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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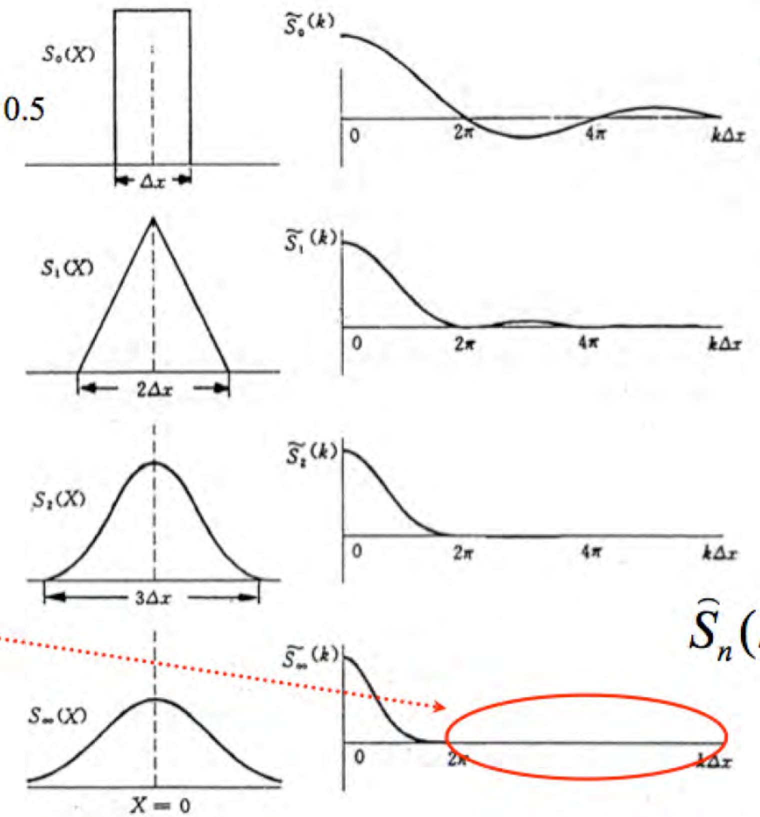
Context

- Filtering action
- Integration of equations
- Aliasing and Reducing noises
- Collisions
- Finite-size particle effects
- Restriction of time step and grid size
- Accuracy and stability of the time integration
- Current deposition seven-boundary move
- Current deposition ten-boundary move
- Charge and current deposition
- Zigzag scheme in two-dimensional systems

Filtering Action of Shape Functions

$$S_0(x) = \begin{cases} \dfrac{1}{\Delta x}, & -0.5 \le \dfrac{x}{\Delta x} \le 0.5 \\ 0, & \text{otherwise} \end{cases}$$



High-frequency components are filtered by a smooth shape function.

$$\hat{S}_0(k) = \sin\left(\tfrac{k\Delta x}{2}\right) \Big/ \tfrac{k\Delta x}{2}$$

$$\hat{S}_n(k) = [\hat{S}_0(k)]^{n+1}$$

$\hat{S}_n(k)$ decays with $k^{-(n+1)}$

Shape Functions of different orders

Corresponding Functions in Fourier Space

Integration of the field equations

$$E_x = -\frac{\partial\phi}{\partial x}$$

$$\frac{\partial E_x}{\partial x} = \rho$$

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

$$\downarrow \text{finit defference}$$

$$E_j = \frac{\phi_{j-1} - \phi_{j+1}}{2\Delta x}$$

$$\frac{\phi_{j-1} - 2\phi_j + \phi_{j+1}}{(\Delta x)^2} = -\rho_j$$

Fourier transform →

$$\hat{E}(k_l) = -ik_l\hat{\phi}(k_l)$$

$$\hat{\phi}(k_l) = \frac{\hat{\rho}(k_l)}{k_l^2} \quad k_l = \frac{2\pi l}{L}$$

$$\uparrow \Delta x = 0$$

$$\hat{E}(k_l) = -iK_l\hat{\phi}(k_l)$$

$$\hat{\phi}(k_l) = \frac{\hat{\rho}(k_l)}{K_l^2}$$

$$K_l^2 = k_l^2\left(\frac{\sin(\frac{1}{2}k_l\Delta x)}{\frac{1}{2}k_l\Delta x}\right)^2$$

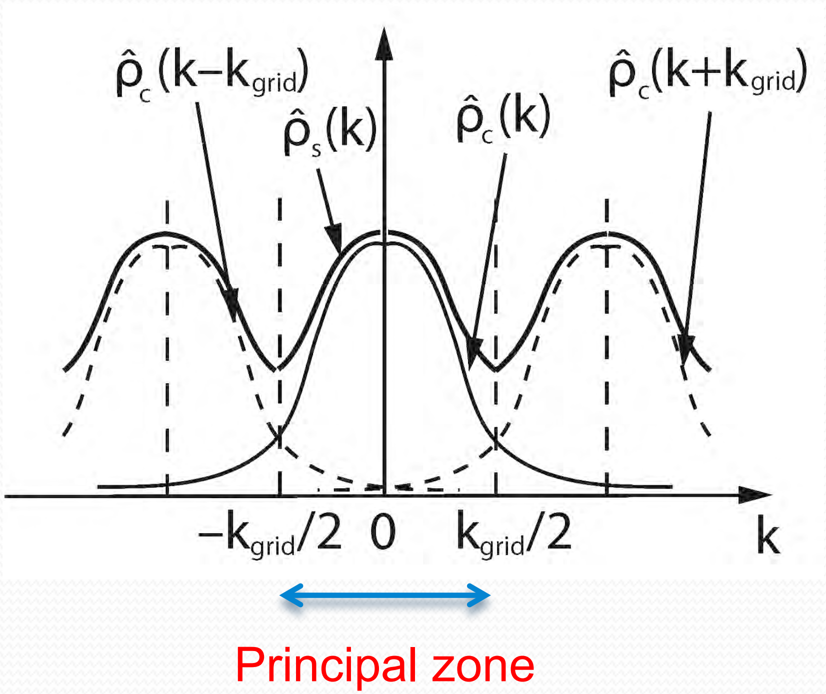
Aliasing

The spurious fluctuation which appears as as result of the loss of displacement invariance, manifest themselves in ***k***-space as non-physical mode coupling, known as `aliasing'.

By introducing a mesh we reduced our representation of $\rho(x)$ from a continuous representation $\rho_c(x)$ to a sampled representation $\rho_s(x)$.

$$\hat{\rho}_c(k) = \int_{-\infty}^{\infty} dx \rho_c(x) e^{-ikx}$$

$$\hat{\rho}_s(k) = \sum_{n=-\infty}^{n=\infty} \hat{\rho}_c(k + nk_{grid})$$



The extra contributions (from |n|>0) to inside the principal zone are called aliasing

Aliasing and reducing noise

- The spurious fluctuations of high frequency cause the noise and error in the main lobe, which might make the numerical system to be unstable.
- The high-k components of $S(k)$ is determined by the smoothness of $S(x)$; The high-k components of $n_c(k)$ is determined by the smoothness of $n(x)$, The number of particles.
- The major noise exists in the particle-in-cell method mainly comes from the aliasing effect. Two methods for reducing the aliasing effects:
  1. Increase the particle number.
  2. Increase the order of the shape function S(x).

Collisional effects

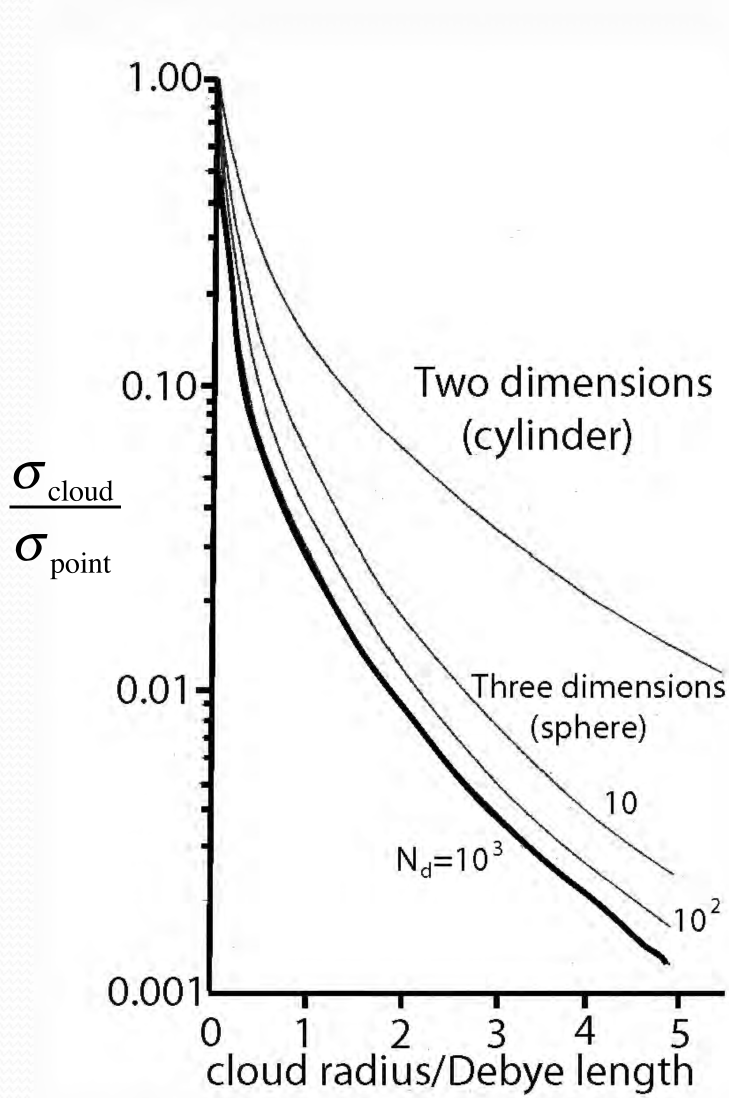
The ratio of the cross sections for finite–sized particles to that for point particles in in two and three dimensions (taken from Okuda and Birdsall 1970)

Examples of collision rates:
(a) two dimensions:

System $100\lambda_D \times 100\lambda_D$
$N = 3\times10^5$ particles
$n\lambda_D^2 = N_p=30$
particle radius $a = \lambda_D$
$v=R\omega_{pe}/16N_D \approx 2\times10^{-4}\omega_p$

(b) three dimensions:

System $50\lambda_D \times 50\lambda_D \times 50\lambda_D$
$N = 10^6$ particles
$n\lambda_D^2 = N_p=10$
particle radius $a = \lambda_D$
$v=R\omega_{pe}/16N_D \approx 10^{-3}\omega_p$



Finite-size particle effects

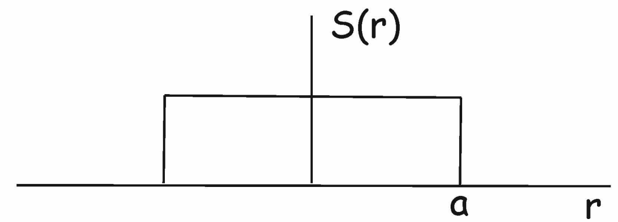
$$\frac{\partial f}{\partial t}+\boldsymbol{v}\cdot\frac{\partial f}{\partial \boldsymbol{r}}+\frac{F}{m}\cdot\frac{\partial f}{\partial \boldsymbol{v}}=0$$

$$F(\boldsymbol{r}_j)=q\int S(\boldsymbol{r}-\boldsymbol{r}_j)\boldsymbol{E}(\boldsymbol{r})d^n r$$

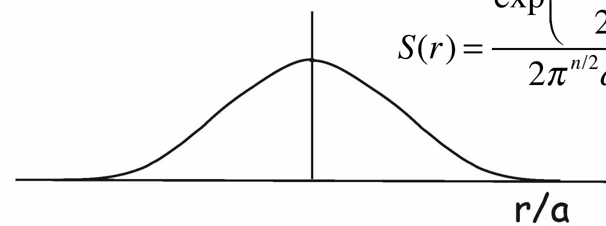
$$\nabla\cdot\boldsymbol{E}=4\pi q\int f(\boldsymbol{r}',\boldsymbol{v}')S(\boldsymbol{r}-\boldsymbol{r}')d^n r' d^n v'$$

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

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



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



Dispersion function with finite-size particles

$$\varepsilon(\boldsymbol{k},\omega)=1+\frac{\omega_p\left|S(\boldsymbol{k})\right|^2}{k^2}\int_{-\infty}^{\infty}\frac{\boldsymbol{k}\cdot\partial f_0/\partial v}{(\omega-\boldsymbol{k}\cdot\boldsymbol{v}+i\nu)}d^n v$$

Plasma frequency is modified by smoothing

$$\omega^2(k)=\omega_p^2\left|S(k)\right|^2$$

$$\left|S(\boldsymbol{k})\right|^2=\frac{e^{-k^2a^2}}{(2\pi)^{n_a n}}$$

Fourier space modification reduces collisions

Restrictions on time step and grid size

1. Courant condition (Cartesian coordinate) this condition comes from the electromagnetic code (light wave)

$$cdt < 1/\sqrt{1/dx_1^2 + 1/dx_2^2 + 1/dx_3^2}$$

2. $\omega_{\max} dt < 0.25 \quad \omega_{\max} = \max(\omega_{pe}, \omega_{ce})$

3. $v_{\max} dt < \min(dx_1, dx_2, dx_3)$

   particle move in one step < 1 cell (grid size)

4. More particles are better, however it takes more memory and computing time

Accuracy and stability of time integration

In vacuum (***E***, ***B***) = (***E***$_0$, ***B***$_0$)exp(i***k•x*** −iωt) ***J***=0 from Maxwell equations

$$\Omega \boldsymbol{B} = cK \times \boldsymbol{E}$$

$$\Omega \boldsymbol{E} = -cK \times \boldsymbol{B}$$

$$\Omega = \omega \left| \frac{\sin(\omega \Delta t/2)}{\omega \Delta t/2} \right|, K = k \left| \frac{\sin(k\Delta x/2)}{k\Delta x/2} \right|$$

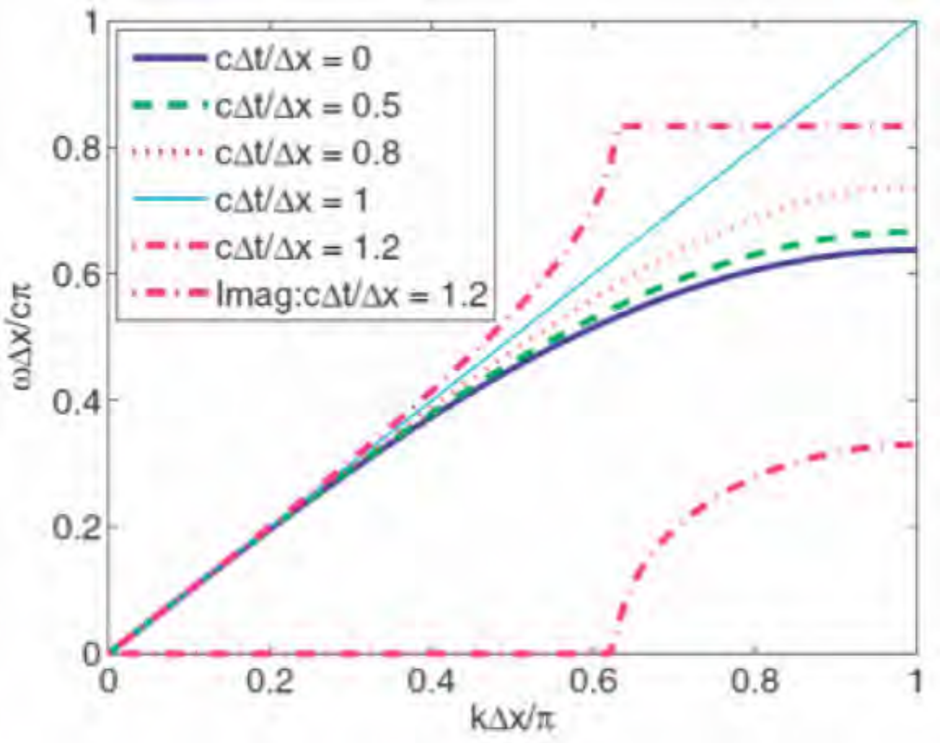
$$\Omega^2 = c^2 K^2$$

$$\left| \frac{\sin(\omega \Delta t/2)}{c\Delta t/2} \right|^2 = \left| \frac{\sin(k\Delta x_1/2)}{\Delta x_1/2} \right|^2 + \left| \frac{\sin(k\Delta x_2/2)}{\Delta x_2/2} \right|^2$$

$$\cos(\omega \Delta t) = \left(c\frac{\Delta t}{\Delta x} \right)^2 [\cos(k\Delta x) - 1] + 1$$

Courant-Levy stability criterion

$$\Delta t \le \frac{1}{c}\left(\sum_i \frac{1}{(\Delta x_i)^2} \right)^{-1/2}$$



Vacuum dispersion curve for leapfrog difference for wave equation

Relativistic particles which move faster than numerical speed of light cause numerical Cherenkov radiation in high wave-numbers

Calculation of vacuum dispersion solution (homework)

$$\cos(\omega\Delta t) = \left(c\frac{\Delta t}{\Delta x} \right)^2 [\cos(k\Delta x) - 1] + 1$$

$$\cos\left(\frac{\omega\Delta x}{c}\frac{cdt}{dx}\right) - 1 = \left(c\frac{\Delta t}{\Delta x} \right)^2 [\cos(k\Delta x) - 1]$$

$$\cos(\alpha y) - 1 = (\alpha)^2 [\cos(x) - 1]$$

$$y = \frac{\omega\Delta x}{c}, \qquad x = k\Delta x, \qquad \alpha = \frac{cdt}{dx}$$

$$\frac{\cos(\alpha y) - 1}{(\alpha)^2} = \cos(x) - 1, \qquad \cos(x) = \sum_{n=1}^{\infty} \frac{(-1)^n (x)^{2n}}{(2n)!}$$

$$-0.5y^2 + \cancel{\tfrac{1}{24} y^4 \alpha^2 + \cdot} = \cos(x) - 1$$

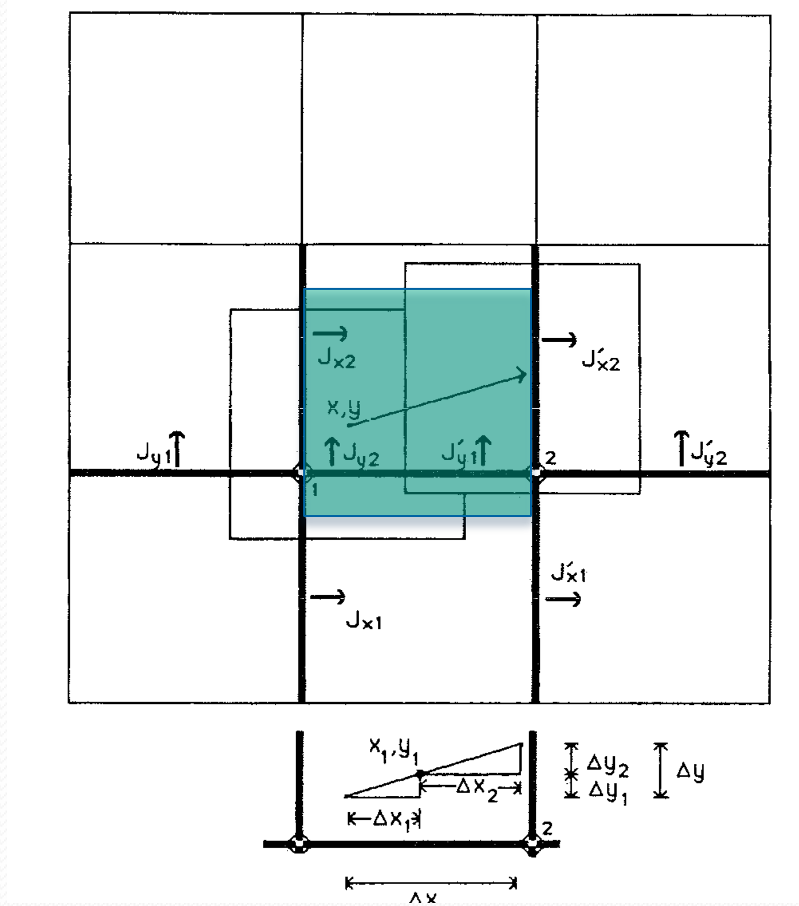
$$y = \sqrt{2 \cdot (1 - \cos(x))} \qquad (\alpha = 0)$$

Current deposition seven-boundary move

$\Delta x_1 = 0.5 - x,$
$\Delta y_1 = (\Delta y/\Delta x)\Delta x_1,$
$x_1 = -0.5,$
$y_1 = y + \Delta y_{1,}$
$\Delta x_2 = \Delta x - \Delta x_1,$
$\Delta y_2 = \Delta y - \Delta y_1$

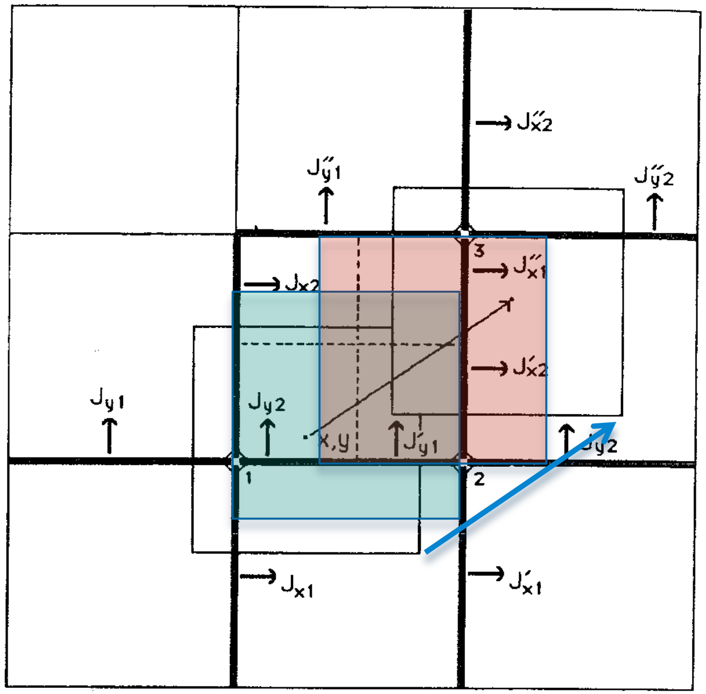
$$J_{x1} = q\Delta x_1(\tfrac{1}{2} - y - \tfrac{1}{2}\Delta y_1)$$
$$J_{x2} = q\Delta x_1(\tfrac{1}{2} + y + \tfrac{1}{2}\Delta y_1)$$
$$J_{y1} = q\Delta y_1(\tfrac{1}{2} - x - \tfrac{1}{2}\Delta x_1)$$
$$J_{y2} = q\Delta y_1(\tfrac{1}{2} + x + \tfrac{1}{2}\Delta x_1)$$

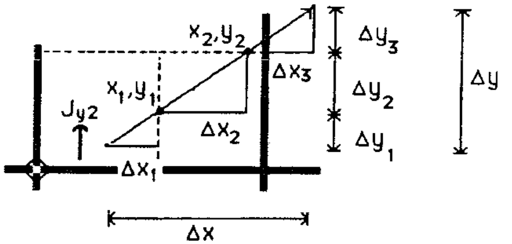
$$J'_{x1} = q\Delta x_2(\tfrac{1}{2} - y_1 - \tfrac{1}{2}\Delta y_2)$$
$$J'_{x2} = q\Delta x_2(\tfrac{1}{2} + y_1 + \tfrac{1}{2}\Delta y_2)$$
$$J'_{y1} = q\Delta y_2(\tfrac{1}{2} - x_1 - \tfrac{1}{2}\Delta x_2)$$
$$J'_{y2} = q\Delta y_2(\tfrac{1}{2} + x_1 + \tfrac{1}{2}\Delta x_2)$$



Current deposition ten-boundary move

$\Delta x_1 = 0.5 - x,$
$\Delta y_1 = (\Delta y/\Delta x)\Delta x_1,$
$x_1 = -0.5,$
$y_1 = y + \Delta y_{1,}$
$\Delta y_2 = 0.5 - y - \Delta y_1,$
$\Delta x_2 = (\Delta x/\Delta y)\Delta y_2,$
$x_2 = \Delta x_2 - 0.5,$
$y_2 = 0.5,$
$\Delta x_3 = \Delta x - \Delta x_1 - \Delta x_2,$
$\Delta y_3 = \Delta y - \Delta y_1 - \Delta y_2$





Current deposit scheme (2-D)

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

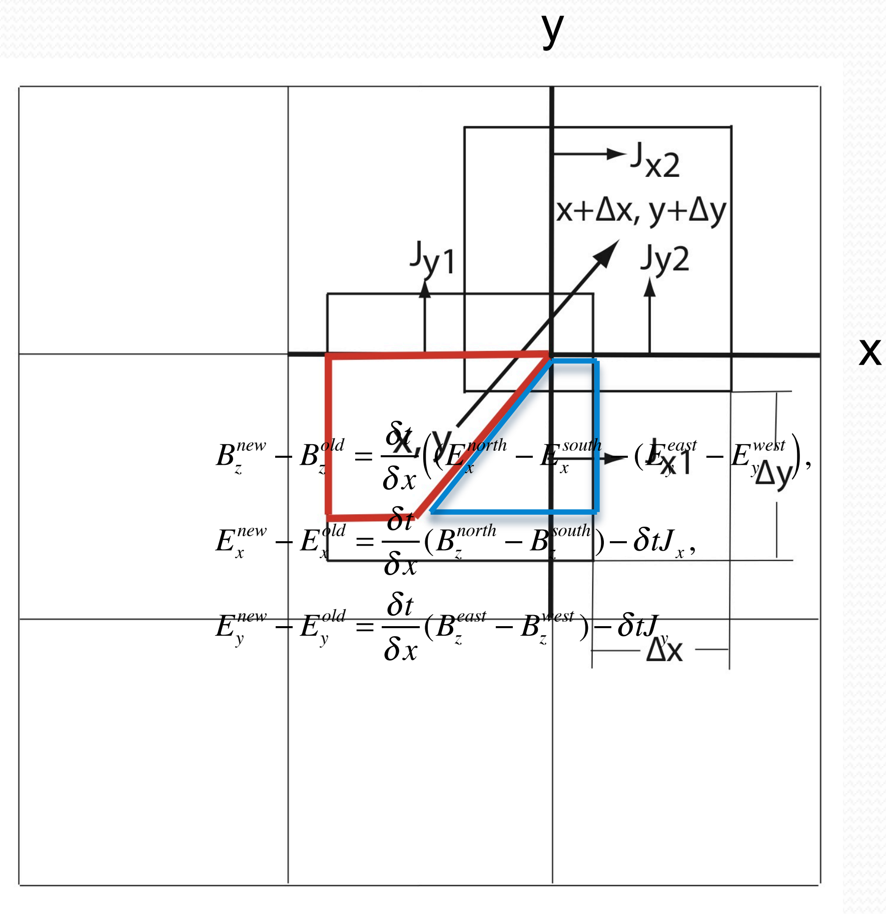
$$\frac{\partial \rho}{\partial t} = -\nabla \bullet J$$

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

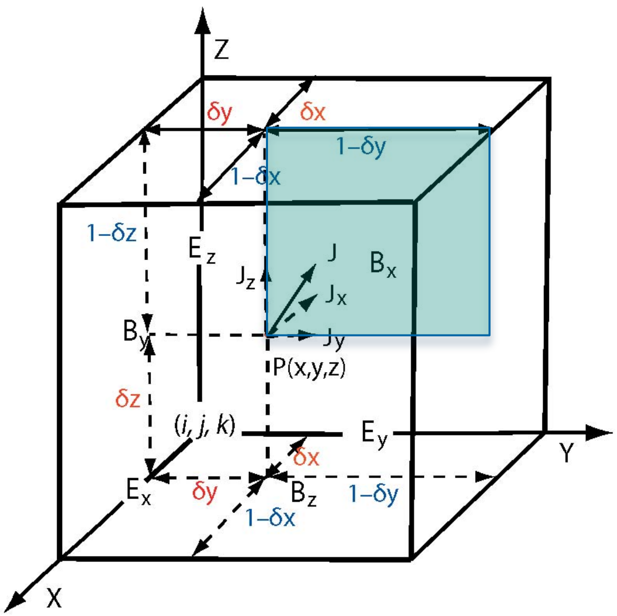
$$J_{x2} = q\Delta x\left(\frac{1}{2} + y + \frac{1}{2}\Delta y\right)$$

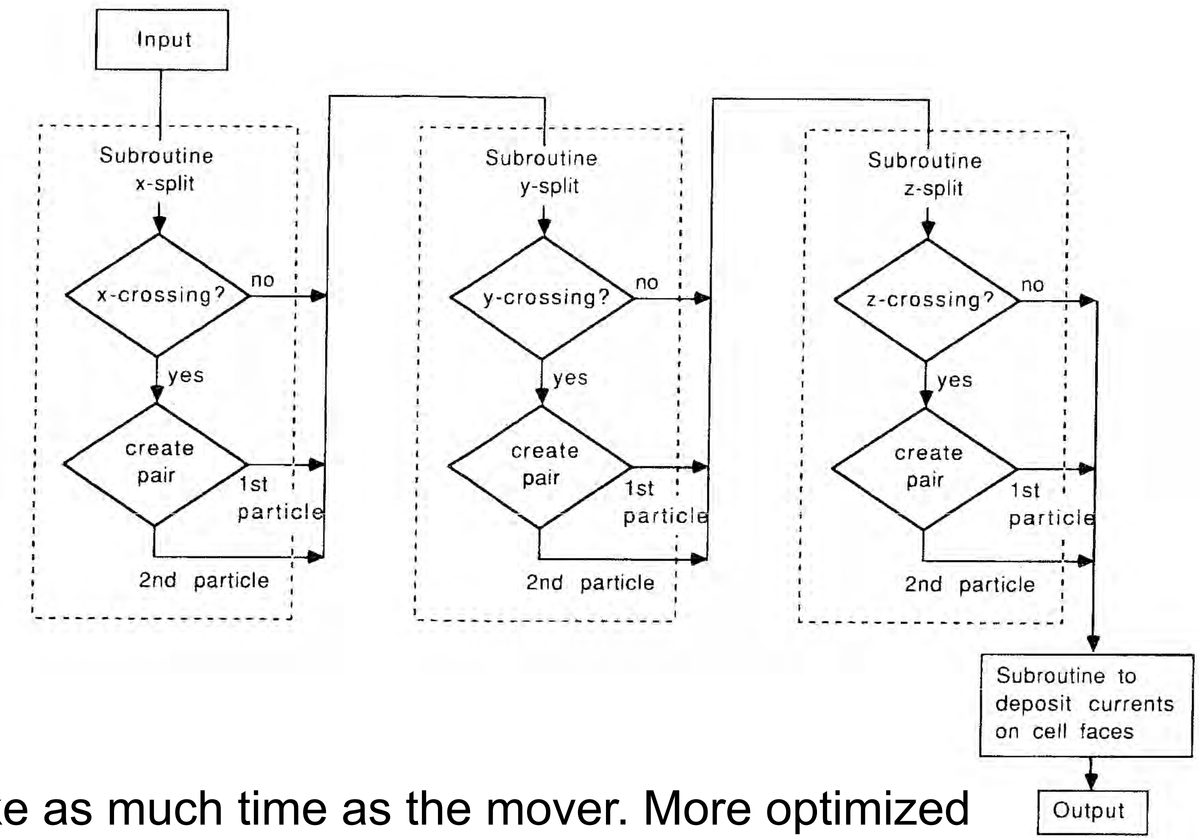
$$J_{y1} = q\Delta y\left(\frac{1}{2} - x - \frac{1}{2}\Delta x\right)$$

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



Charge and current deposition





Current deposition can take as much time as the mover. More optimized deposits exist (Umeda 2003).

Charge conservation makes the whole Maxwell solver local and hyperbolic. Static fields can be established dynamically.

Zigzag scheme in two-dimensional systems

$$\frac{J_x^{t+\Delta t/2}(i+\frac{1}{2},j) - J_x^{t+\Delta t/2}(i-\frac{1}{2},j)}{\Delta x} + \frac{J_y^{t+\frac{\Delta t}{2}}(i,j+\frac{1}{2}) - J_y^{t+\Delta t/2}(i,j-\frac{1}{2})}{\Delta y}$$

$$= \frac{\rho^t(i,j) - \rho^{t+\Delta t}(i,j)}{\Delta t}.$$

$$J_x\left(i_1+\tfrac{1}{2}, j_1\right) = \frac{1}{\Delta x \Delta y} F_x (1 - W_y), \qquad J_x\left(i_1+\tfrac{1}{2}, j_1+1\right) = \frac{1}{\Delta x \Delta y} F_x W_y,$$

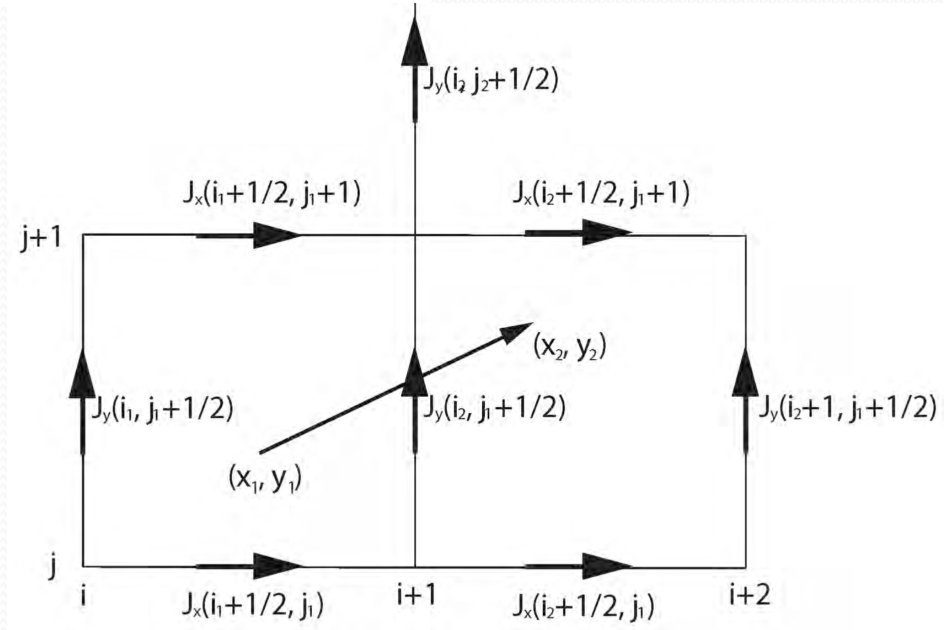
$$J_y\left(i_1, j_1+\tfrac{1}{2}\right) = \frac{1}{\Delta x \Delta y} F_y (1 - W_x), \qquad J_y\left(i_1+1, j_1+\tfrac{1}{2}\right) = \frac{1}{\Delta x \Delta y} F_y W_x,$$

$$i_1 \equiv \mathrm{floor}(x_1/\Delta x), \qquad i_2 \equiv \mathrm{floor}(x_2/\Delta x),$$

$$j_1 \equiv \mathrm{floor}(y_1/\Delta y), \qquad j_2 \equiv \mathrm{floor}(y_2/\Delta y),$$

$$F_x = q\frac{x_2 - x_1}{\Delta t}, \qquad F_y = q\frac{y_2 - y_1}{\Delta t},$$

$$W_x = \frac{x_1 + x_2}{2\Delta x} - i_1, \qquad W_y = \frac{y_1 + y_2}{2\Delta y} - j_1.$$



see Umeda (2003) for detailed numerical method