Particle in Cell for Plasma Simulation

Imran Khan

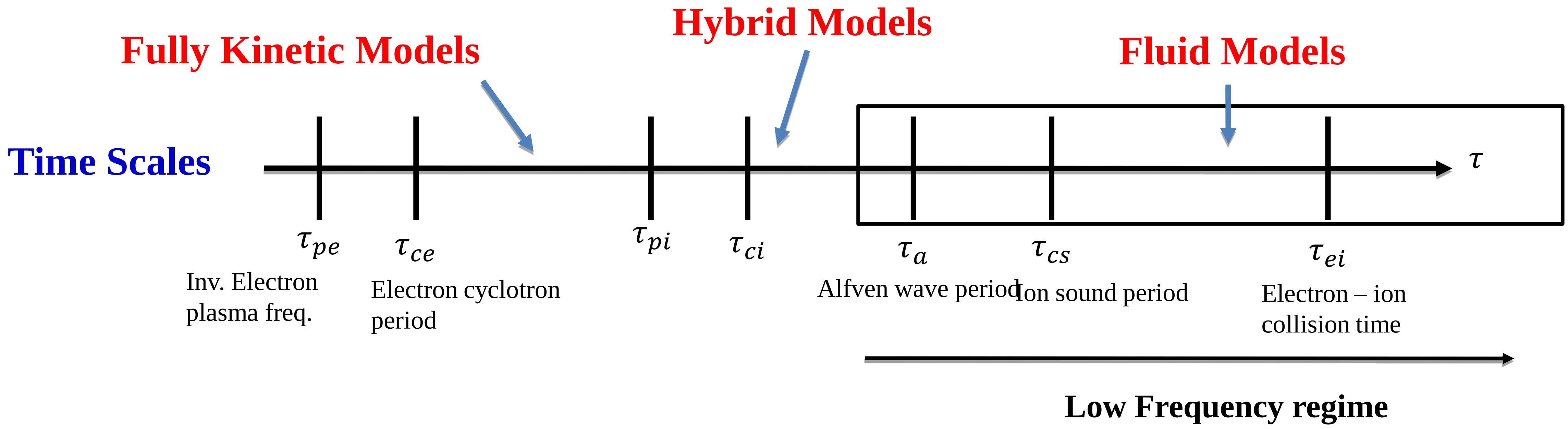
(phz198491)

Under the guidance of

Dr. Vikrant Saxena

Physics Department, IIT Delhi

Why PIC ?


Fully Kinetic Models
Hybrid Models
Fluid Models
Time Scales
τ
τ_{pe}
τ_{ce}
τ_{pi}
τ_{ci}
τ_{a}
τ_{cs}
τ_{ei}
Inv. Electron plasma freq.
Electron cyclotron period
Alfven wave period
Ion sound period
Electron – ion collision time
Low Frequency regime

Why PIC ?

- **Single Pasticle (example)**

Consider electrostatic case and a fully ionized copper plasma with 10 μm x 10 μm x 100 μm.
$m \approx 0.90$ g or $N_{mol} \approx 14$ nmol so $N_{ion} \approx 9\text{x}10^{15}$ ions and $N_e = Z\,N_{ion}$ with $Z = 28$.
Number of force pair calculations for electrons alone is roughly $N_e^2 \approx 10^{34}$.
At 1 calc/cycle and 1000 3 GHz processors, that would take roughly 10^{15} years.

- **If we study each particle it will take very large time**

Why PIC ?

Numerical

Kinetic

Fluid

Vlasov Equation

PIC

$$\frac{\partial f}{\partial t}+\vec{v}\cdot\vec{\nabla}f+\frac{q}{m}\left(\vec{E}+\vec{v}\times\vec{B}\right)\cdot\frac{\partial f}{\partial\vec{v}}=0$$

0^{th} order moment → continuity equation

1^{sh} order moment → momentum equation

2^{nd} order moment → heat flow equation

6D phase space, numericaly expensive

- **Deals with macroscopic phenomena**
- **Does not deal with wave-particle interaction**
- **Information of individual particle get lost**

- **Solve system of equation in the physical observable quantity**
- **Fully kinetic approach**
- **Least physics approximation**
- **Have high noise**
- **Some time difficult to understand the physics**

Cost : Vlasov Equation > PIC > Fluid

Basic Equations

- **Equations for plasma dynamics**

Maxwell Equations

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

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

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

$$c\vec{\nabla} \times \vec{B} = 4\pi\vec{J} + \frac{\partial \vec{E}}{\partial t}$$

Lorentz Force

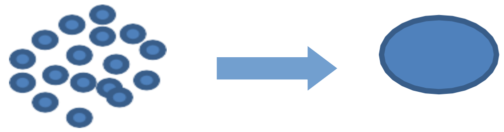
$$\frac{\partial \vec{P}}{\partial t} = q\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right)$$

Equation of Continuity

$$\vec{\nabla} \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0$$

PIC Steps

- Replace the charges by a small no of large size particles with same charge to mass ratio.



- Discretise the system.
- Replace the continuous EM fields by values on a discrete mesh.
- Advances the time related quantities by **leap-frog**method.
- Couples the particles and fields by **interpolation**.

Assigns particle related quantities to mesh points. Compute mesh related quantities at particle position.

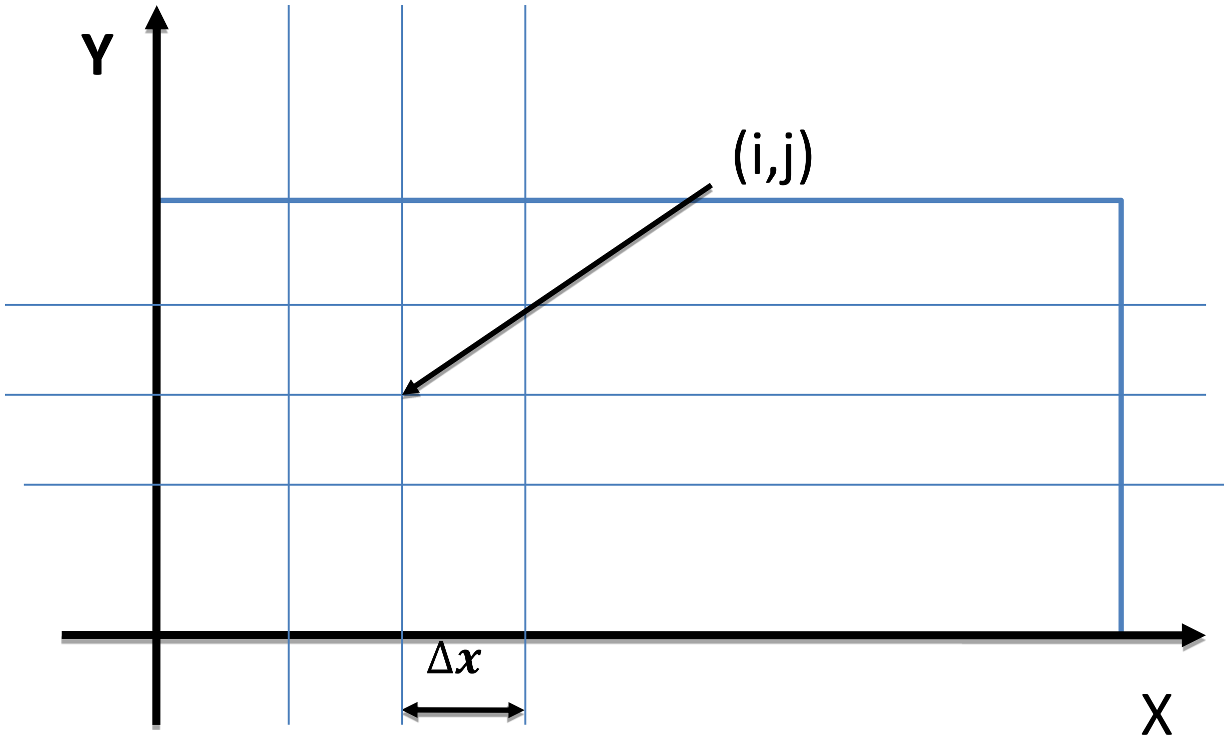
Discretising Computational Space

- **The computational space is reduced to a mesh by drawing lines parallel to the boundaries.**

- **Each mesh point accessed by a set of 3 integer indices [i],[j],[k].**

- **The mesh spacing is determined by smallest length scale of the simulation which needs to be accurately resolved.**

$$\Delta x \leq 3.4\lambda_d$$
$$\omega_p \Delta t \leq 2$$
$$C\Delta t \leq \Delta x$$



Weighting (connection b/w grid and particle)

- **Charge density on the discrete grid points from continuous particle position**

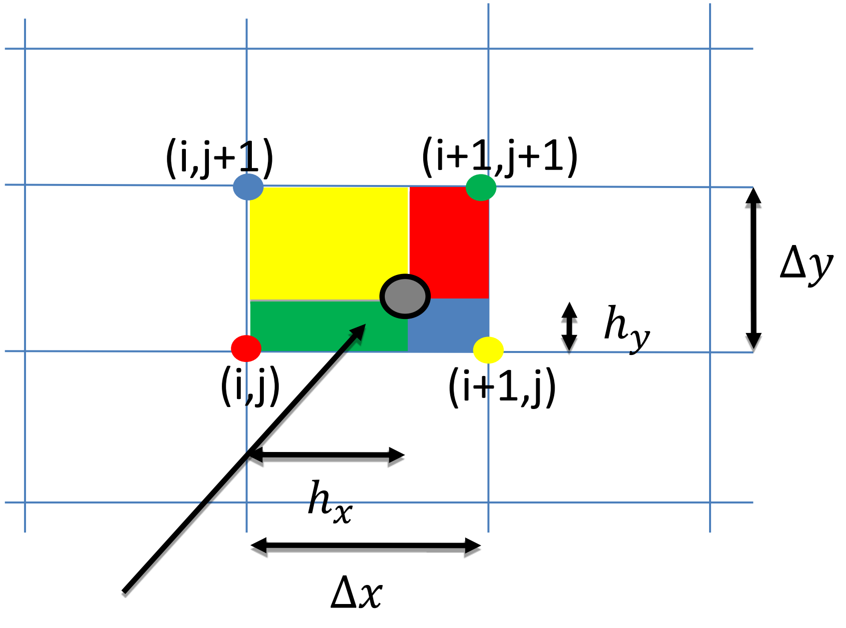
$$A_r = (\Delta x - h_x)(\Delta y - h_y)$$

$$A_y = h_x(\Delta y - h_y)$$

$$A_b = (\Delta x - h_x)h_y$$

$$A_g = h_x h_y$$

Area Weighting

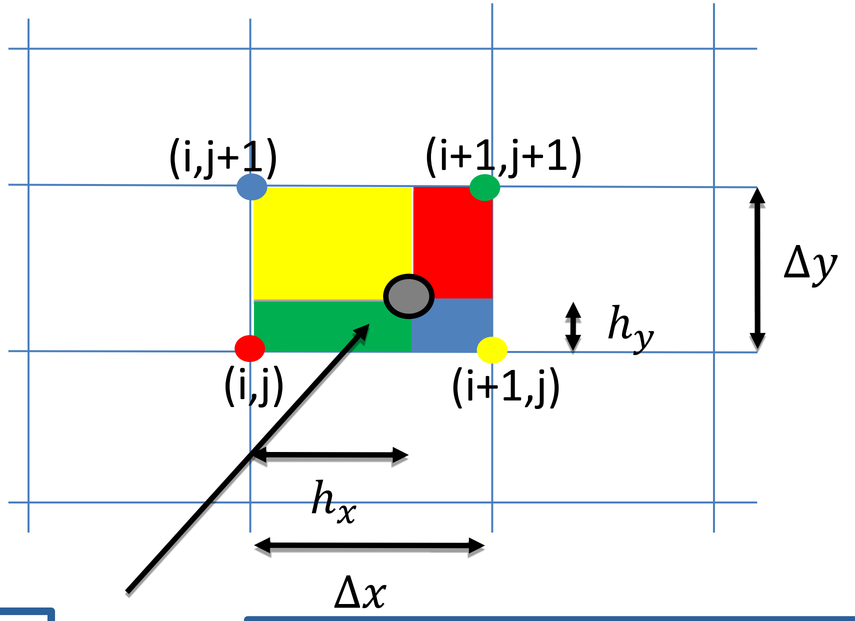


$q_m e$

Weighting (connection b/w grid and particle)

- **Charge density on the discrete grid points from continuous particle position**

Area Weighting



q_m macroscopic charge

$A_{red} = (\Delta x - h_x)(\Delta y - h_y)$

$A_{yellow} = h_x(\Delta y - h_y)$

$A_{blue} = (\Delta x - h_x)$

$A_{green} = h_x h_y$

$q_m e$

$W_{i,j} = A_{red}/(\Delta x \Delta y)$

$W_{i+1,j} = A_{yellow}/(\Delta x \Delta y)$

$W_{i,j+1} = A_{blue}/(\Delta x \Delta y)$

$W_{i+1,j+1} = A_{green}/(\Delta x \Delta y)$

$q_{i,j} = q_m W_{i,j}$

$q_{i+1,j} = q_m W_{i+1,j}$

$q_{i,j+1} = q_m W_{i,j}$

$q_{i+1,j+1} = q_m W_{i+1,j+1}$

The Yee Cell

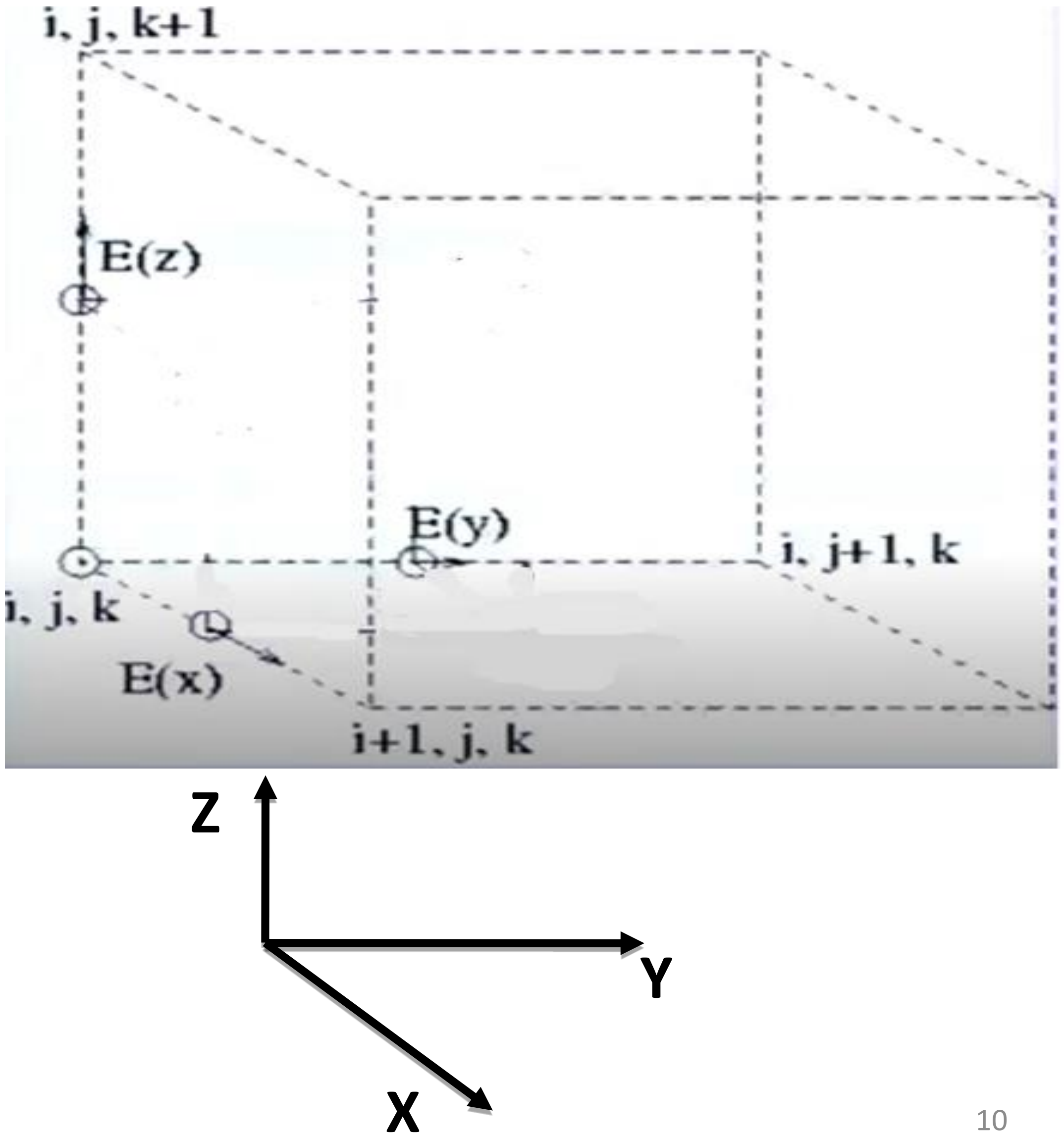
- **The charge density is located at the mesh points.**

- **Central differencing place the electric field between them.**

$$E_x = -\frac{\emptyset_{i+1,j,k} - \emptyset_{i,j,k}}{\Delta x}$$

$$E_y = -\frac{\emptyset_{i,j+1,k} - \emptyset_{i,j,k}}{\Delta y}$$

$$E_z = -\frac{\emptyset_{i,j,k+1} - \emptyset_{i,j,k}}{\Delta z}$$

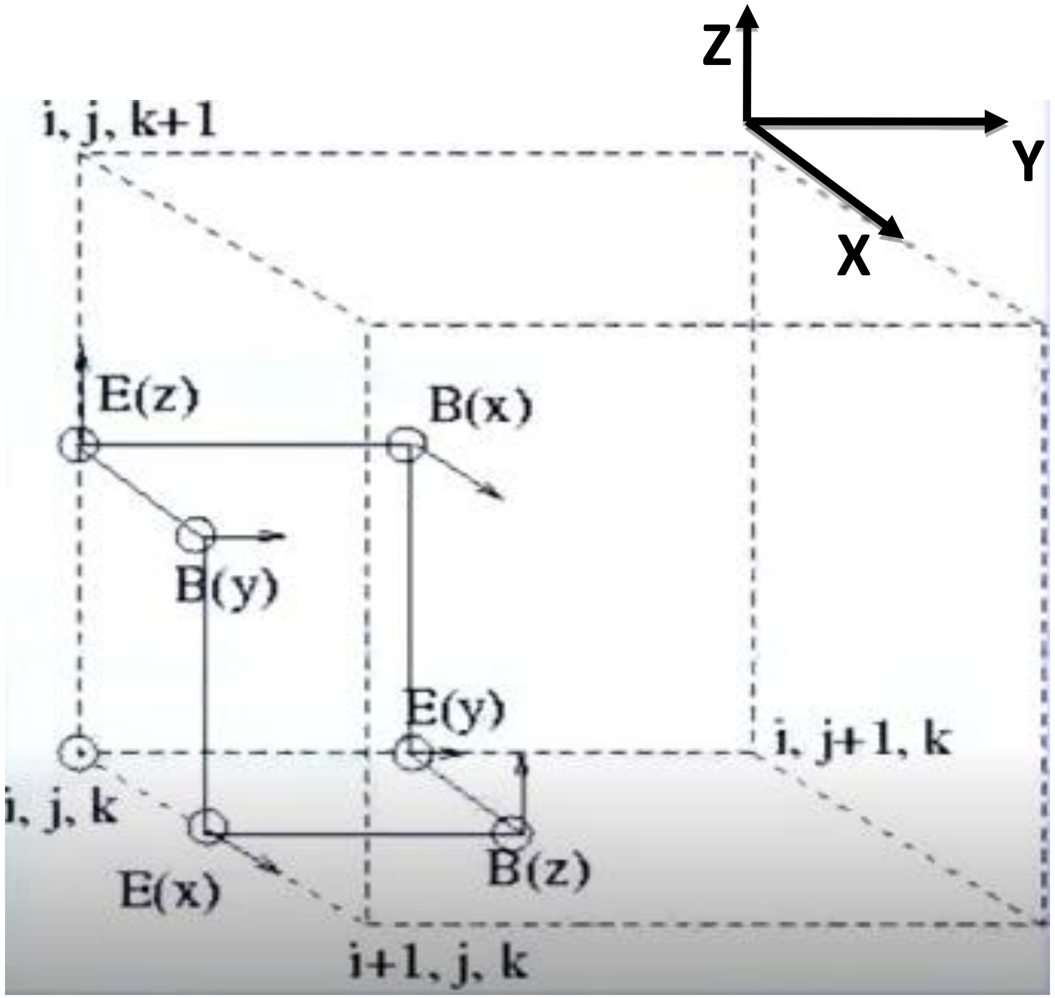


The Yee Cell

- Hence the magnetic field must lie at the face centres.

- This placement is the key to the Finite Difference Time Domain (FDTD) method.

- Current density coincides with the Electric fields.



$$\nabla \times E = \begin{bmatrix} i & j & k \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ E_x & E_y & E_z \end{bmatrix}$$

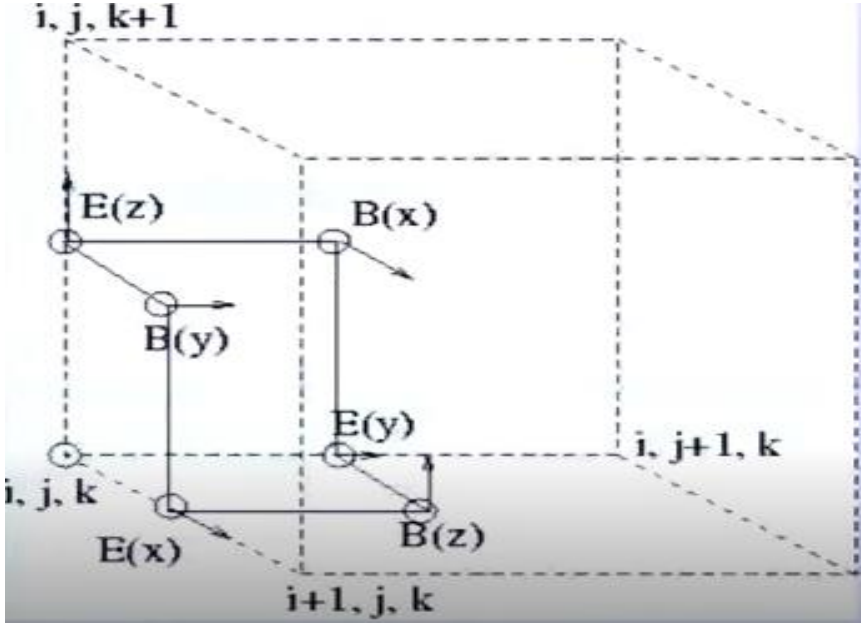
$$-\frac{1}{c}\left(\frac{\partial B_x}{\partial t} i + \frac{\partial B_y}{\partial t} \mathrm{j} + \frac{\partial B_z}{\partial t} k\right) = \left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}\right) i - \left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z}\right) j + \left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right) k$$

Advancing Field (E)

- The advance of E from step (n) to (n+1) is done via central difference using B at step (n+1/2)

- The x-component of curl-B is:

$$\frac{\partial \overrightarrow{B_z}}{\partial y} - \frac{\partial \overrightarrow{B_y}}{\partial z} = \frac{4\pi}{c}\overrightarrow{J_x} + \frac{1}{c}\frac{\partial \overrightarrow{E_x}}{\partial t}$$



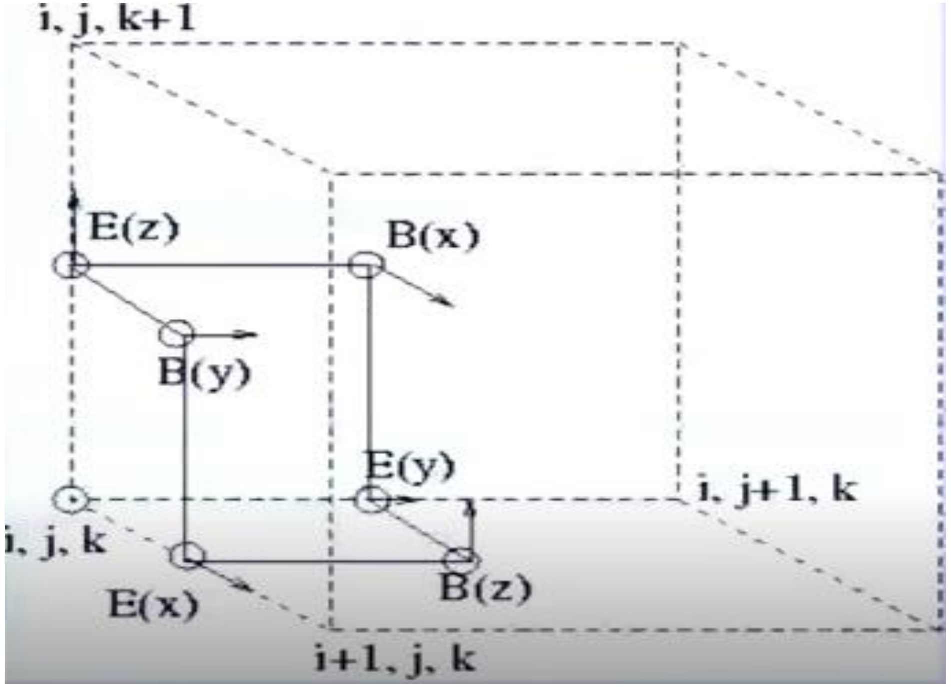
Time


$$\frac{\vec{B}^{z,n+1/2}_{i+1/2,j+1/2,k} - \vec{B}^{z,n+1/2}_{i+1/2,j-1/2,k}}{\Delta} - \frac{\vec{B}^{y,n+1/2}_{i+1/2,j,k+1/2} - \vec{B}^{y,n+1/2}_{i+1/2,j,k-1/2}}{\Delta z} = \frac{4\pi}{c}\vec{J}^{x,n+1/2}_{i+1/2,j,k} + \frac{1}{c}\frac{\vec{E}^{x,n+1}_{i+1/2,j,k} - \vec{E}^{x,n}_{i+1/2,j,k}}{\Delta t}$$

Advancing Dield (B)

- The advance of B from step (n-1/2) to (n+1/2) is done via central difference using E at step n

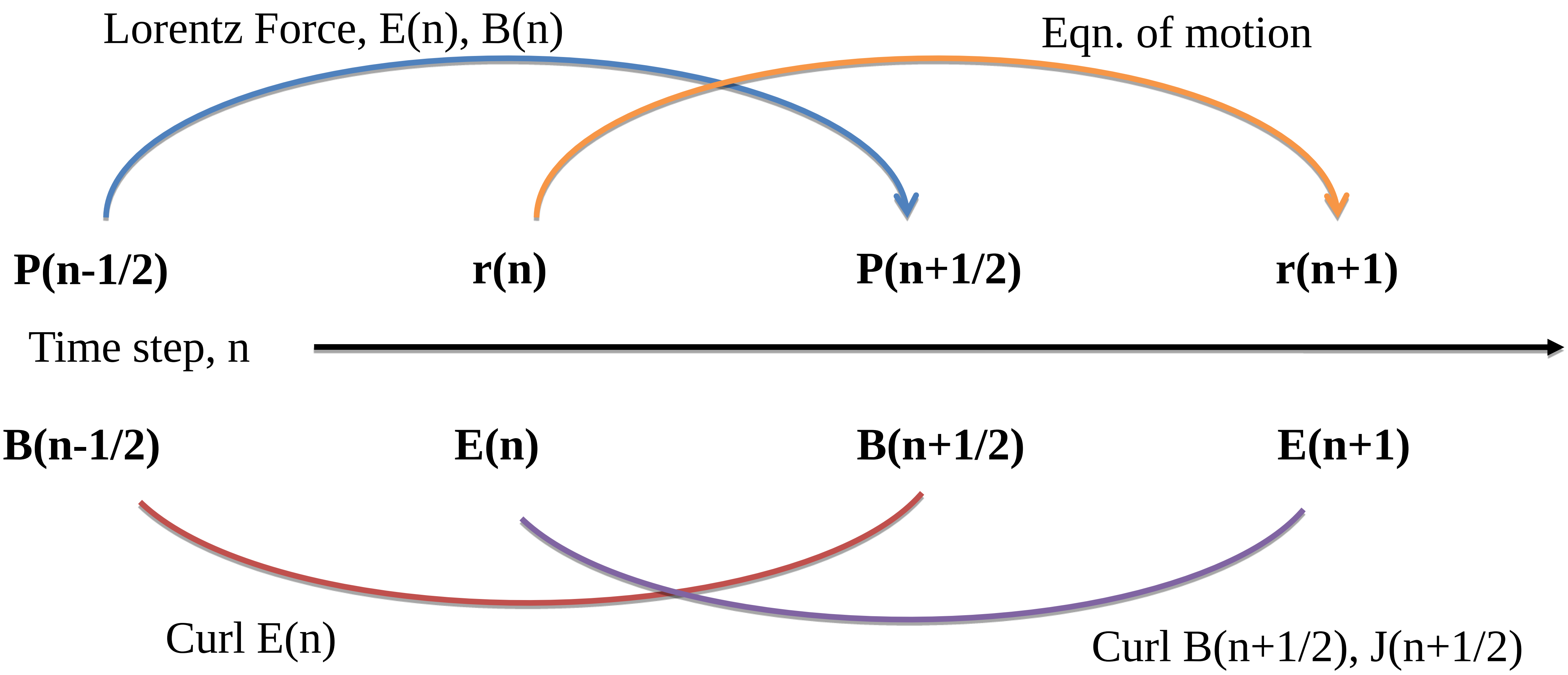
- The x-component of curl-E is:



$$\frac{\partial \overrightarrow{E_z}}{\partial y} - \frac{\partial \overrightarrow{E_y}}{\partial z} = -\frac{1}{c}\frac{\partial \overrightarrow{B_x}}{\partial t}$$

$$\frac{\vec{E}^{z,n}_{i,j+1,k+1/2} - \vec{E}^{z,n}_{i,j,k+1/2}}{\Delta} - \frac{\vec{E}^{y,n}_{i,j+1/2,k+1} - \vec{E}^{y,n}_{i,j+1/2,k}}{\Delta z} = +\frac{1}{c}\frac{\vec{B}^{x,n+1/2}_{i,j+1/2,k+1/2} - \vec{B}^{x,n-1/2}_{i,j+1/2,k+1/2}}{\Delta t}$$

Leap - Frogging



Updating Position and Velocity

Lorentz force $\vec{F}_n = q\left(\vec{E}_n + \vec{v}_n \times \vec{B}_n\right)$

- **Convert second order equation into two first order equation**

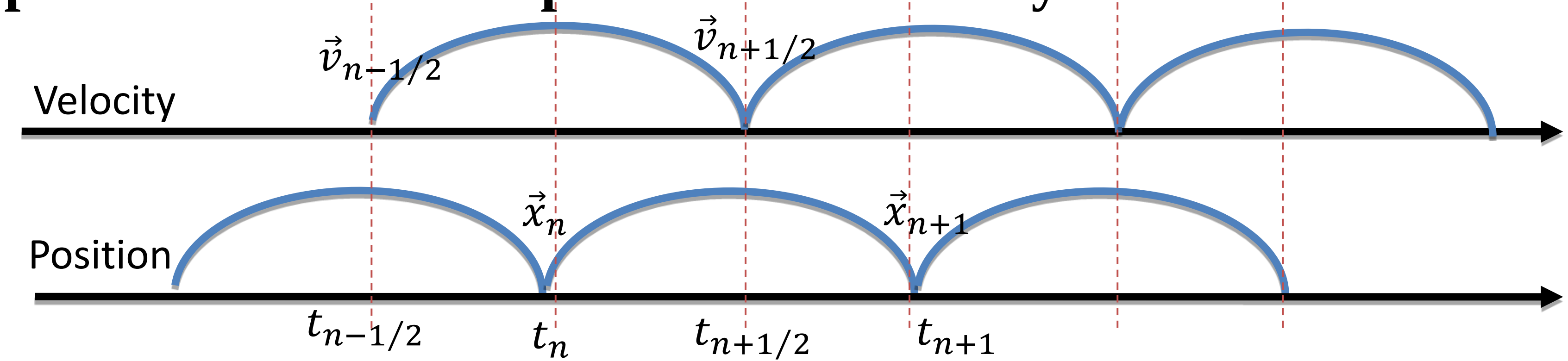
$$\vec{F}_n = m\frac{\partial \vec{v}_n}{\partial t}$$

$$\vec{F}_n = m\left(\frac{\vec{v}_{n+1/2} - \vec{v}_{n-1/2}}{\Delta t}\right)$$

$$\vec{v}_{n+1/2} = \frac{\partial \vec{x}_{1/2}}{\partial t}$$

$$\vec{v}_{n+1/2} = \left(\frac{\vec{x}_{n+1} - \vec{x}_n}{\Delta t}\right)$$

- **Half time step difference between position and velocity**



Updating Position and Velocity

Lorentz force $\vec{F}_n = q\left(\vec{E}_n + \vec{v}_n \times \vec{B}_n\right)$

Boris Method

- **Half-step acceleration in Electric field**

$$m\frac{\vec{v}_n - \vec{v}_{n-1/2}}{Vt/2} = q\vec{E}_n \quad \Rightarrow \quad v_n^{(1)} = v_{n-1/2} + \frac{q}{m}E_n\frac{\Delta t}{2}$$

- **Full step rotation in magnetic field:** Let **B**$_n$ z-axis and resolve v_n^1 into components parallel and perpendicular to z

$$\|\vec{B}_n\colon v_{z,n}^{(2)} = v_{z,n}^{(1)}$$

$$\perp \vec{B}_n\colon \begin{bmatrix} v_{x,n}^{(2)} \\ v_{y,n}^{(2)} \end{bmatrix} = \begin{bmatrix} cos\left(\omega_{c,n}\Delta t\right) & sin\left(\omega_{c,n}\Delta t\right) \\ -sin\left(\omega_{c,n}\Delta t\right) & cos\left(\omega_{c,n}\Delta t\right) \end{bmatrix} \begin{bmatrix} v_{x,n}^{(1)} \\ v_{y,n}^{(1)} \end{bmatrix}$$

- **Half step acceleration in electric field**

$$v_{n+1/2} = v_{n+1/2}^{(3)} = v_n^{(2)} + \frac{q}{m}E_n\Delta\frac{t}{2}$$

Where $\omega_{c,n} = \frac{qB_n}{m}$

Reason For Cenral Difference

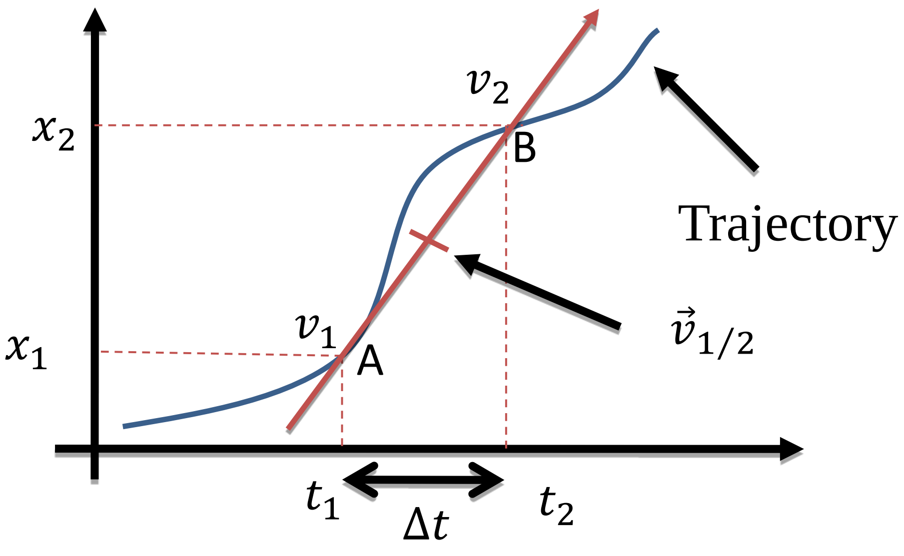
- **Forward Difference**

$$\vec{v}_1 = \frac{\vec{x}_2 - \vec{x}_1}{t_2 - t_1}$$

- **Backward Difference**

$$\vec{v}_2 = \frac{\vec{x}_1 - \vec{x}_2}{t_1 - t_2}$$

$$\vec{v}_1 = \vec{v}_2$$



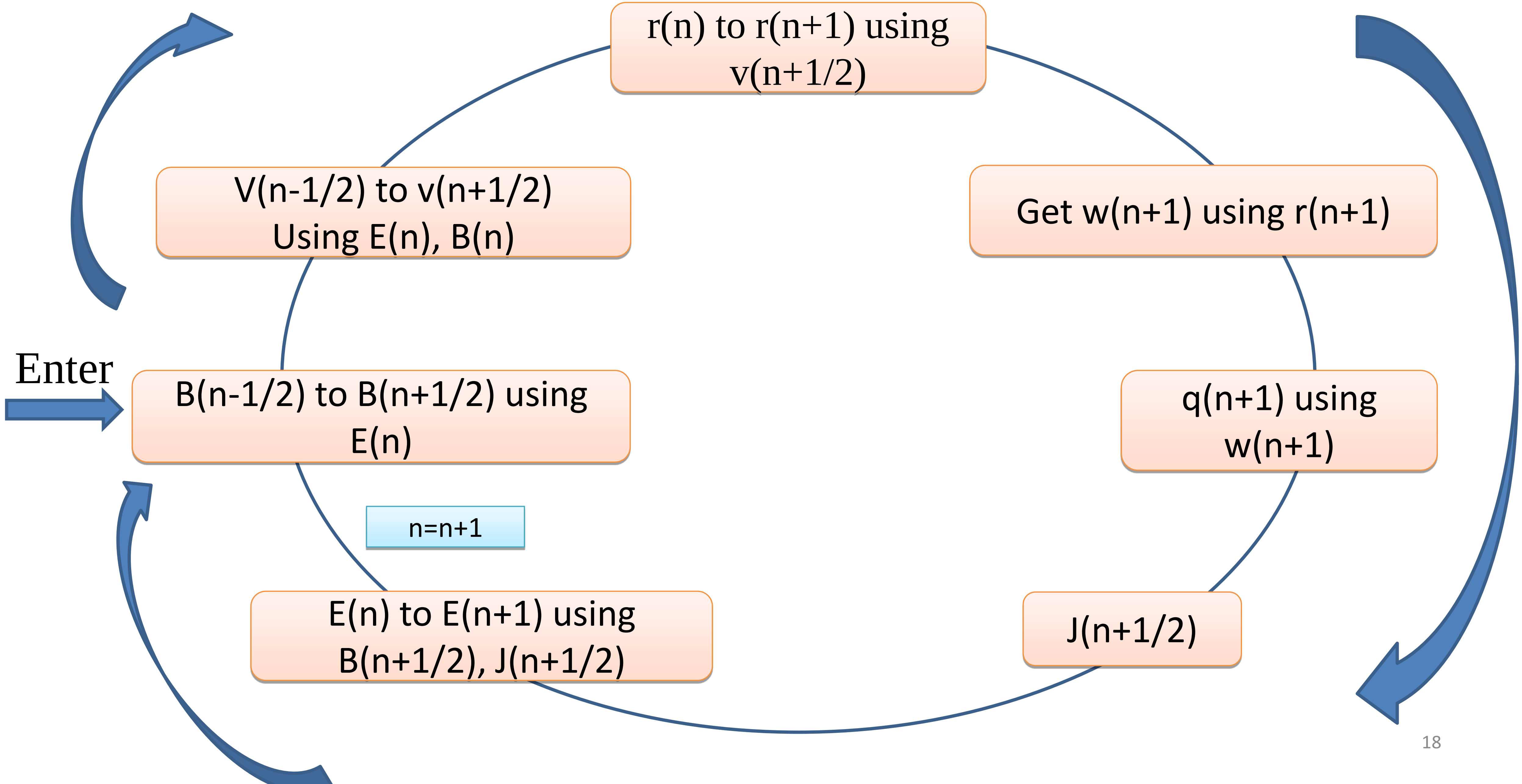
- **But, actually** $\vec{v}_1 \neq \vec{v}_2$

- **Time symmetry is not maintained**

- **So, take central difference**

- **Result in separation of half time step in position and velocity**

Computational Cycle



Boundary

- **Radiation Boundary Condition**

Open: boundaries are at infinity
Perfectly Matched Layer (PML)
Mur BC's
Periodic: wave re-enters from opposite side

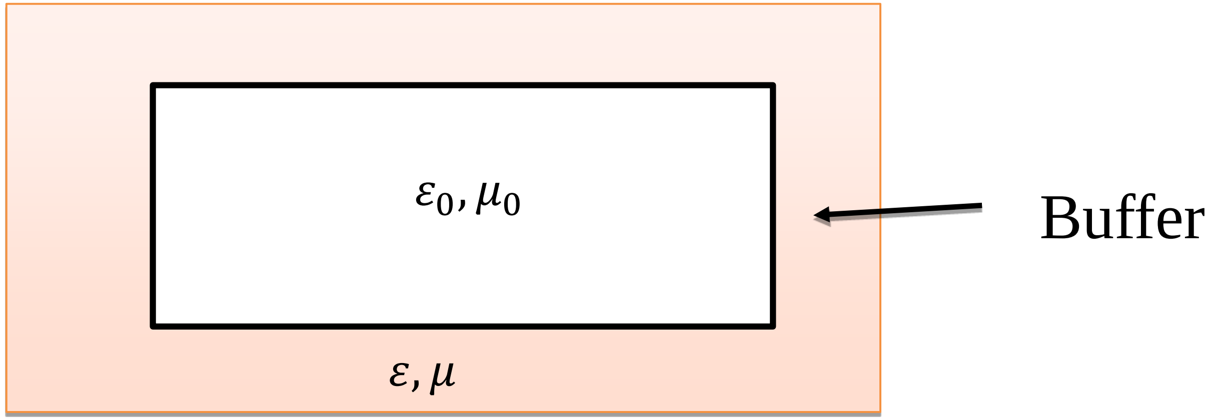
- **Particle Boundary conditions**

Absorbing: charge vanishes as it exits the space
Reflective: charge is reflect back
Periodic: charge re-enters from opposite boundary

Boundary Conditions (radation)

PML BC's

- **System is surrounded by buffer layer of different**
- **Adjust electric and magnetic conductivities so that impedance is equal to that of system**
- **The wave propagating outward without reflection and get attenuated until…**
- **… it hit the real boundary, and there the reflection is negligibly small**

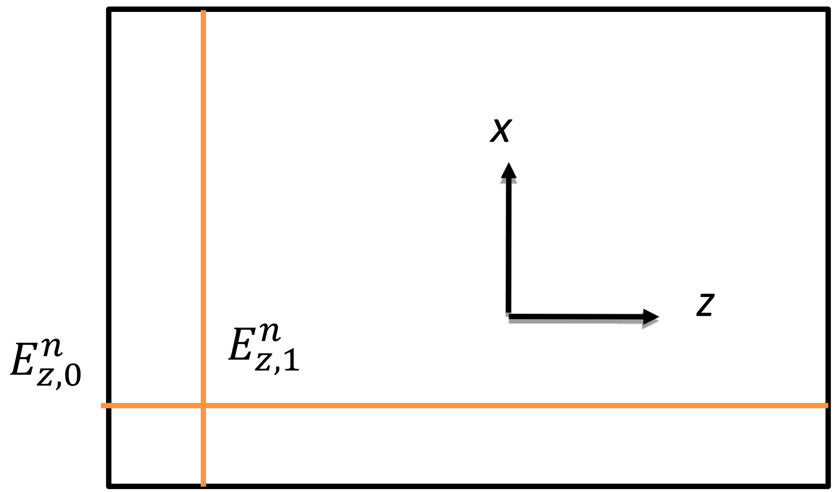


Boundary Condition (radation)

Mur BC's (radiation)

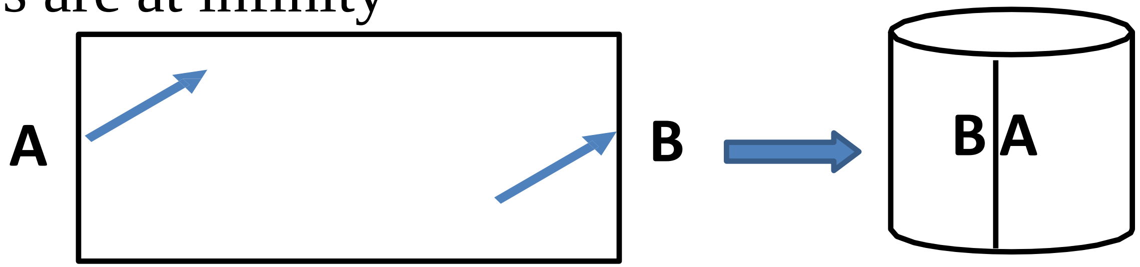
- Take the wave hitting the boundary
- Calculate the change in phase and magnitude
- No need of magnetic field outside the boundary

$$E_{z,0}^{n+1} = E_{z,1}^{n} + \frac{c\Delta t - \Delta x}{c\Delta t + \Delta x}\left(E_{z,1}^{n+1} + E_{z,0}^{n}\right)$$



Periodic Boundary condition (radiation/particle)

- Wave/particle exit form the system will re-enter from apposite side.
- The initial conditions of the wave/particle which enter to the system are same as that of wave/particle which exit from opposite side
- System behave as its boundaries are at infinity



THANK YOU