Computational Methods for Kinetic Processes in Plasma Physics

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Basics of PIC Simulation methods

* Collisionless plasmas
* Finite-size particles
* Electrostatic codes
* Charge assignment and force interpolation (already in 3-D system)
* Filtering action of shape function
* Summary

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Context

- Collisionless plasmas
- Finite-size particles
- Electrostatic codes
- Charge assignment and force interpolation
  (already in 3-D system)
- Filtering action of shape function
- Summary

Characteristic time and length scales

$$\omega_P = \left(\frac{4\pi\, ne^2}{m}\right)^{1/2}$$

Plasma frequency

$$\lambda_D = \frac{V_{thermal}}{\omega_p} \propto \left(\frac{T}{n}\right)^{1/2}$$

Debye length

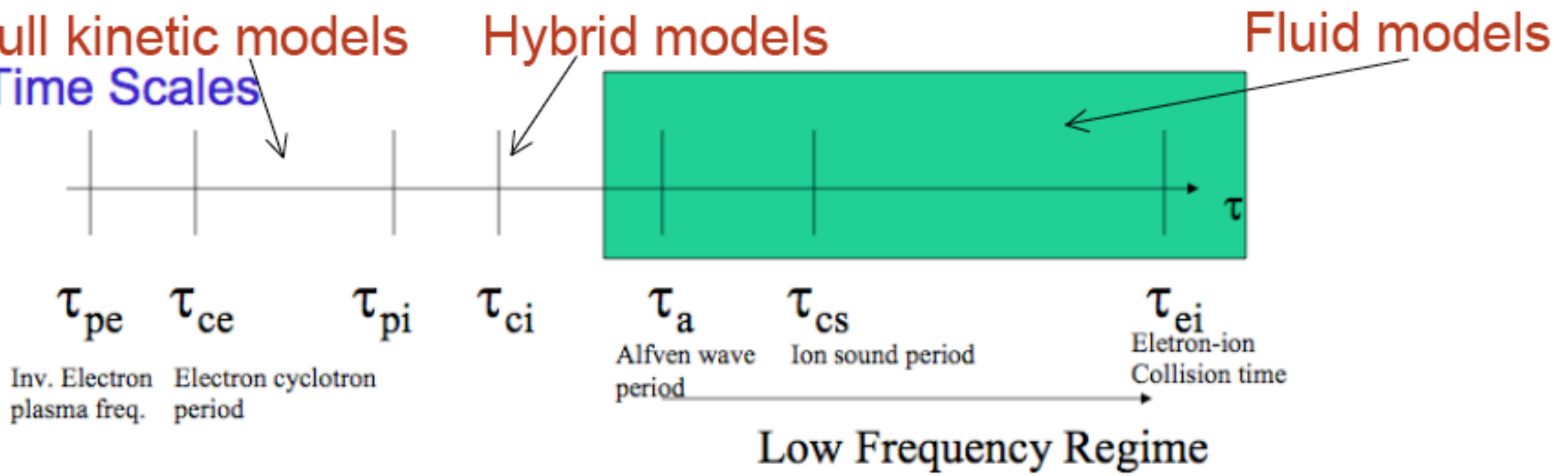
$$\lambda_{skin} = c/\omega_p$$

skin depth

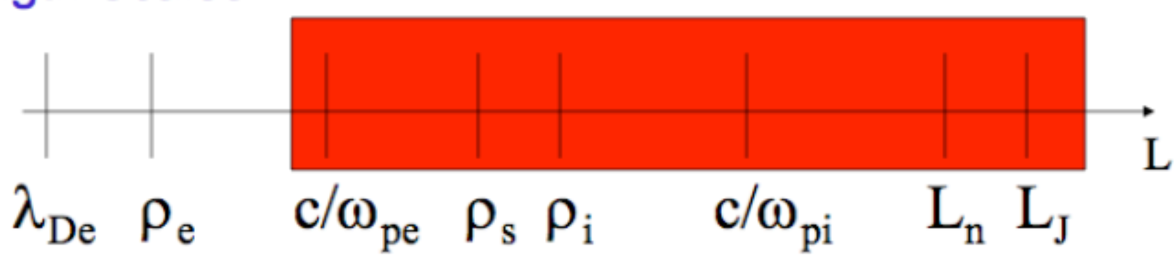
$$\omega_c = \frac{eB}{mc}$$

Larmor

•Time Scales

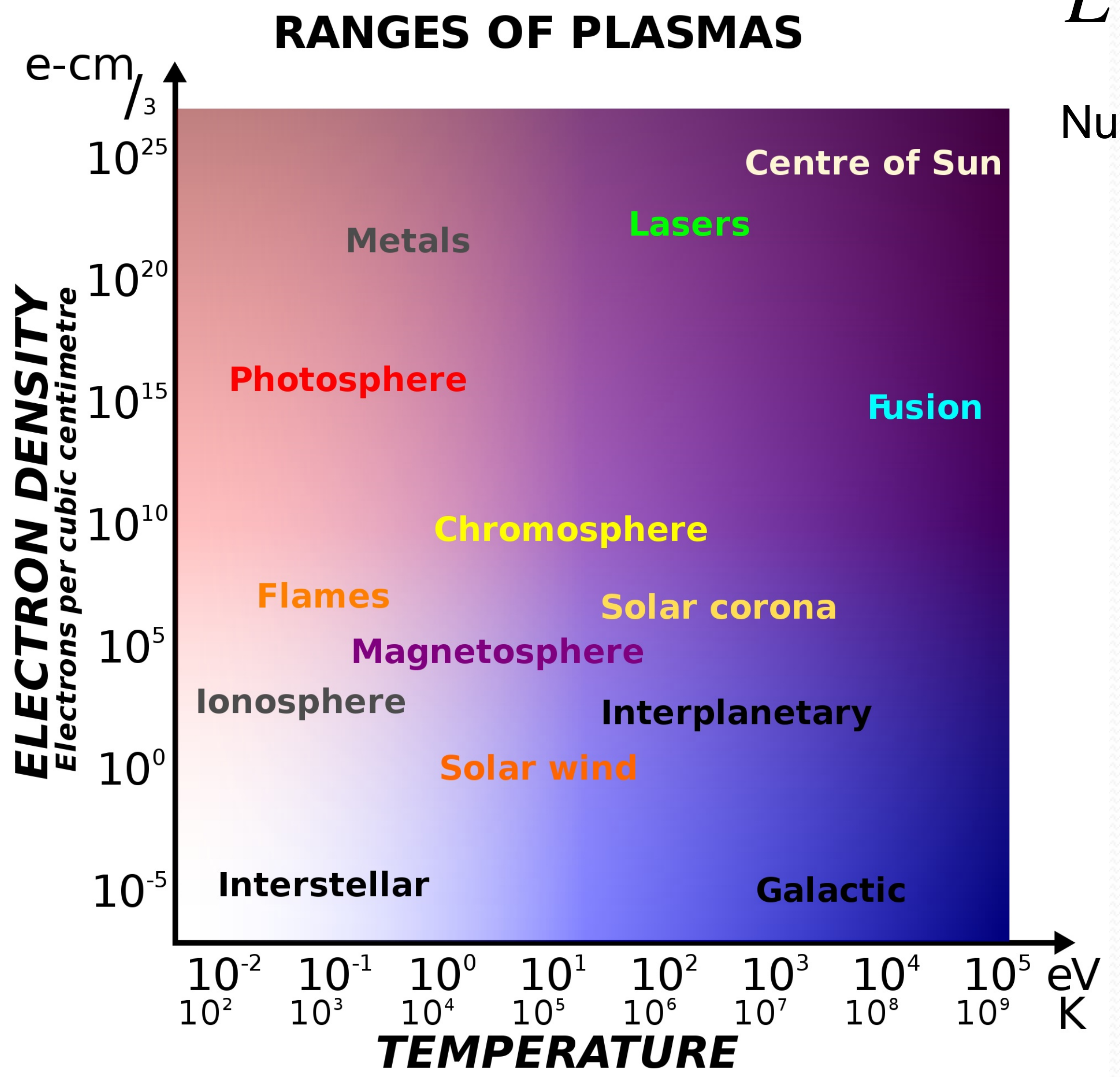


•Length Scales



$$\rho_e = v_{te}/\omega_{ce} \qquad \rho_s = \sqrt{T_i/T}\,\rho_i \qquad L_n = \nabla n/n$$

Collisionless plasmas



$$L \gg \lambda_D, \quad t \gg \omega_p^{-1}, \omega_c^{-1}$$

Number of particles in Debye cubes

$$N_D \equiv n\lambda_D^3 \gg 1$$

Collisionless plasma can be described by Vlasov-Maxwell equations with distribution function f(**x**, **v**, t) (6 dimensions):

$$\frac{\partial f}{\partial t} + \vec{v} \bullet \frac{\partial f}{\partial \vec{x}} + \frac{q}{m}(\vec{E} + \frac{\vec{v} \times \vec{B}}{c}) \bullet \frac{\partial f}{\partial \vec{v}} = 0,$$

$$\nabla \bullet \vec{E} = 4\pi \int qfd^3\vec{v}$$

$$\nabla \times \vec{B} = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c}\int q\vec{v}fd^3\vec{v},$$

$$\nabla \bullet \vec{B} = 0, \quad \nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}.$$

Direct calculation of this set of equations – 6D
Improvements have been made, but difficult to calculate using this method

Particle method

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

$$\frac{d\vec{x}}{dt} = \vec{v}$$

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

$$\nabla \times B = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} + \frac{4\pi \vec{J}}{c}$$

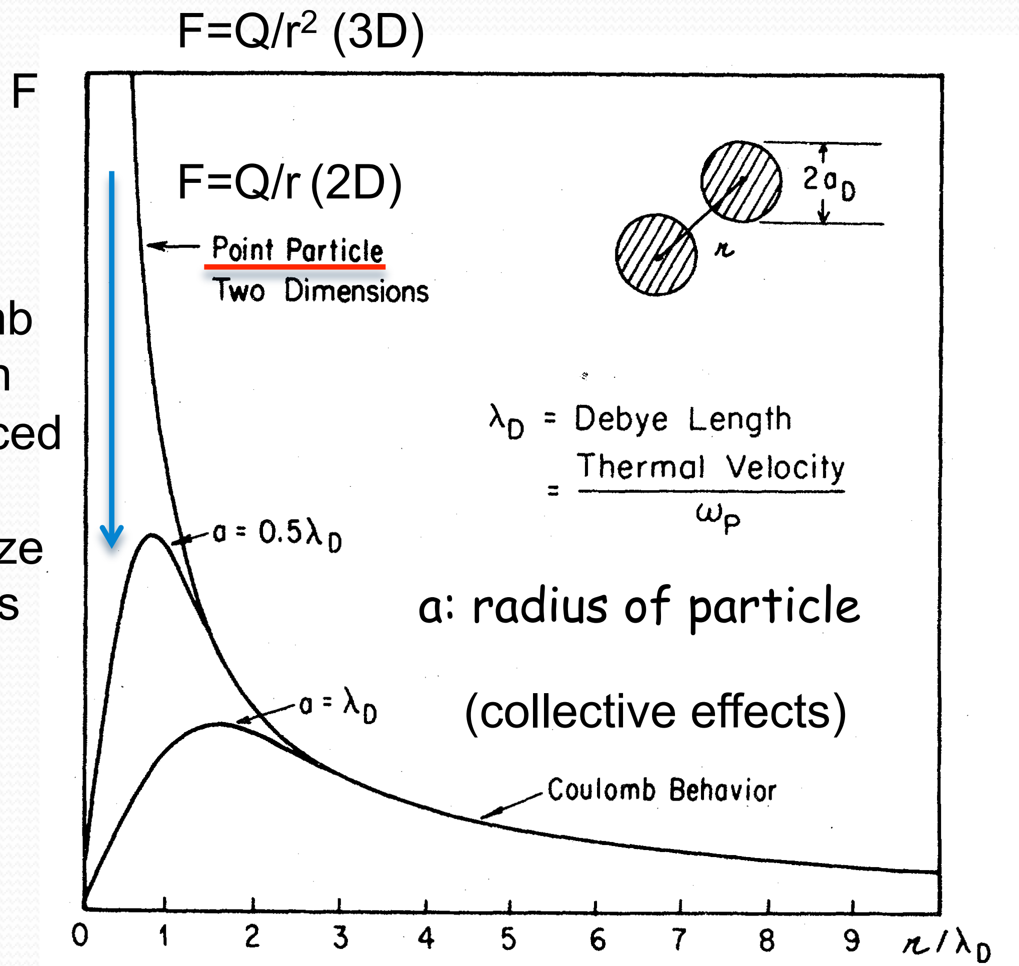
$$\nabla \bullet B = 0, \quad \nabla \bullet E = 4\pi\rho$$

$$\rho(\vec{x}) = \sum_j q_j \delta(\vec{x} - \vec{x}_j)$$

$$\vec{j}(\vec{x}) = \sum_j q_j \vec{v}_j \delta(\vec{x} - \vec{x}_j)$$

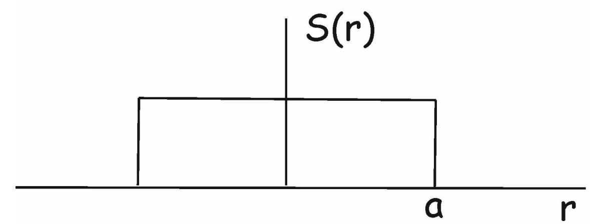
Coulomb force and force law

Coulomb collision is reduced using finite-size particles

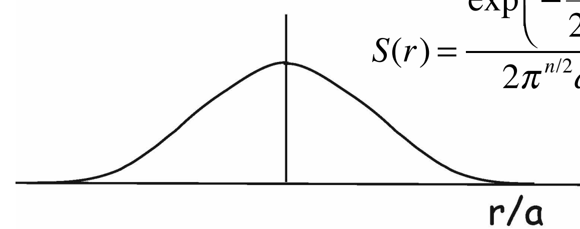


$$S(r) = \frac{1}{V_n a^n}, \quad r < a$$

$$S(r) = 0, \quad r > a$$



$$S(r) = \frac{\exp\left(-\frac{r^2}{2a_0^2}\right)}{2\pi^{n/2} a_0^n}$$



(Dawson 1983)

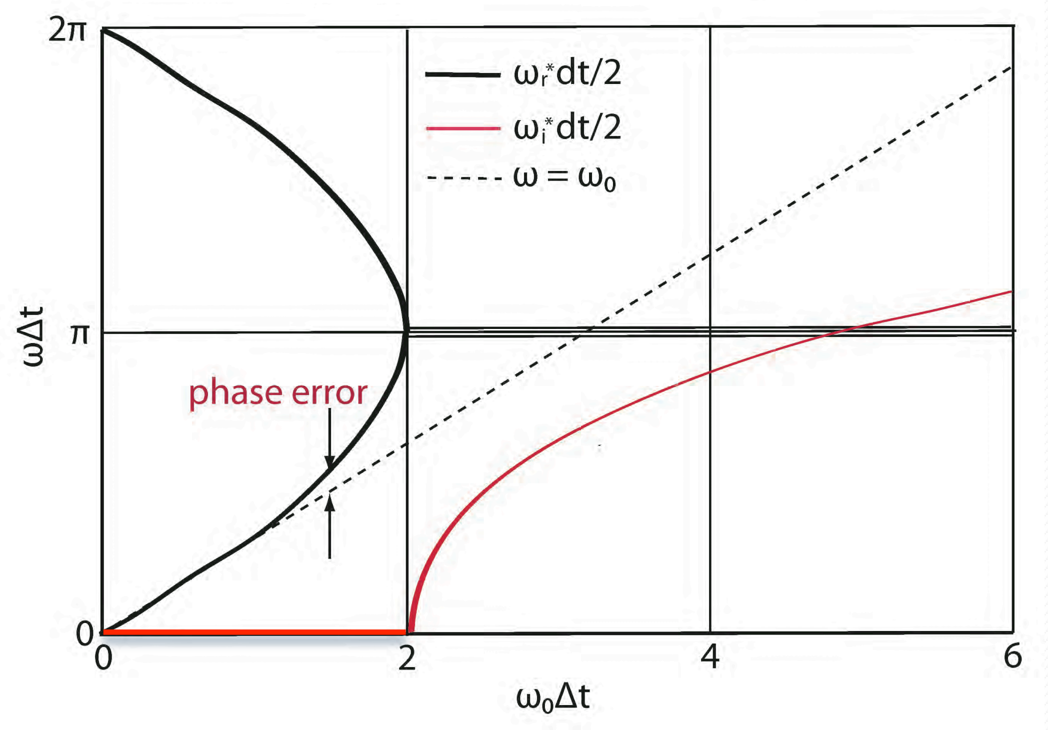
Particle mover accuracy: Simple harmonic motion test

$$\frac{d^2x}{dt^2} = -\omega_0^2 x$$

$$x = Ae^{-i\omega t}$$

$$\frac{x^{t+\Delta t} - 2x^t + x^{t-\Delta t}}{dt^2} = -\omega_0^2 x^t$$

$$\sin\left[\omega \frac{\Delta t}{2}\right] = \pm\omega_0 \frac{\Delta t}{2}$$



Two major methods of calculating current

1. Spectral method (UPIC code) (note by Decyk)
   We will review this method in details later after we do handout exercises

2. Charge-conserving current deposit (Villasenor & Buneman 1992)
   We will review this method with Umeda's method later

Electrostatic codes

Time scales of the system >> light crossing time, static magnetic field

$$\nabla^2 \phi = -\rho(x)$$

$$E(x) = -\nabla \phi$$

$$F_i = q_i E(x_i)$$

Four major criteria to choose an Algorism for integration of equation of motion

- **Convergence:** the numerical solution converges to the exact solution of the differential equation in the limit of Δt and Δx tend to zero
- **Accuracy:** the truncation error associated with approximating derivatives with differences
- **Stability:** depends on how total errors (including truncation error and round-off errors) grows in time
- **Efficiency:** the code needs to be efficient to handle large number of particles

Need asses two physical quantities to know how well the codes work

- **Dissipation:** The truncation error associated with approximating derivatives with differences causes the dissipation of some physical quantities
- **Conservation:** The truncation error also causes the deviation of the conservation law

Integration of equations of motion

The simple second order leapfrog achieves the best balanced between accuracy stability, and efficiency

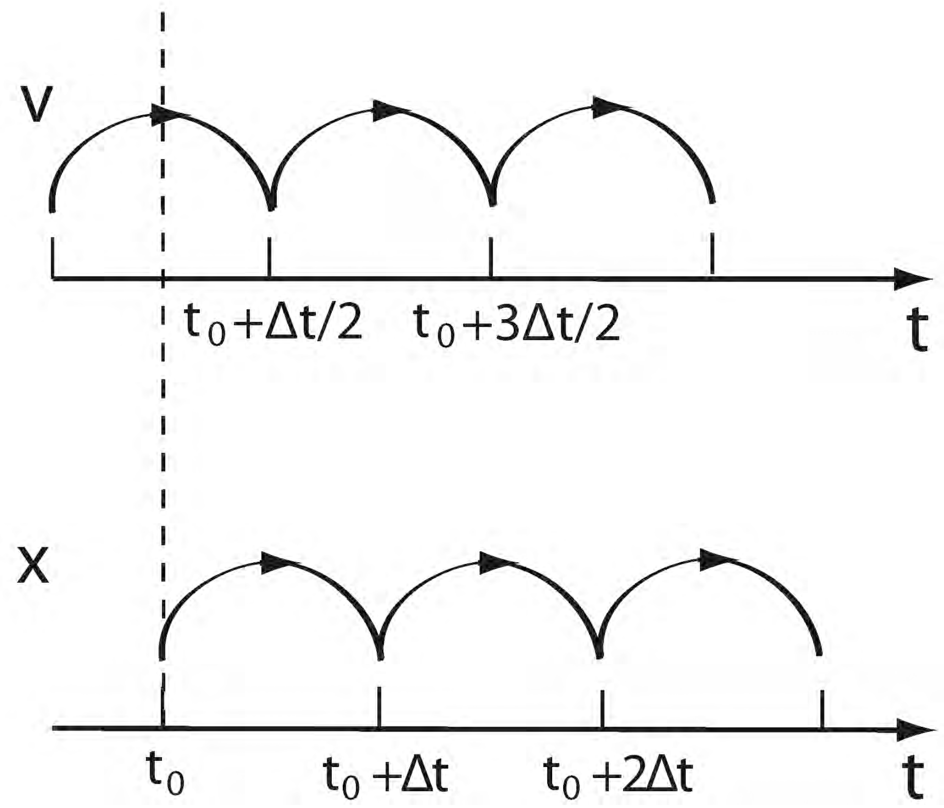
$$\frac{dx_i}{dt} = v_i$$

$$\frac{dv_i}{dt} = \frac{F_i}{m_i}$$

$$\downarrow$$

$$m_i \frac{v_i^{n+1/2} - v_i^{n-1/2}}{\Delta t} = F_i^n$$

$$\frac{x_i^{n+1} - x_i^n}{\Delta t} = v_i^{n+1/2}$$



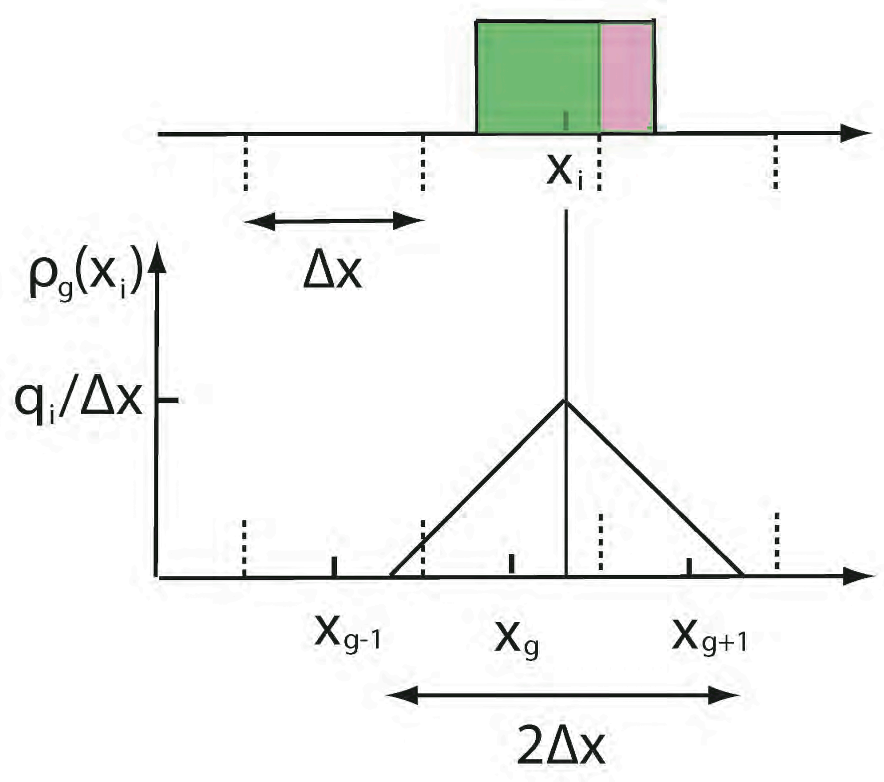
Charge assignment and force evaluation by cloud-in-cell in 1D

As assigned in 3D system the same interpolation scheme is used in 1D

$$\rho_g = \rho_i \frac{x_{g+1} - x_i}{\Delta x}$$

$$\rho_{g+1} = \rho_i \frac{x_i - x_g}{\Delta x}$$

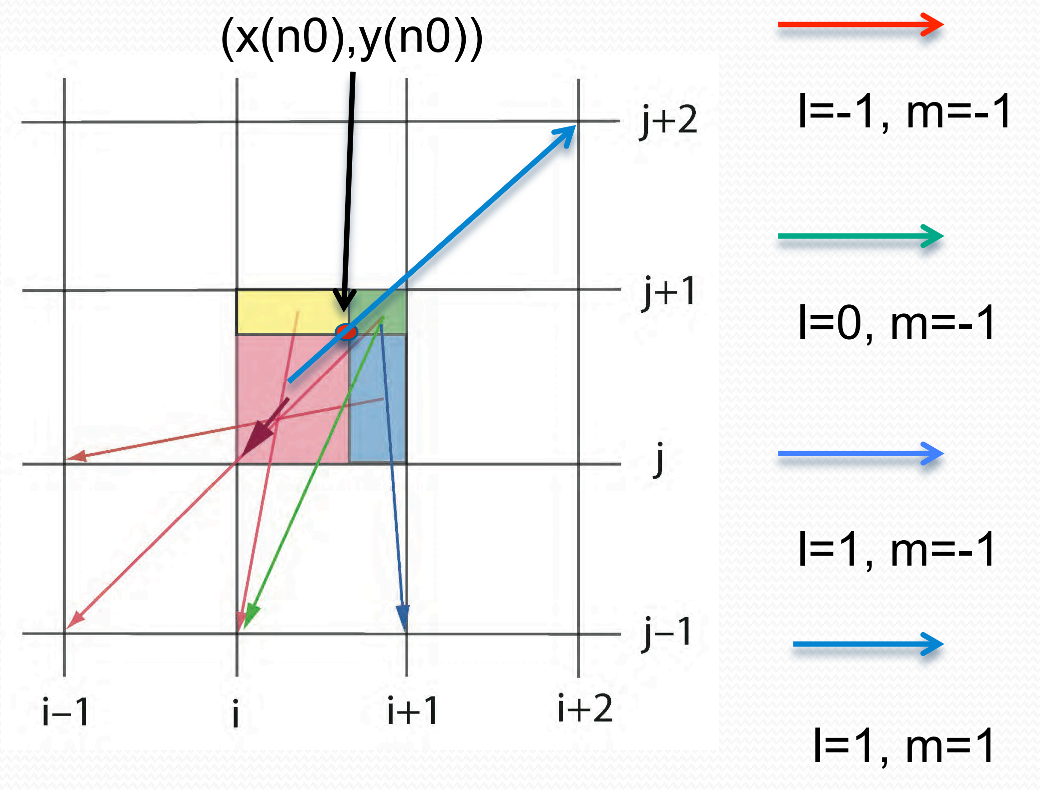
$$F_x = q_i \left(\frac{x_{g+1} - x_i}{\Delta x} E_g + \frac{x_i - x_g}{\Delta x} E_{g+1} \right)$$



Density assignment in 3D system (2D)

```
c for electrons
      do 3 n0=1,lecs
      i=x(n0)
      dx=x(n0)-i
      cx=1.-dx
      j=y(n0)
      dy=y(n0)-j
      cy=1.-dy
      k=z(n0)
      dz=z(n0)-k
      cz=1.-dz
C  Smoothing with the (.25,.5,.25)
profile in each dimension:
      sl=.5
      do 121 l=-1,1
      sl=.75-sl
      sr=.5
      do 121 m=-1,1
      sr=.75-sr
      sn=.5
      do 121 n=-1,1
      sn=.75-sn
      s=sl*sr*sn
```

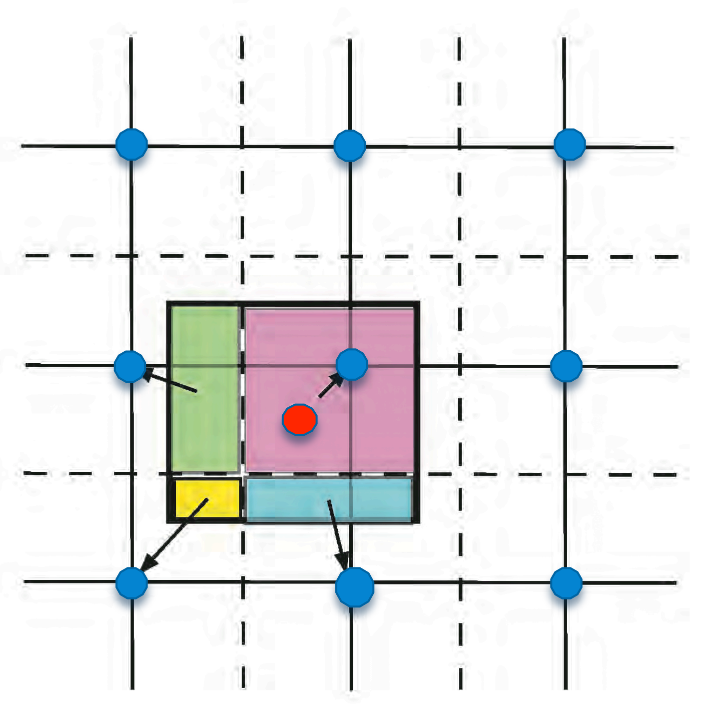
```
      rhe(i+l  ,j+m  ,k+n  )=rhe(i+l  ,j+m  ,k+n  )
+s*cx*cy*cz
      rhe(i+l+1,j+m  ,k+n  )=rhe(i+l+1,j+m  ,k+n  )
+s*dx*cy*cz
      rhe(i+l  ,j+m+1,k+n  )=rhe(i+l  ,j+m+1,k+n  )
+s*cx*dy*cz
      rhe(i+l+1,j+m+1,k+n  )=rhe(i+l+1,j+m+1,k+n  )
+s*dx*dy*cz
```



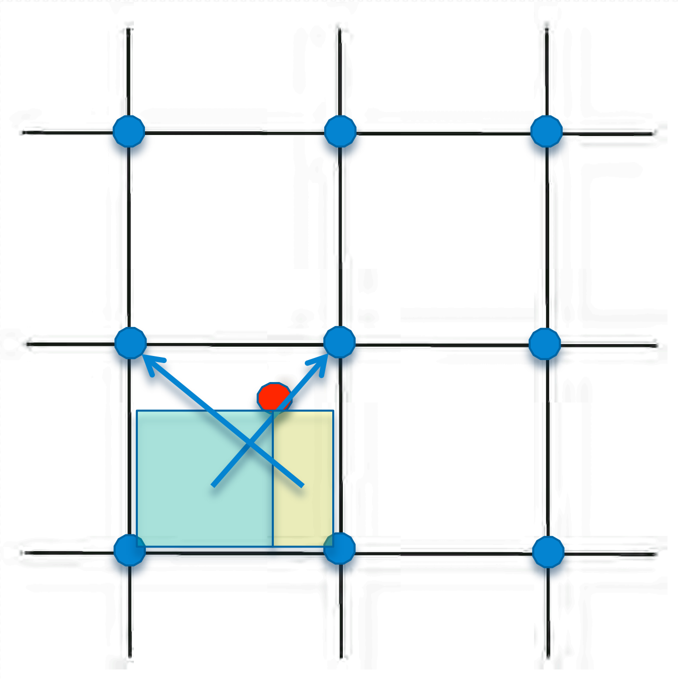
PIC Approach to Vlasov Equation

Lorentz-Force: $$\frac{d\vec{v}_j}{dt} = \frac{q_j}{m_j}(\vec{E} + \frac{\vec{v}_j \times \vec{B}}{c})$$

Solving Maxwell equations on grid



Charge assignment
(conserving charge current)



Force Interpolation

Current deposit scheme (2-D)

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

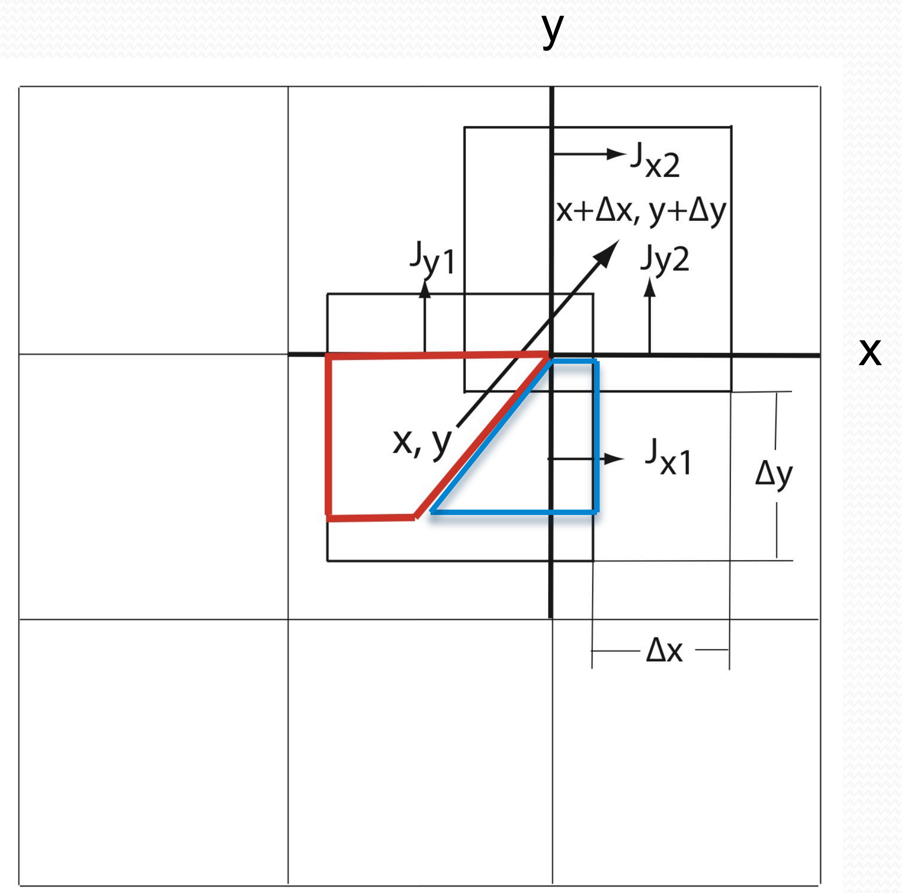
$$\frac{\partial \rho}{\partial t} = -\nabla \bullet J$$

$$J_{x1} = q\Delta x(\frac{1}{2} - y - \frac{1}{2}\Delta y)$$

$$J_{x2} = q\Delta x(\frac{1}{2} + y + \frac{1}{2}\Delta y)$$

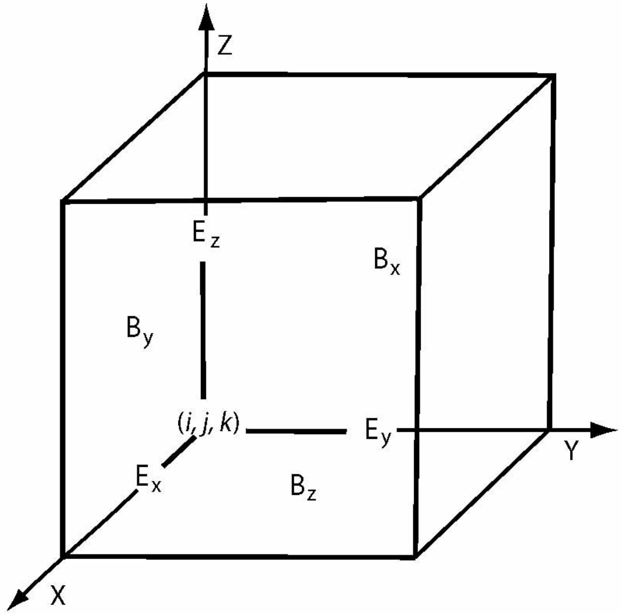
→ $$J_{y1} = q\Delta y(\frac{1}{2} - x - \frac{1}{2}\Delta x)$$

→ $$J_{y2} = q\Delta y(\frac{1}{2} + x + \frac{1}{2}\Delta x)$$



Ampere equation

$$\frac{\partial \mathbf{B}}{\partial t} = -c\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ e_x & e_y & e_z \end{vmatrix} = c[\,\mathbf{i}(\frac{\partial e_y}{\partial z} - \frac{\partial e_z}{\partial y}) + \mathbf{j}(\frac{\partial e_z}{\partial x} - \frac{\partial e_x}{\partial z}) + \mathbf{k}(\frac{\partial e_x}{\partial y} - \frac{\partial e_y}{\partial x})]$$



Yee lattice

In Yee Lattice e_x, e_y, e_z, b_x, b_y, b_z are, respectively staggered and shifted on 0.5 from (*I, j, k*) and located at the position

$$\begin{aligned} e_x(i,j,k) &\rightarrow e_x(i+.5,j,k), \\ e_y(i,j,k) &\rightarrow e_y(i,j+.5,k), \\ e_z(i,j,k) &\rightarrow e_z(i,j,k+.5), \end{aligned}$$

and

$$\begin{aligned} b_x(i,j,k) &\rightarrow b_x(i,j+.5,k+.5), \\ b_y(i,j,k) &\rightarrow b_y(i+.5,j,k+.5), \\ b_z(i,j,k) &\rightarrow b_z(i+.5,j+.5,k). \end{aligned}$$

Field update

$$\frac{\partial}{\partial t} b_x = (b_x^{new}(i, j + .5, k + .5) - b_x^{old}(i, j + .5, k + .5))/\delta t$$
$$= c[(e_y(i, j + .5, k + 1) - e_y(i, j + .5, k))/\delta z$$
$$-(e_z(i, j + 1, k + .5) - e_z(i, j, k + .5))/\delta y].$$

Here $\partial t = \partial x = \partial y = \partial z = 1$

$$b_x^{new}(i, j, k) = b_x^{old}(i, j, k) + c[\, e_y(i, j, k + 1) - e_y(i, j, k) - e_z(i, j + 1, k) + e_z(i, j, k)\,].$$

$$b_y^{new}(i, j, k) = b_y^{old}(i, j, k) + c[\, e_z(i + 1, j, k) - e_z(i, j, k) - e_x(i, j, k + 1) + e_x(i, j, k)\,],$$

$$b_z^{new}(i, j, k) = b_z^{old}(i, j, k) + c[\, e_x(i, j + 1, k) - e_x(i, j, k) - e_y(i + 1, j, k) + e_y(i, j, k)].$$

Electric field update

$$\frac{\partial \mathbf{E}}{\partial t} = c \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ b_x & b_y & b_z \end{vmatrix} = c[\ \mathbf{i}(\frac{\partial b_z}{\partial y} - \frac{\partial b_y}{\partial z}) \\ + \mathbf{j}(\frac{\partial b_x}{\partial z} - \frac{\partial b_z}{\partial x}) \\ + \mathbf{k}(\frac{\partial b_y}{\partial x} - \frac{\partial b_x}{\partial y})]$$

$$\begin{aligned} \frac{\partial}{\partial t} e_x &= (e_x^{new}(i+.5,j,k) - e_x^{old}(i+.5,j,k))/\delta t \\ &= c[(b_z(i+.5,j+.5,k) - b_z(i+.5,j-.5,k))/\delta y \\ &- (b_y(i+.5,j,k+.5) - b_y(i+.5,j,k-.5))/\delta z], \end{aligned}$$

$$\begin{aligned} e_x^{new}(i,j,k) = e_x^{old}(i,j,k) \\ +c[\ b_y(i,j,k-1) - b_y(i,j,k) - b_z(i,j-1,k) + b_z(i,j,k)\ ], \end{aligned}$$

Particle update

Newton-Lorentz equation

$$\mathbf{v}^{new} - \mathbf{v}^{old} = \frac{q\delta t}{m} < \mathbf{E} + \frac{1}{2}(\mathbf{v}^{new} + \mathbf{v}^{old}) \times \mathbf{B} >$$

$$\mathbf{r}^{next} - \mathbf{r}^{present} = \delta t \mathbf{v}^{new}$$

Buneman-Boris method

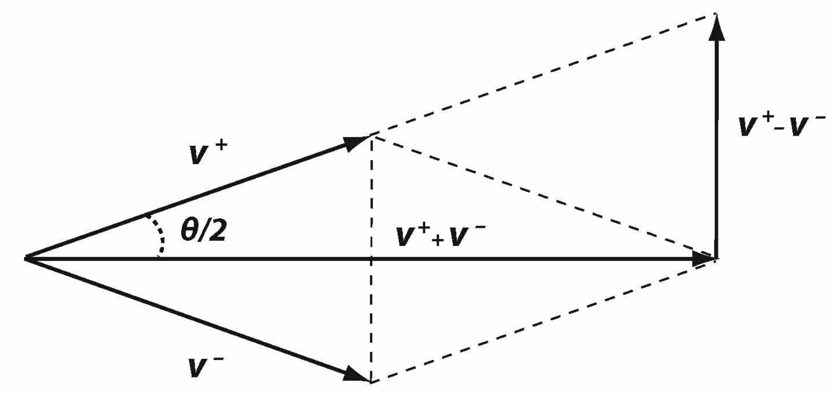
Half an electric acceleration

Pure magnetic rotation

Another half electric acceleration

Buneman-Boris method

$$\frac{\mathbf{v}^{n+1/2}-\mathbf{v}^{n-1/2}}{\Delta t}=\frac{q}{m}\left(\mathbf{E}^n+\frac{\mathbf{v}^{n+1/2}+\mathbf{v}^{n-1/2}}{2}\times\mathbf{B}^n\right)$$



$$\mathbf{v}^{-}=\mathbf{v}^{n-1/2}+\frac{q}{m}\mathbf{E}^n\frac{\Delta t}{2}$$

$$\mathbf{v}^{+}=\mathbf{v}^{n+1/2}-\frac{q}{m}\mathbf{E}^n\frac{\Delta t}{2}$$

rotation $$\frac{\mathbf{v}^{+}-\mathbf{v}^{-}}{\Delta t}=\frac{1}{2}\frac{q}{m}(\mathbf{v}^{+}+\mathbf{v}^{-})\times\mathbf{B}^n$$

$$\mathbf{v}^{+}=\mathbf{v}^{-}+\frac{2}{1+\mathbf{T}^2}(\mathbf{v}^{-}+\mathbf{v}^{-}\times\mathbf{T})\times\mathbf{T}$$

$$\mathbf{T}=\frac{q}{2m}\Delta t\mathbf{B}^n$$

Buneman-Boris method (cont)

4 steps

$$\mathbf{v}^- = \mathbf{v}^{n-1/2} + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2}$$

$$\mathbf{v}^0 = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{T}$$

$$\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}^0 \times \mathbf{S}$$

$$\mathbf{S} = 2\mathbf{T} / (\mathbf{1} + \mathbf{T}^2)$$

$$\mathbf{v}^{n+1/2} = \mathbf{v}^+ + \frac{q}{m}\mathbf{E}^n \frac{\Delta t}{2}$$

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \mathbf{v}^{n+1/2}\Delta t$$

Relativistic generalization

$$\mathbf{u} = \gamma_v \mathbf{v}, \quad \gamma_v^2 = 1 - \frac{v^2}{c^2} \qquad \gamma^2 = \left(1 + \frac{u^2}{c^2}\right)$$

$$\frac{\mathbf{u}^{n+1/2} - \mathbf{u}^{n-1/2}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}^n + \frac{\mathbf{u}^{n+1/2} + \mathbf{u}^{n-1/2}}{2\gamma^n} \times \mathbf{B}^n\right)$$

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \mathbf{v}^{n+1/2}\Delta t = \mathbf{r}^n + \frac{\mathbf{u}^{n+1/2}}{\gamma^{n+1/2}}\Delta t$$

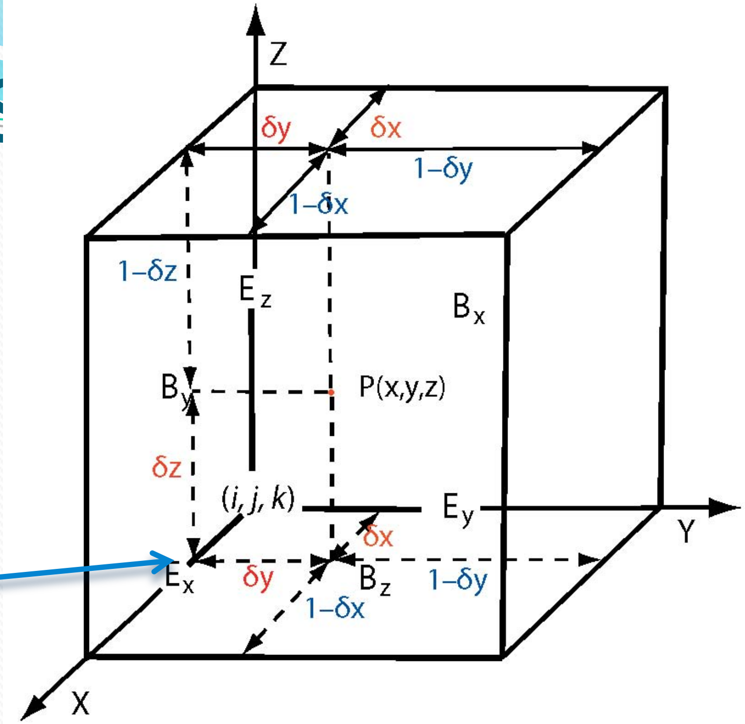
$$\left(\gamma^{n+1/2}\right)^2 = 1 + \left(\frac{u^{n+1/2}}{c}\right)^2$$

Force interpretations

"volume" weight

$$(i,j,k) \Leftarrow (1-\delta x)(1-\delta y)(1-\delta z) = cx \bullet cy \bullet cz$$

$$(i+1,j+1,k+1) \Leftarrow \delta x \bullet \delta y \bullet \delta z$$



$$\mathbf{F}_{e_x}^{(x,j,k)} = \overline{e}_x(i,j,k) + \left[\overline{e}_x(i+1,j,k) - \overline{e}_x(i,j,k)\right]\delta x$$

$$\overline{e}_x(i,j,k) = \frac{1}{2}\{e_x(i,j,k) + e_x(i-1,j,k)\} \qquad \overline{e}_x(i+1,j,k) = \frac{1}{2}\{e_x(i+1,j,k) + e_x(i,j,k)\}$$

on (*x*, *j*, *k*)

$$2\mathbf{F}_{e_x}^{(x,j,k)} = e_x(i,j,k) + e_x(i-1,j,k) + \left[e_x(i+1,j,k) - e_x(i-1,j,k)\right]\delta x$$

similarly on (x, *j*+1, *k*), (x, *j*, *k*+1), (x, *j*+1, *k*+1)

$$2\mathbf{F}_{e_x}^{(x,j+1,k)} = e_x(i,j+1,k) + e_x(i-1,j+1,k) + \left[e_x(i+1,j+1,k) - e_x(i-1,j+1,k)\right]\delta x$$

$$2\mathbf{F}_{e_x}^{(x,j,k+1)} = e_x(i,j,k+1) + e_x(i-1,j,k+1) + \left[e_x(i+1,j,k+1) - e_x(i-1,j,k+1)\right]\delta x$$

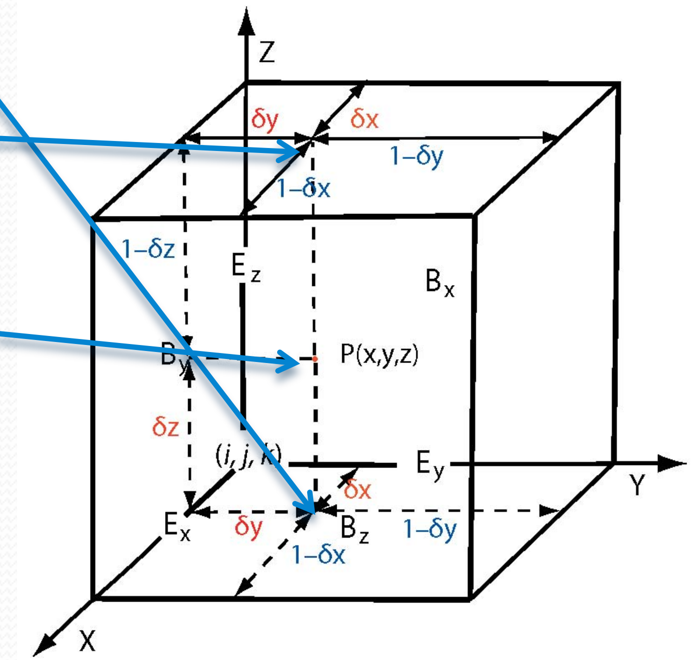
$$2\mathbf{F}_{e_x}^{(x,j+1,k+1)} = e_x(i,j+1,k+1) + e_x(i-1,j+1,k+1) + \left[e_x(i+1,j+1,k+1) - e_x(i-1,j+1,k+1)\right]\delta x$$

$$\mathbf{F}_{e_x}^{(x,y,k)} = \mathbf{F}_{e_x}^{(x,j,k)} + \left[\mathbf{F}_{e_x}^{(x,j+1,k)} - \mathbf{F}_{e_x}^{(x,j,k)}\right]\delta y$$

$$\mathbf{F}_{e_x}^{(x,y,k+1)} = \mathbf{F}_{e_x}^{(x,j,k+1)} + \left[\mathbf{F}_{e_x}^{(x,j+1,k+1)} - \mathbf{F}_{e_x}^{(x,j,k+1)}\right]\delta y$$

$$\mathbf{F}_{e_x}^{(x,y,z)} = \mathbf{F}_{e_x}^{(x,y,k)} + \left[\mathbf{F}_{e_x}^{(x,y,k+1)} - \mathbf{F}_{e_x}^{(x,y,k)}\right]\delta z$$

$$\mathbf{F}_{e_y}^{(x,y,z)}, \mathbf{F}_{e_z}^{(x,y,z)}, \mathbf{F}_{b_x}^{(x,y,z)}, \mathbf{F}_{b_y}^{(x,y,z)}, \mathbf{F}_{b_z}^{(x,y,z)}$$

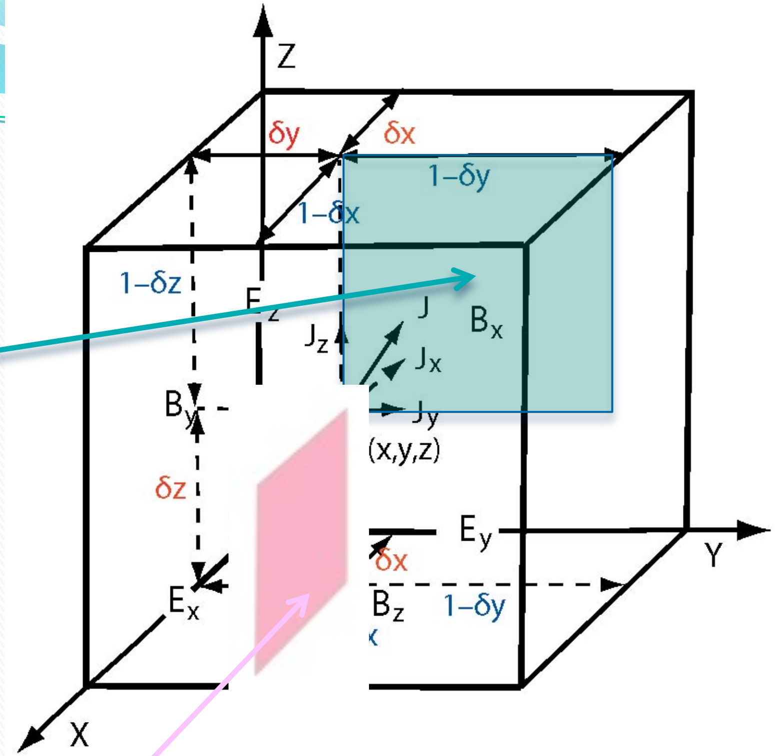


Current deposit

Charge conservation $$\frac{\partial \rho}{\partial t} = -\nabla \bullet \mathbf{J}$$

$$\begin{aligned}
e_x(i,j,k) &= e_x(i+.5,j,k) \\
&= e_x(i,j,k) - J_x \bullet cy \bullet cz \\
e_x(i,j+1,k) &= e_x(i+.5,j+1,k) \\
&= e_x(i,j+1,k) - J_x \bullet \delta y \bullet cz \\
e_x(i,j,k+1) &= e_x(i+.5,j,k+1) \\
&= e_x(i,j,k+1) - J_x \bullet cy \bullet \delta z \\
e_x(i,j+1,k+1) &= e_x(i+.5,j+1,k+1) \\
&= e_x(i,j+1,k+1) - J_x \bullet \delta y \bullet \delta z
\end{aligned}$$

$$\begin{aligned}
e_y(i,j,k) &= e_y(i,j+.5,k) \\
&= e_y(i,j,k) - J_y \bullet cx \bullet cz \\
e_y(i,j+1,k) &= e_y(i+1,j+.5,k) \\
&= e_y(i+1,j,k) - J_y \bullet \delta x \bullet cz \\
e_y(i,j,k+1) &= e_y(i,j+.5,k+1) \\
&= e_y(i,j,k+1) - J_y \bullet cx \bullet \delta z \\
e_y(i,j+1,k+1) &= e_y(i+1,j+.5,k+1) \\
&= e_y(i+1,j,k+1) - J_y \bullet \delta x \bullet \delta z
\end{aligned}$$



Villasenor and Buneman 1992

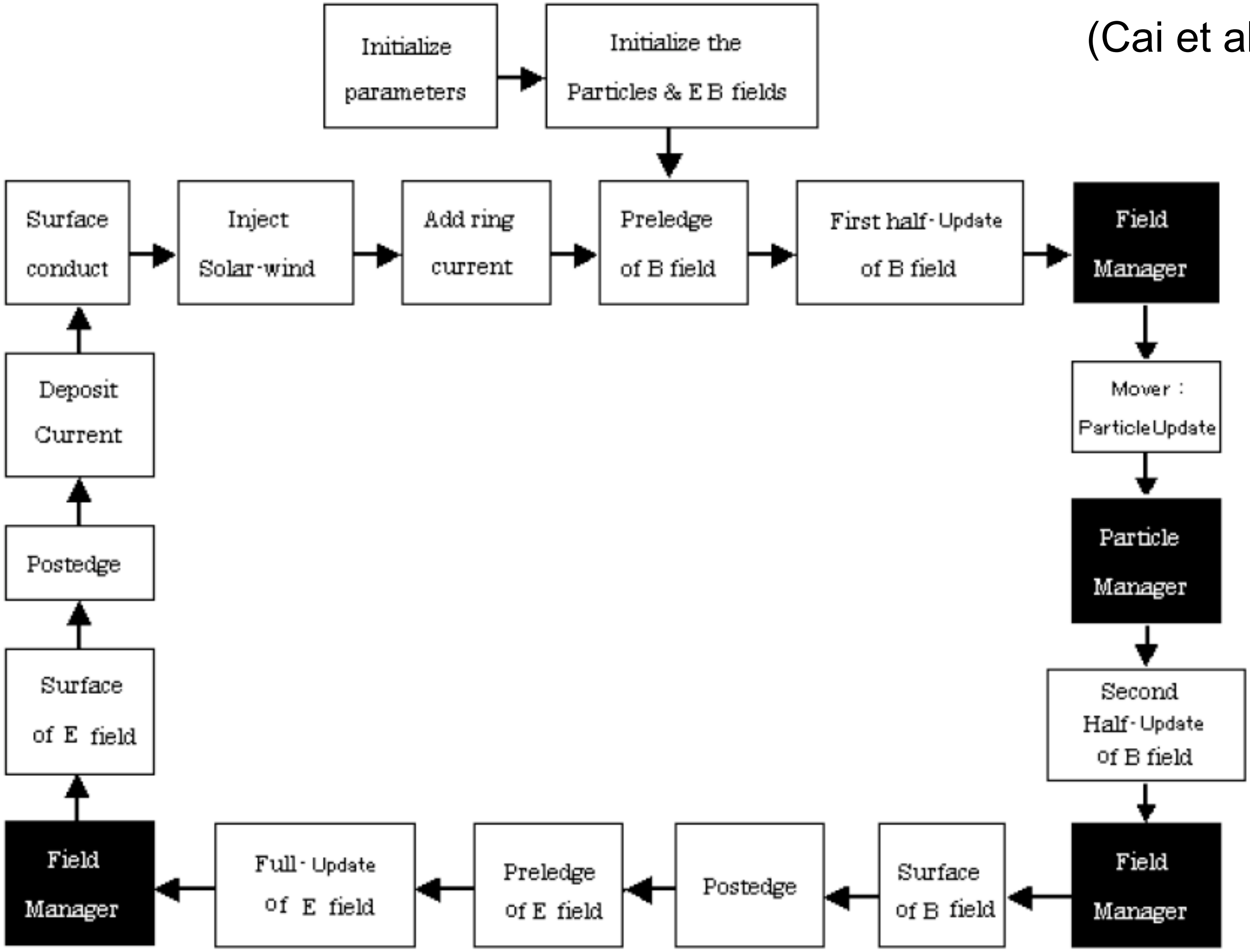
$$cx = 1 - \delta x$$

$$cy = 1 - \delta y$$

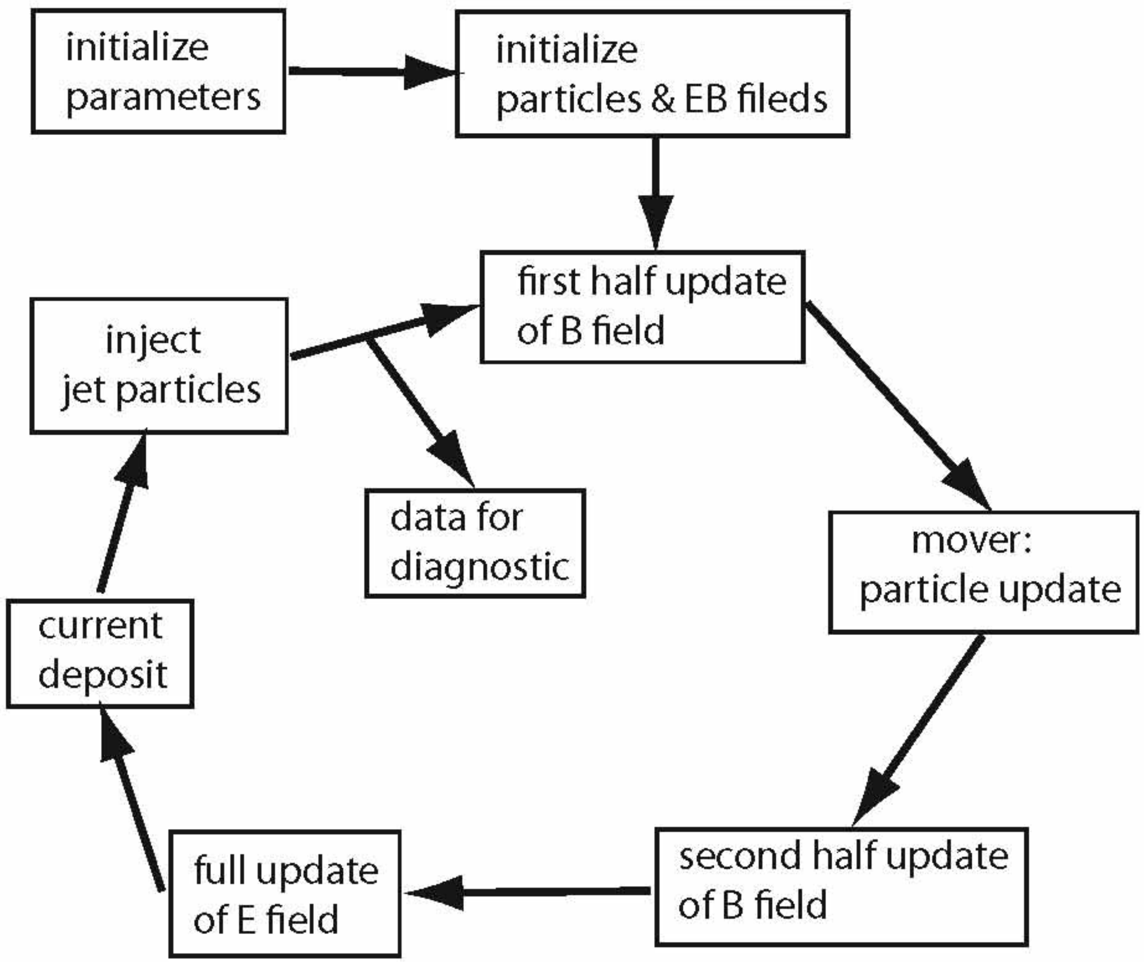
$$cz = 1 - \delta z$$

Schematic computational cycle

(Cai et al. 2006)



Time evolution of RPIC code



Code development

Combine these components

Set initial conditions for each problem you would like to investigate

Apply MPI for speed-up

Develop graphics using NCARGraphic, AVSExpress, IDL, etc

Analyze simulation results and compare with theory and other simulation results

Prepare report