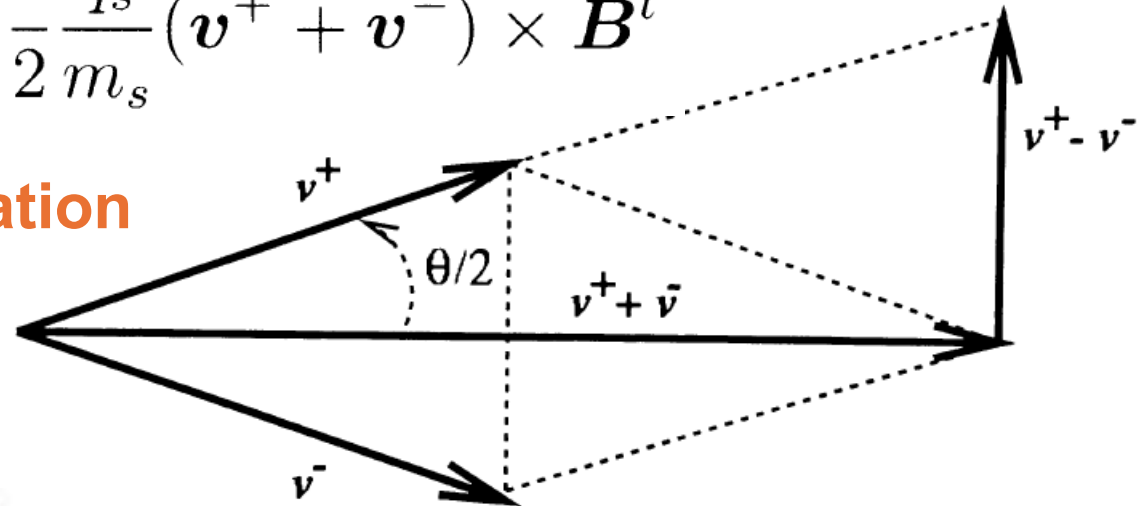
**Kinetic Energy Conservation**

$$(\mathbf{v}^+)^2 = (\mathbf{v}^-)^2$$

**Small Phase Delay**

$$\Omega_c = \frac{\tan^{-1} \omega_c \Delta t / 2}{\Delta t / 2}$$

$$\Omega_c / \omega_c = 0.9967 \text{ with } \omega_c \Delta t = 0.2$$



# Relativistic equation of motion

$$\frac{d}{dt}(m\mathbf{v}) = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

$$m = \gamma m_0$$
$$\gamma = \frac{1}{\sqrt{1 - \left(\frac{v}{c}\right)^2}}$$

$$\mathbf{u} = \frac{c}{\sqrt{c^2 - |\mathbf{v}|^2}} \mathbf{v}$$

$$\mathbf{B}_u = \frac{c}{\sqrt{c^2 + |\mathbf{u}|^2}} \mathbf{B}$$

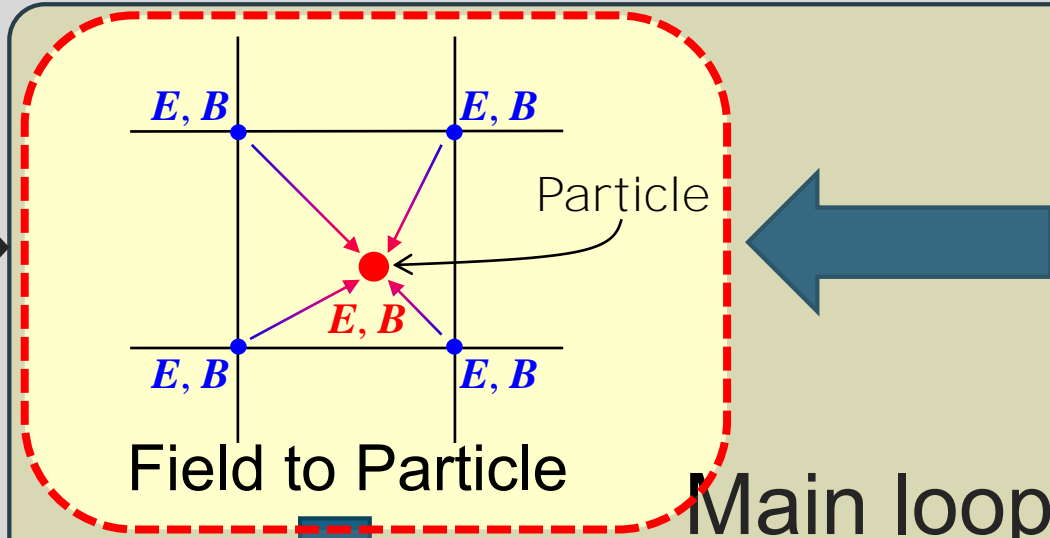
$$\frac{d\mathbf{u}}{dt} = \frac{q}{m_0} (\mathbf{E} + \mathbf{u} \times \mathbf{B}_u)$$

$$\mathbf{v} = \frac{c}{\sqrt{c^2 + |\mathbf{u}|^2}} \mathbf{u}$$

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Main loop  
 $\Delta t$

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

Update of particle velocities/positions

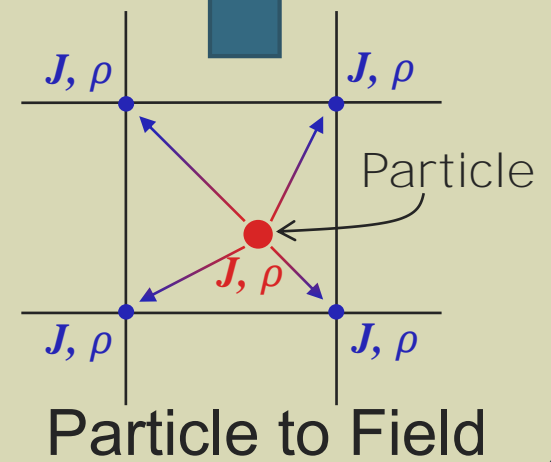
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or

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \text{ in ES approx.}$$

Update of EM-field

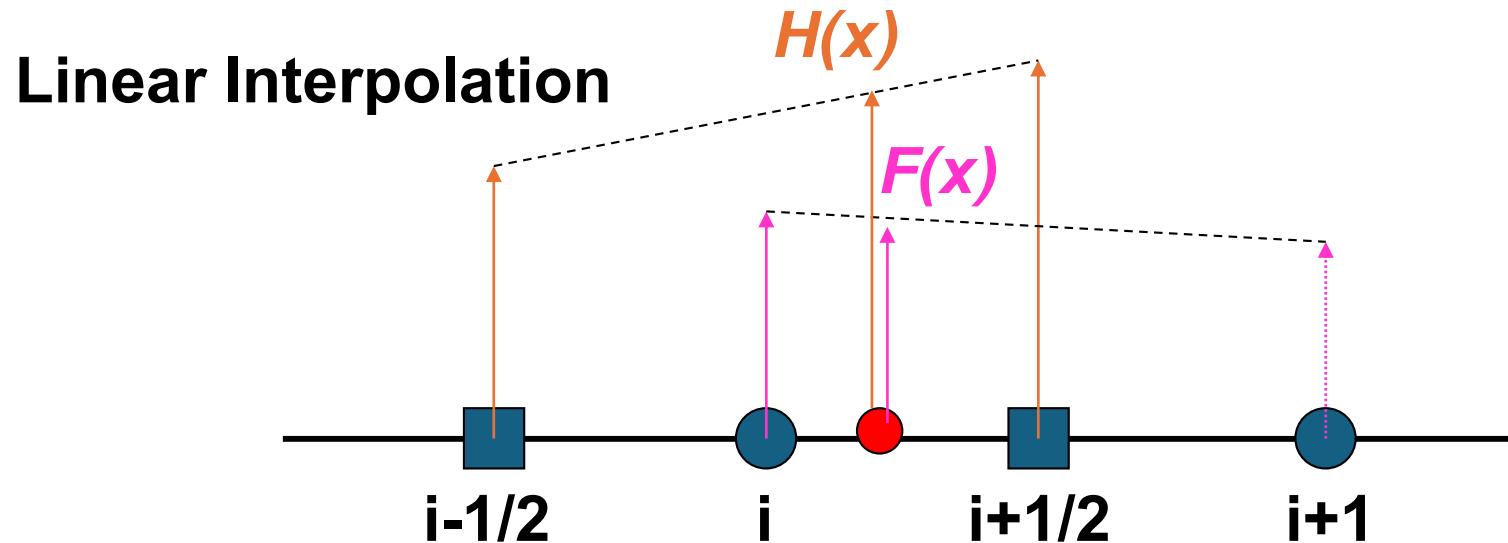


Job completion  
Diagnostics

# Field interpolation to particle position

$$F(x) = \sum_{i=1}^{N_x} F_i W(x - X_i)$$

$$H(x) = \sum_{i=1}^{N_x} H_{i+1/2} W(x - X_{i+1/2})$$



# Electrostatic self-force cancellation

$$\rho_i = \frac{1}{\Delta x} \sum_j^{N_p} q_j \underline{W(x_j - X_i)}$$

$$\frac{E_{x,i+1/2} - E_{x,i-1/2}}{\Delta x} = \frac{\rho_i}{\epsilon_0}$$

$$E_x(x) = \sum_{i=1}^{N_x} E_{x,i+1/2} \underline{W(x - X_{i+1/2})}$$

 **Self-force**

**Relocation**  $E_{x,i} = \frac{E_{x,i-1/2} + E_{x,i+1/2}}{2}$

$$E_x(x) = \sum_{i=1}^{N_x} E_{x,i} \underline{W(x - X_i)}$$

 **No Self-force**



# Magnetostatic self-force cancellation

Magnetostatic equation (Ampere's Law)  $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$

$$J_{yz, i+1/2} = \frac{1}{\Delta x} \sum_j^{N_p} q_j v_{yz} W(x_j - X_{i+1/2})$$

**Source Relocation**  $J_y$  &  $B_z$

$$J_{y,i} = \frac{J_{y,i-1/2} + J_{y,i+1/2}}{2}$$

$$\frac{B_{z,i+1/2} - B_{z,i-1/2}}{\Delta x} = -\mu_0 J_{y,i}$$

**Field Relocation**  $J_z$  &  $B_y$

$$\frac{B_{y,i+1} - B_{y,i}}{\Delta x} = \mu_0 J_{z,i+1/2}$$

$$B_{y,i+1/2} = \frac{B_{y,i} + B_{y,i+1}}{2}$$

$B_{yz}(x)$

$$= \sum_{i=1}^{N_x} B_{yz,i+1/2} W(x - X_{i+1/2})$$

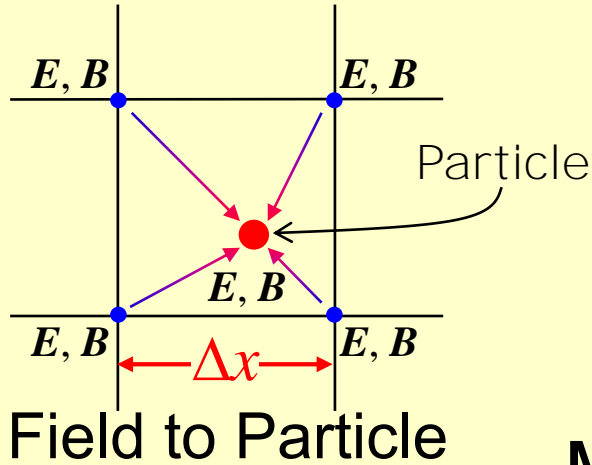


**No Self-force**

# Numerical procedures of PIC simulations

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Field to Particle

$$\frac{d(m_i \mathbf{v}_i)}{dt} = q_i (\mathbf{E} + \mathbf{v}_i \times \mathbf{B})$$

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Update of particle velocities/positions

Main loop

$\Delta t$

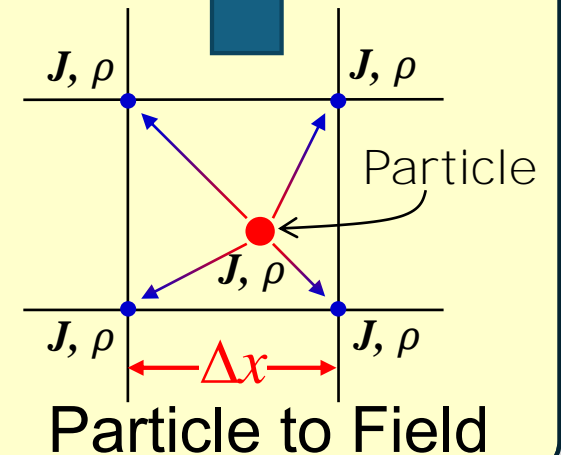
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$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \text{ in ES approx.}$$

Update of EM-field

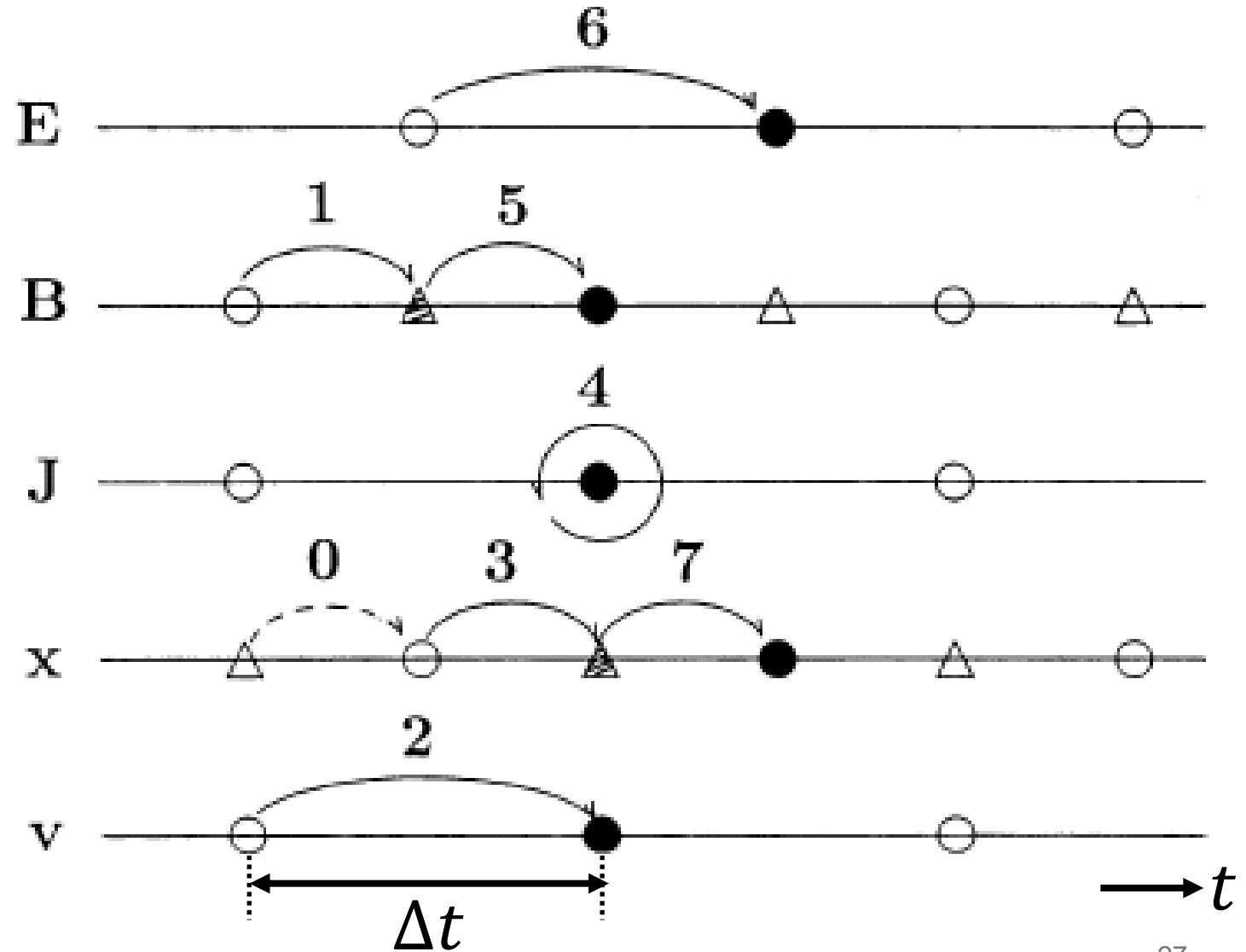
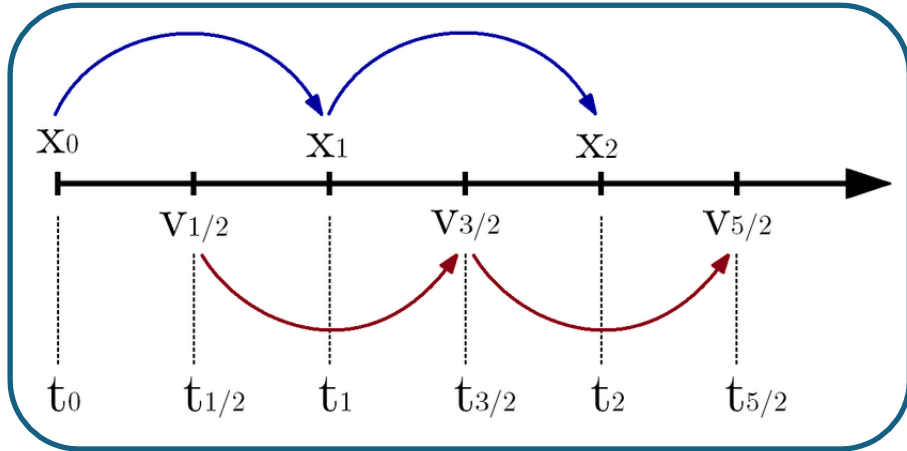


Particle to Field

Job completion  
Diagnostics

# Time Step Chart

Leap-frog scheme




# Effect of centered differentiation


$$E(X_i, t) = E_o \exp(ikX_i - i\omega t)$$

$$\frac{\partial E(X_i, t)}{\partial x} = \frac{E(X_i + \Delta x/2, t) - E(X_i - \Delta x/2, t)}{\Delta x}$$

$$= \frac{1}{\Delta x} [\exp(ik\Delta x/2) - \exp(-ik\Delta x/2)] E(X_i, t)$$

$$= i \frac{\sin(k\Delta x/2)}{\Delta x/2} E(X_i, t) = iK E(X_i, t)$$


$$k \longrightarrow K = \frac{\sin(k\Delta x/2)}{\Delta x/2}$$


$$\omega \longrightarrow \Omega = \frac{\sin(\omega\Delta t/2)}{\Delta t/2}$$

# Modified dispersion relation of light mode

Electromagnetic modes in vacuum

$$\omega^2 = c^2 k^2$$

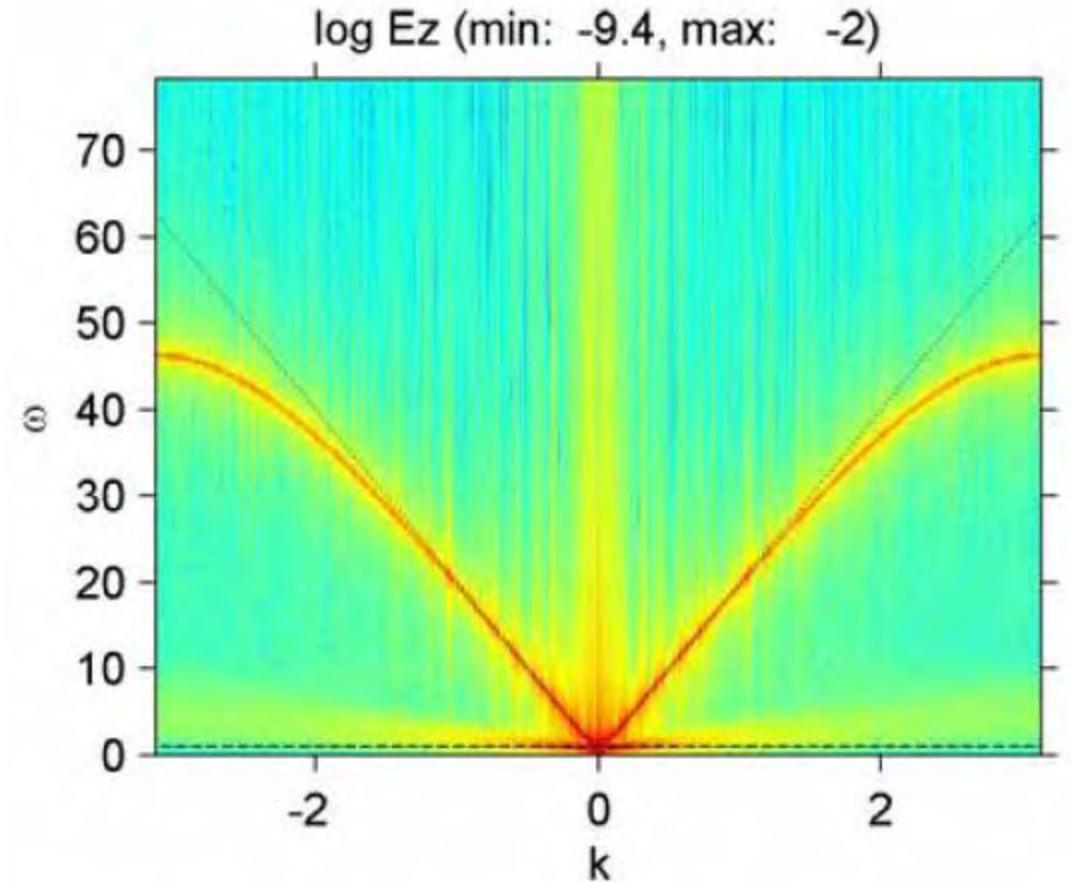


In centered difference scheme,

$$\Omega^2 = c^2 K^2$$

$$\Omega = \frac{\sin(\omega \Delta t / 2)}{\Delta t / 2},$$

$$K = \frac{\sin(k \Delta x / 2)}{\Delta x / 2}$$



# Condition for numerical stability 1

Centered Difference Scheme in space and time

$$\Omega^2 = c^2 K^2 \quad \Omega = \frac{\sin(\omega \Delta t / 2)}{\Delta t / 2}, \quad K = \frac{\sin(k \Delta x / 2)}{\Delta x / 2}$$

For  $k = \frac{\pi}{\Delta x}$  we have  $\sin\left(\frac{\omega \Delta t}{2}\right) = \frac{\Delta t}{\Delta x} c < 1$

Courant Condition

$$c \Delta t < \Delta x$$

# Condition for numerical stability 2

Shortest wavelength scale to solved in the explicit PIC is

$$|k| \sim \frac{1}{\lambda_D} \quad \text{where } \lambda_D \text{ is the Debye length.}$$

Replacing  $k$  with  $K$

$$|\sin(k\Delta x/2)| \sim \frac{\Delta x}{2\lambda_D} < 1$$

Explicit PIC should satisfy the following stability condition

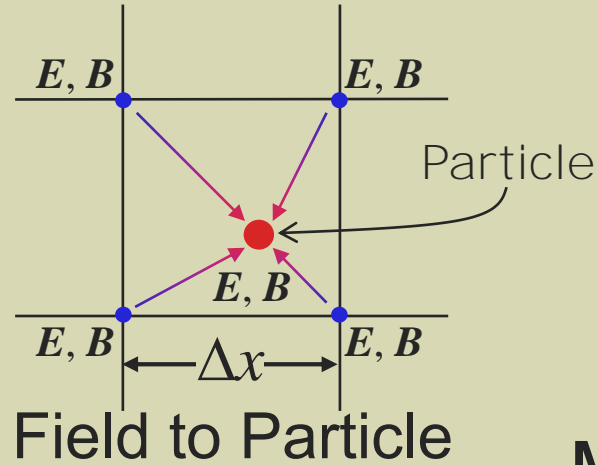
$$\Delta x < 2\lambda_D$$

Violation of the condition leads to numerical (unphysical) heating.

# Numerical procedures of PIC simulations

## Initialization

- Variable definition
- Memory allocation
- Particle initialization
- Field initialization



Field to Particle

Main loop  
 $\Delta t$

$$\frac{d(m_i \mathbf{v}_i)}{dt} = q_i (\mathbf{E} + \mathbf{v}_i \times \mathbf{B})$$
$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

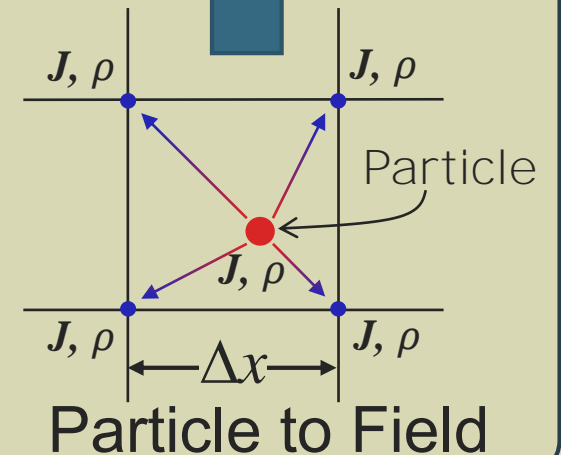
Update of particle velocities/positions

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{B} = \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J}$$

or

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \text{ in ES approx.}$$

Update of EM-field



Particle to Field

Job completion  
Diagnostics



# Initial & boundary conditions

## Initialization

- Particle loading
  - Positions:
  - Velocities: Maxwellian, shifted Maxwellian, loss-cone, ring, etc.
- Initial electrostatic field: Poisson's equation

## Outer boundary condition

- Periodic boundaries
- Reflecting boundaries
- Open boundaries
  - Particle injection from outer edge
  - Non-reflective field boundary: masking method

## Inner boundary condition

- for object-plasma interaction study

# Numerical solutions of Poisson's equation

$\nabla \cdot \mathbf{E} = \rho/\epsilon_0$ ,  $\mathbf{E} = -\nabla\phi$  reduce to  $\nabla^2\phi = -\rho/\epsilon_0$  (Poisson's equation).

In 1D,

$$\frac{\partial^2\phi}{\partial x^2} = -\frac{\rho}{\epsilon_0}$$

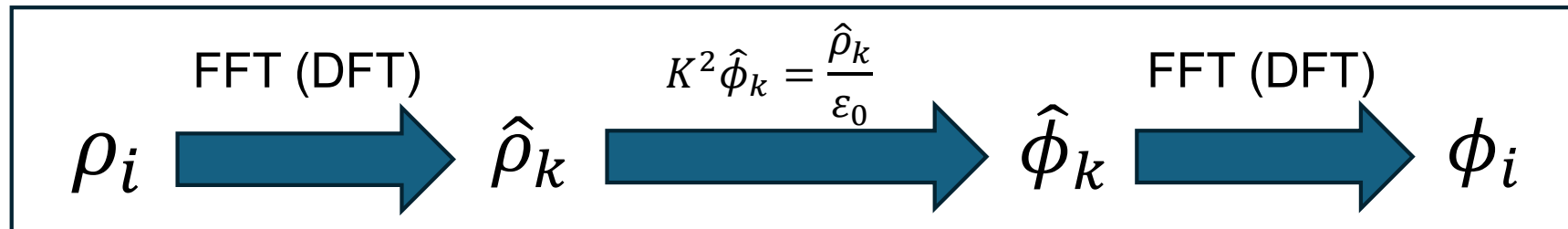
In Fourier space,

$$k^2\hat{\phi} = \frac{\hat{\rho}}{\epsilon_0}$$

In centered difference scheme,

$$K^2\hat{\phi}_k = \frac{\hat{\rho}_k}{\epsilon_0}, \text{ where } K = \frac{\sin(k\Delta x/2)}{\Delta x/2}$$

FFT-based Poisson solver,



In periodic system,

$$K^2\hat{\phi}_0 = \frac{\hat{\rho}_0}{\epsilon_0} = 0 \text{ for } k = 0 \longrightarrow \sum_i \frac{\rho_i}{N_x} = 0 \quad \text{“Charge neutral”}$$

# Cancellation of uniform current

Consider periodic 1D system along x-axis:

$$\frac{\partial \mathbf{J}_u}{\partial t} = \frac{n_e e^2}{m_e} \mathbf{E}_u \quad \frac{\partial \mathbf{E}_u}{\partial t} = -\mathbf{J}_u$$

...provide a solution in the following form:

$$\mathbf{J}_u = \mathbf{J}_o \exp(i\omega_{pe}t) \quad \mathbf{E}_u = \frac{i}{\omega_{pe}} \mathbf{J}_o \exp(i\omega_{pe}t)$$

The uniform component must be subtracted.

(**Periodic system** should also be “current neutral”.)

$$\mathbf{J}_u = \frac{1}{N_x} \sum_{i=1}^{N_x} \mathbf{J}_i \quad \mathbf{J}_{i,sub} = \mathbf{J}_i - \mathbf{J}_u$$

# Initial & boundary conditions

## Initialization

- Particle loading
  - Positions:
  - Velocities: Maxwellian, shifted Maxwellian, loss-cone, ring, etc.
- Initial electrostatic field: Poisson's equation

## Outer boundary condition

- Periodic boundaries
- Reflecting boundaries
- Open boundaries
  - Particle injection from outer edge
  - Non-reflective field boundary: masking method

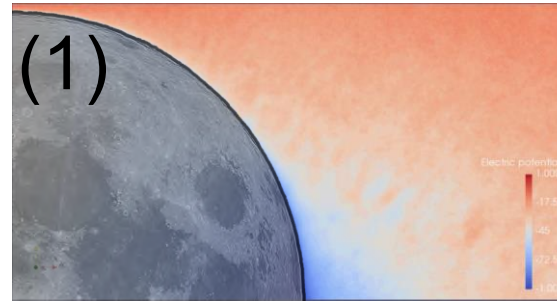
## Inner boundary condition

- for object-plasma interaction study

# Inner boundary conditions for object-in-plasma

## Solid objects in space

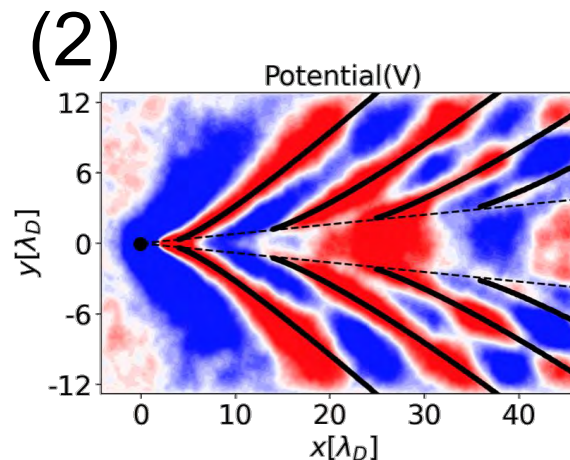
- Celestial bodies ... (1)
  - Dust grains ... (2)
  - Spacecraft / instrument ... (3)
- ...and so on.



## Effects at **object surface**

Inner boundaries

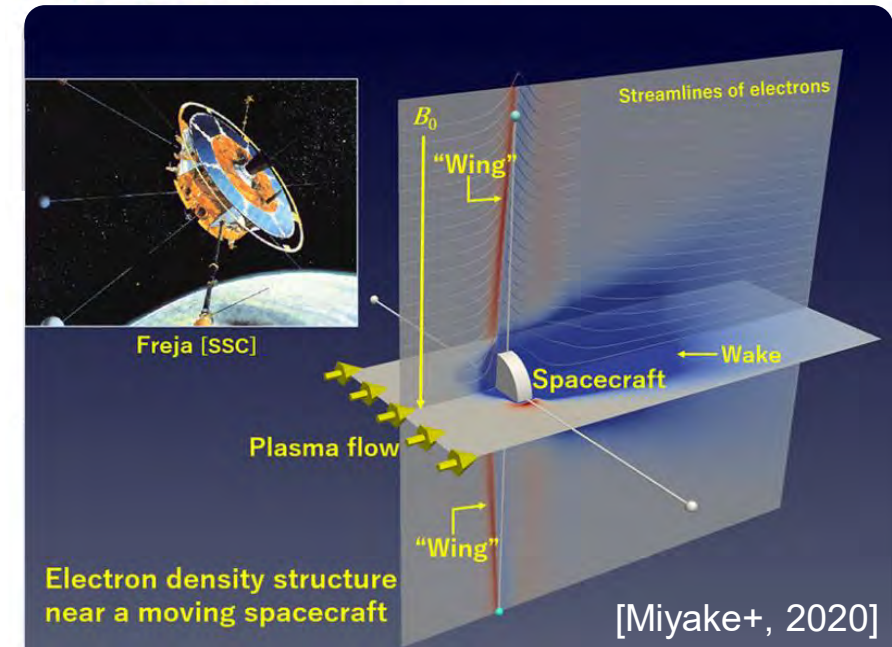
- Particle loss
- Particle emission
- Charge deposition
- **Surface potential**
- Conducting current
- EM scattering



Eos AGU's Eos @AGU\_Eos (3)

Under certain conditions, features called "electron wings" can form around spacecraft, potentially introducing interference and artifacts into data collected by onboard instruments.

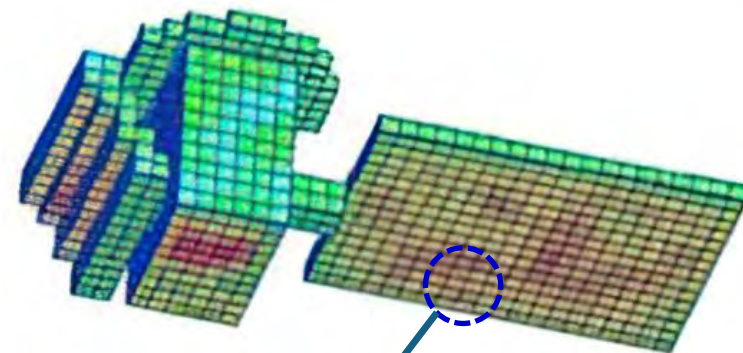
By @MarkZastrow  
@Fysikk\_UniOslo



"Electron Wings" Can Interfere with Spacecraft Measurements - Eos  
Spacecraft sometimes produce a form of electrical self-interference as they zip through plasmas in space—a previously unreported effect that may be lurking in...  
eos.org

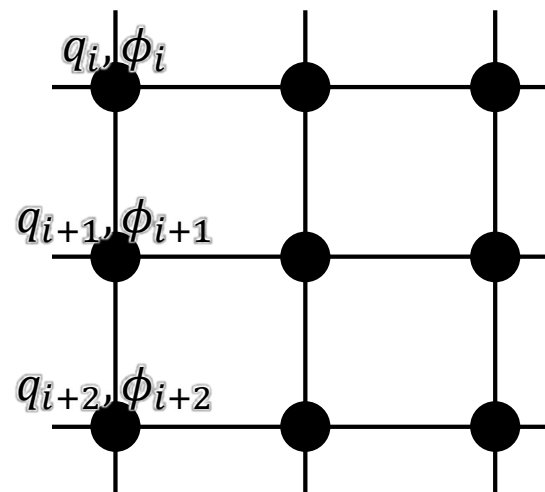
# Capacitance matrix

$$\underset{\text{charge}}{Q} = \underset{\text{potential}}{\overset{\text{capacitance}}{C}} \Phi$$



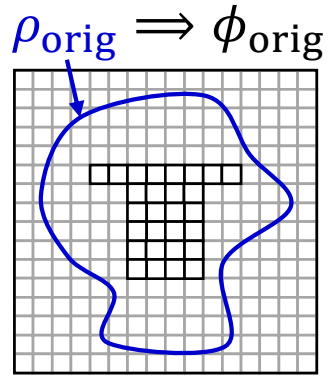
$$\underset{\text{charges}}{\begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ \vdots \\ q_n \end{pmatrix}} = \underset{\text{capacitance matrix}}{\begin{bmatrix} C_{11} & \cdots & C_{n1} \\ C_{12} & & C_{n2} \\ C_{13} & & C_{n3} \\ \vdots & \ddots & \vdots \\ C_{1n} & \cdots & C_{nn} \end{bmatrix}} \underset{\text{potentials}}{\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{pmatrix}}$$

capacitance matrix



# Control of on-grid potential/charge

1. Solve Poisson's eq.



2. Compute  $\Delta\rho_i$

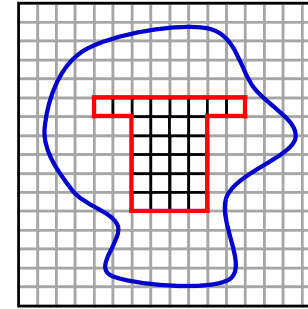
$$\Delta\phi_j = \phi_{\text{target}_j} - \phi_{\text{orig}_j}$$

$$\Delta q_i = \sum_j c_{ij} \Delta\phi_j$$

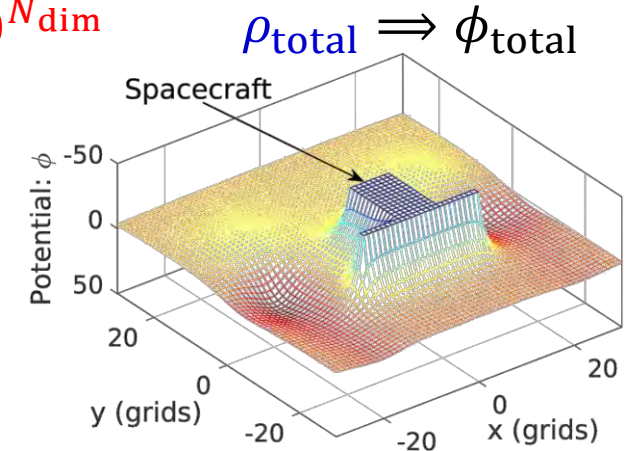
$i, j = 1 \dots N_{\text{grid\_for\_object}}$   
 $c_{ij}$ : capacitance matrix element

3. Add charge correction

$$\rho_{\text{total}} \leftarrow \rho_{\text{orig}} + \Delta q / (\Delta x)^{N_{\text{dim}}}$$



4. Solve Poisson's eq.



## Some applications...

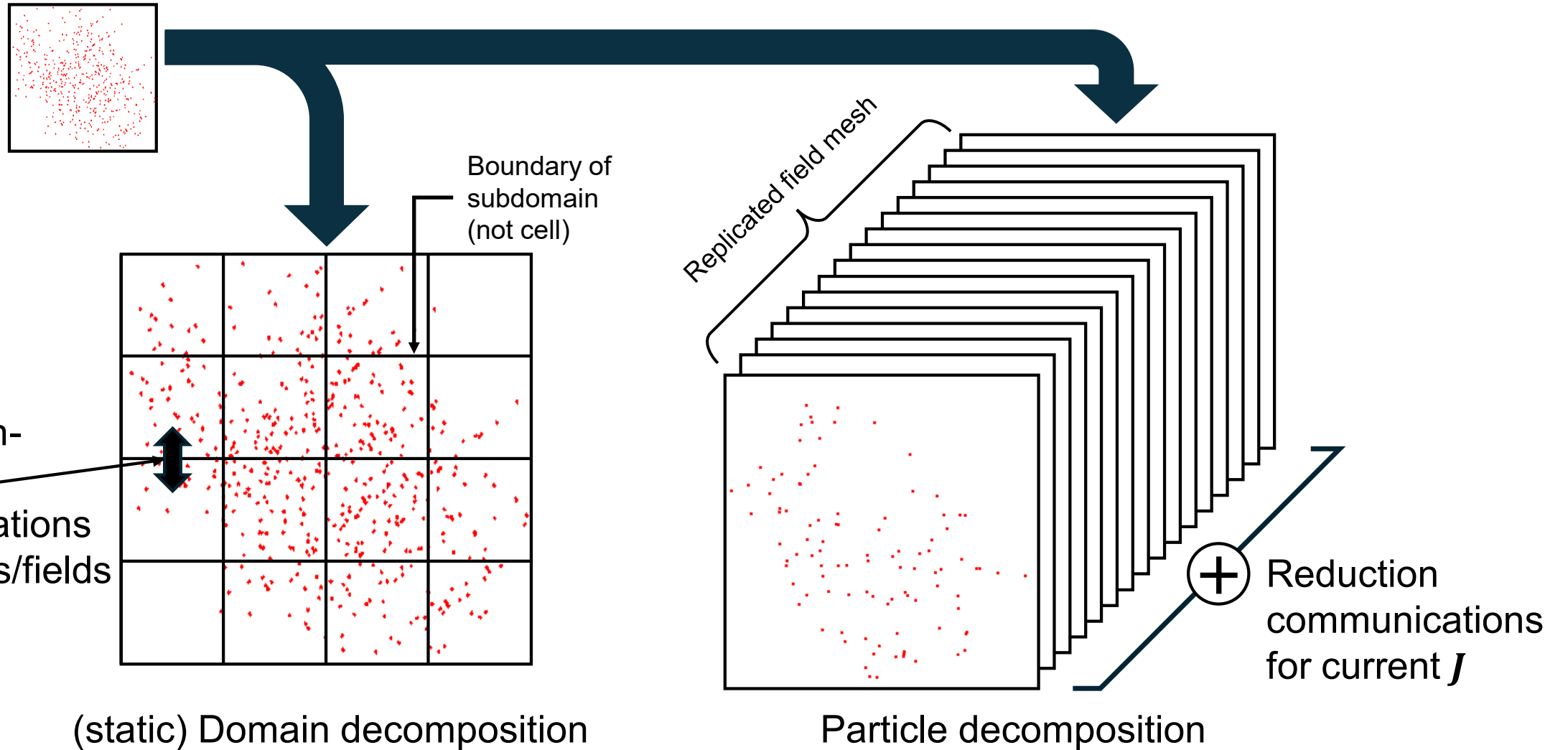
1. Known target potentials on all grids on object surface: Solve  $Q = C\Phi$ .  
 Application: electrodes with applied potential
2. Equi-potential over object surface, but its potential value unknown:  
 Solve  $Q = C\Phi$  with  $\sum_i \Delta q_i = 0$ .  
 Application: conducting objects with floating potential (e.g., spacecraft)



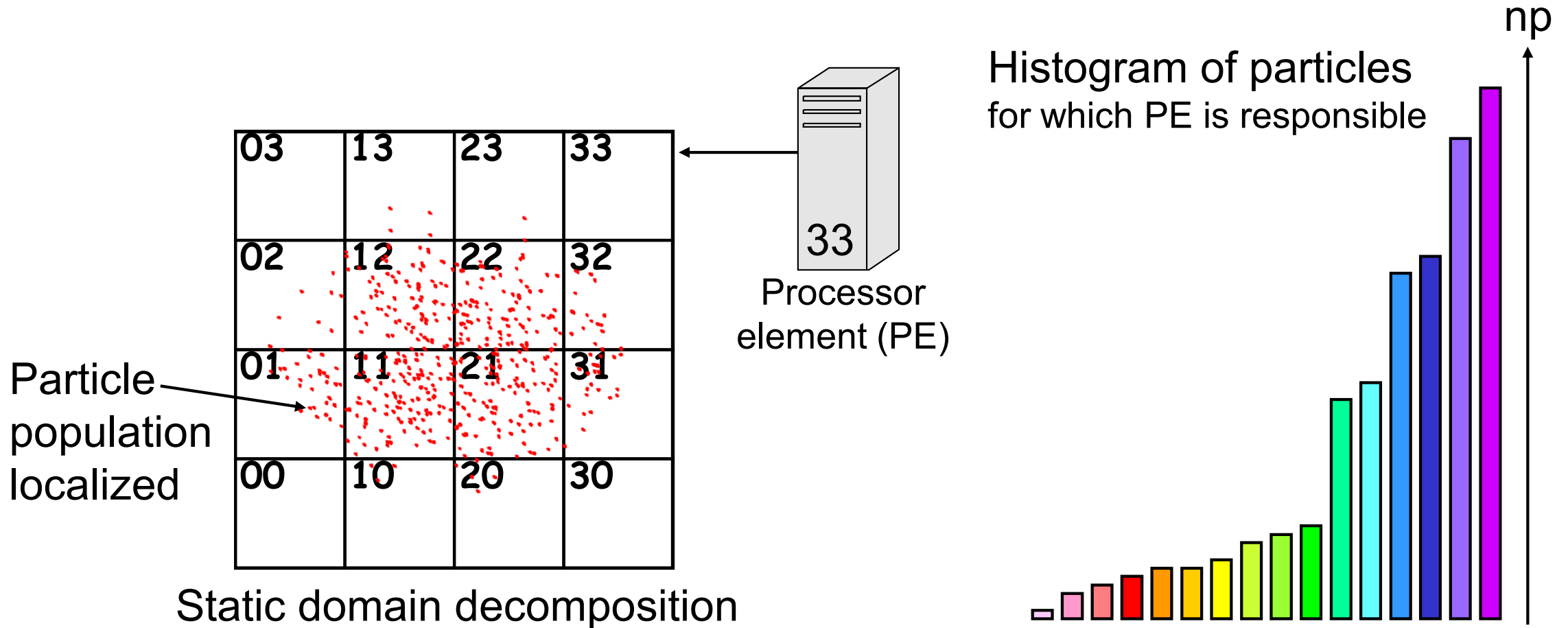
# PIC simulations on Supercomputers



# Fundamental strategies of parallelization

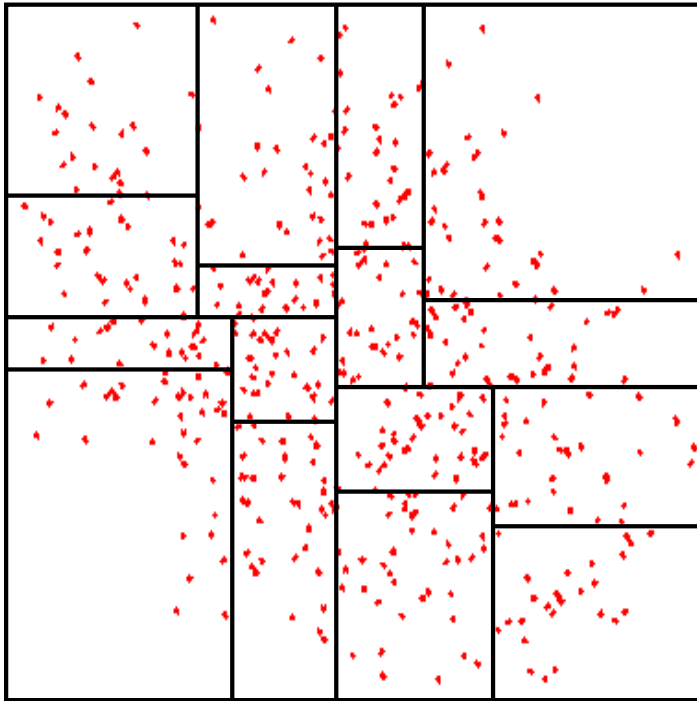


# Load balancing consideration



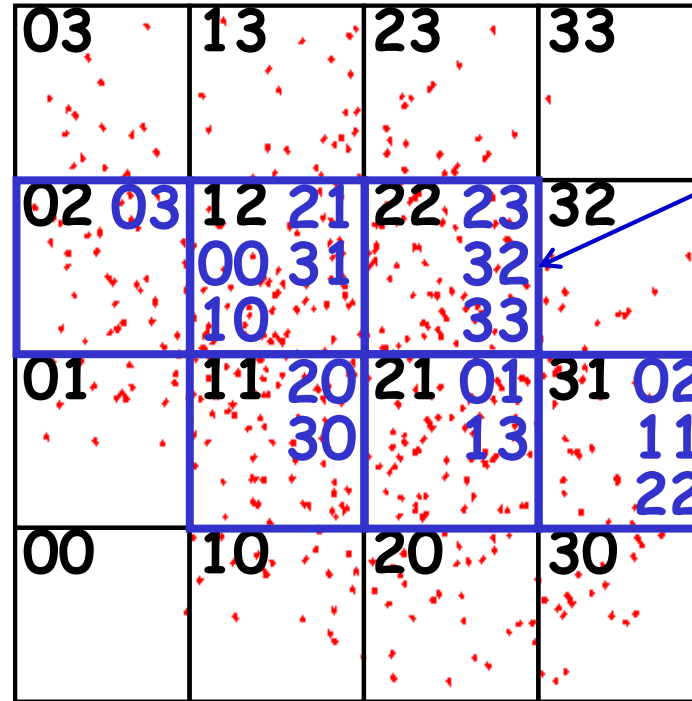
# Advanced strategies for parallelization

Orthogonal recursive bisection  
[Thackera+, 2003]



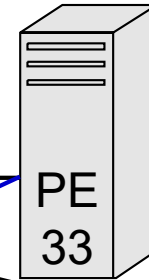
**Dynamic** domain decomposition

OhHelp  
[Nakashima+, 2009]



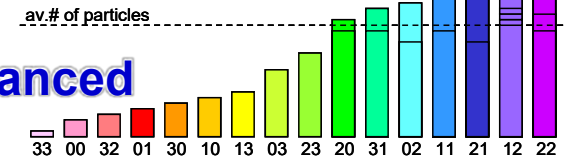
Static domain decomposition

**Dynamic PE assignment**

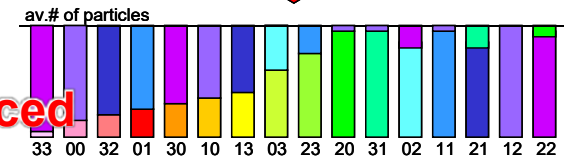


One-handed help  
(OhHelp)

load  
unbalanced



load  
balanced



# References from past ISSSs

## **Advanced Methods for Space Simulations (ISSS-7)**

“One-dimensional Electromagnetic Particle Code: KEMPO1”

Edited by H. Usui and Y. Omura (2007)

## **Computer Space Plasma Physics:**

### **Simulation Technique and Software (ISSS-4)**

“KEMPO1: Technical Guide to one-dimensional electromagnetic particle code”

Edited by H. Matsumoto and Y. Omura (1993)

## **Computer Simulation of Space Plasmas (ISSS-1)**

“Particle simulation of electromagnetic waves and its application to space plasmas”

Edited by H. Matsumoto and T. Sato (1985)