

Electromagnetic Particle-In-Cell codes

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US Particle Accelerator School (USPAS) Summer Session

Self-Consistent Simulations of Beam and Plasma Systems

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- 1 Electromagnetic PIC vs. electrostatic PIC
 - When to use electrostatic or electromagnetic PIC
 - The PIC loop in electrostatic and electromagnetic PIC
- 2 Finite-difference electromagnetic field solvers
 - Staggering in time
 - Staggering in space
 - The equations $\nabla \cdot \mathbf{B} = 0$ and $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$
- 3 Current deposition and continuity equation
 - Direct current deposition and continuity equation
 - Boris correction
 - Charge-conserving deposition

EM-PIC vs. ES-PIC Field solvers Deposition of J References

When to use ES-PIC or EM-PIC

Electrostatics

$$\frac{\partial \mathbf{B}}{\partial t} \approx \mathbf{0}$$

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad \left(\rightarrow \nabla^2 \phi = -\frac{\rho}{\epsilon_0} \right)$$

Approximate set of equations:

- Magnetic fields vary **slowly**.
- Magnetic fields are typically **externally generated**. The magnetic fields generated by beams/plasma are neglected.
- Fast evolutions such as radiation/retardation effects are neglected.

Electromagnetics

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{B} = 0 \quad \nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$$

Full set of equations:

- **Self-consistently** includes magnetic fields generated by the beams/plasmas.
- Supports **fast** evolution of fields and esp. retardation/radiation effects

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EM-PIC vs. ES-PIC Field solvers Deposition of J References

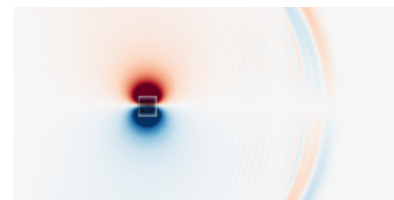
When to use ES-PIC or EM-PIC

Intuitive examples (animations)



- The particles are **slow** compared to c .
- The fields change **adiabatically** and depend only on the **instantaneous** positions of the particles.

→ **Electrostatic PIC is OK**



- The particles move **close to** c , and accelerate abruptly.
- The fields depend on the **history** of the particles (radiation effects)

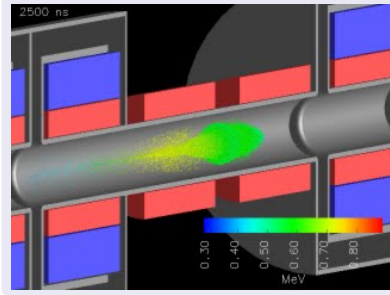
→ **Electromagnetic PIC is needed**

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When to use ES-PIC or EM-PIC

Example using electrostatic PIC:

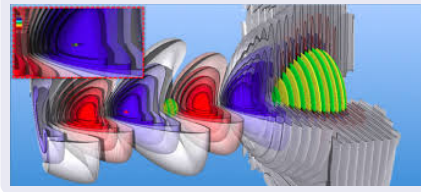
Sub-GeV acceleration of ions in conventional accelerators



- The ions are slower than c .

Example using electromagnetic PIC:

Laser-driven acceleration of electrons in plasmas



- Presence of radiation (the laser)
- The electrons move close to c .

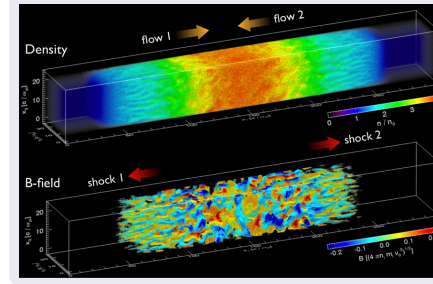
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When to use ES-PIC or EM-PIC

Other examples using **electromagnetic PIC**

Electromagnetic plasma instabilities

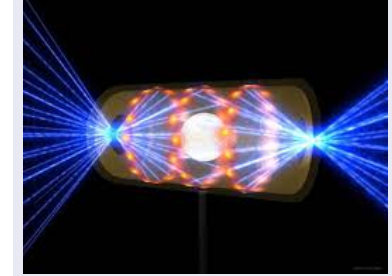
e.g. collisionless astrophysical shocks



- Capturing the **self-consistent** evolution of the \mathbf{B} field is key.

Interaction of intense lasers with plasmas

e.g. inertial fusion



- Presence of radiation (lasers)

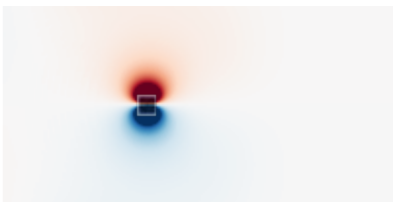
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Field solver in ES-PIC and EM-PIC

Electrostatic field solver

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0} \quad \mathbf{E} = -\nabla \phi$$

The fields are **recalculated from scratch** at each timestep, from the **current** particle charge density. (no dependence on the history)

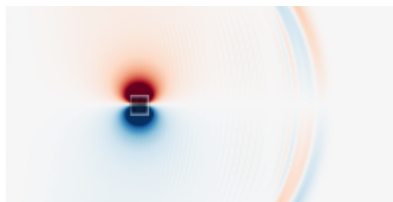


Electromagnetic field solver

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

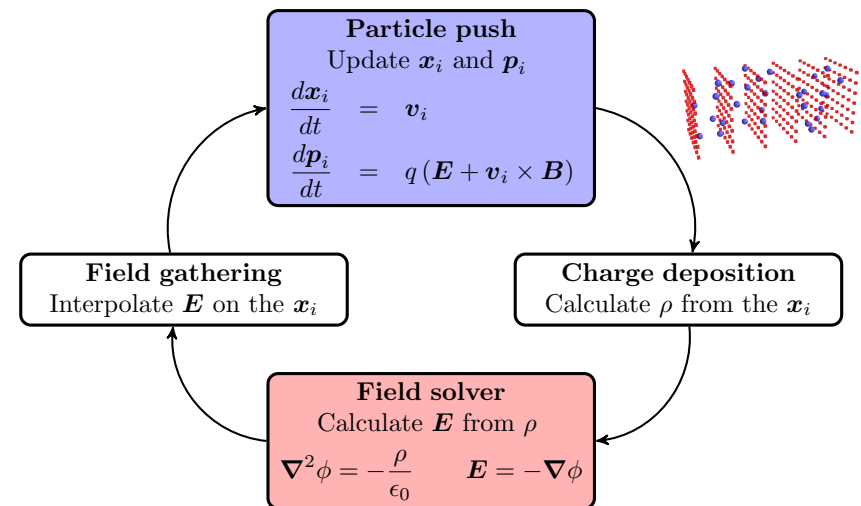
$$\frac{\partial \mathbf{E}}{\partial t} = c^2 \nabla \times \mathbf{B} - \mu_0 c^2 \mathbf{j}$$

The fields are **updated** at each timestep.



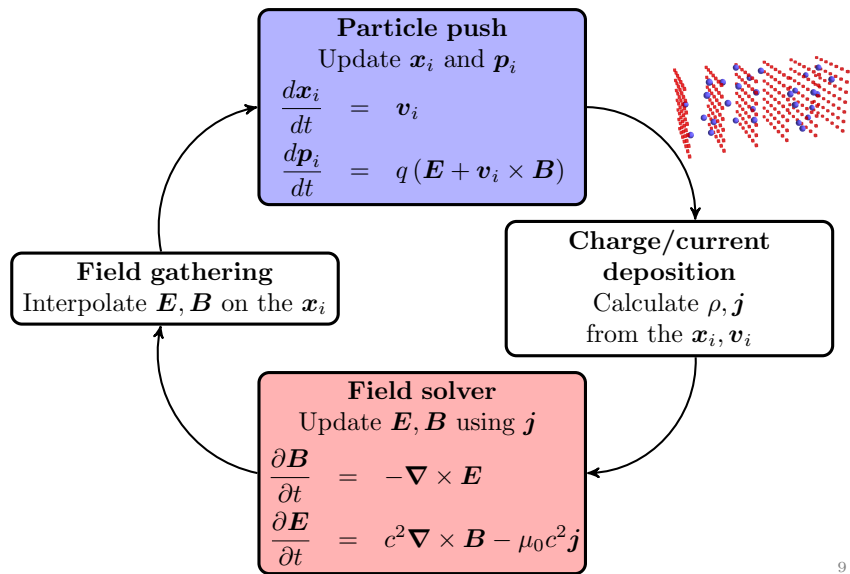
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The PIC loop in Electrostatic-PIC



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The PIC loop in Electromagnetic-PIC



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Staggering in time

Reminder: (Monday's *Overview of Basic Numerical Methods*)
Centered discretization of derivatives is more accurate

Non-centered discretization

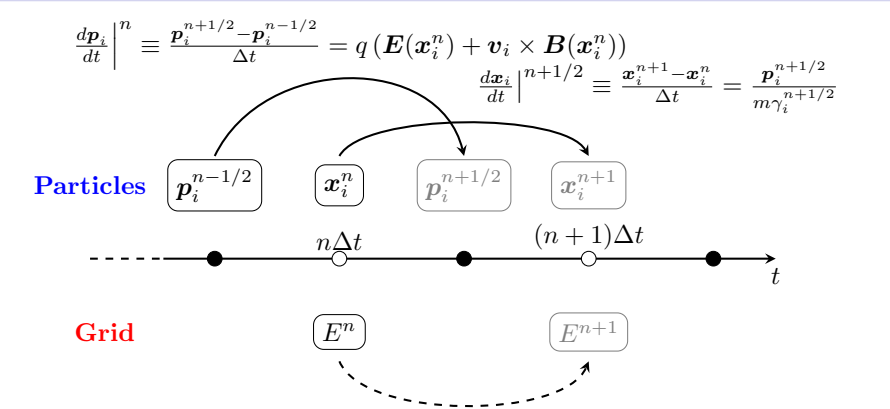
$$\left. \frac{\partial f}{\partial t} \right|_n = \frac{f_{n+1} - f_n}{\Delta t} + \mathcal{O}(\Delta t)$$

Centered discretization

$$\left. \frac{\partial f}{\partial t} \right|_n = \frac{f_{n+1/2} - f_{n-1/2}}{\Delta t} + \mathcal{O}(\Delta t^2)$$

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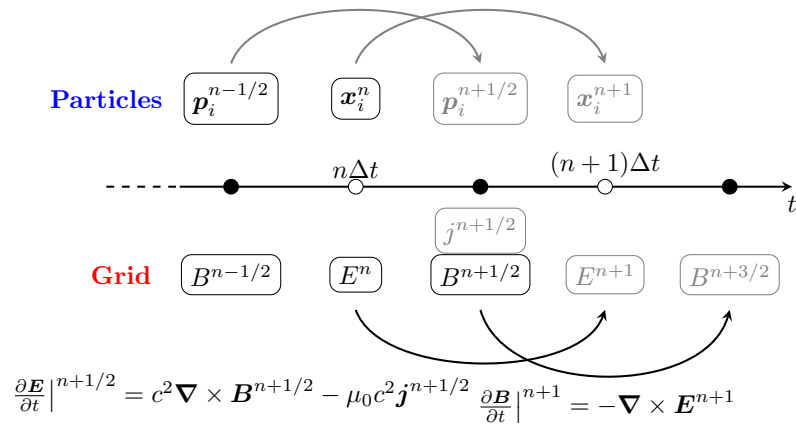
Staggering in time



- How to discretize $\frac{\partial \mathbf{E}}{\partial t} = c^2 \nabla \times \mathbf{B} - \mu_0 c^2 \mathbf{j}$ in time?
- How to stagger \mathbf{E}, \mathbf{B} and \mathbf{j} ?

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Staggering in time

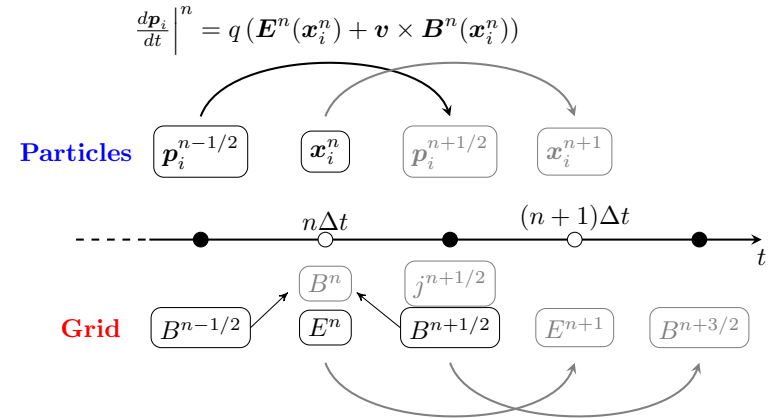


- E is defined at integer timestep.
- B and j are defined at half-integer timestep.

Staggering in time

Implication for field gathering

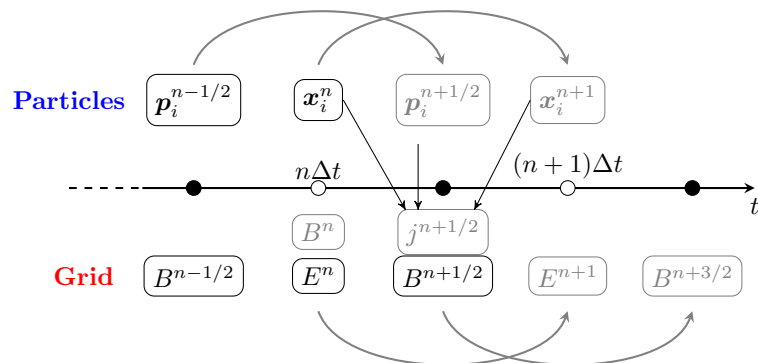
The particle pusher requires B at time $n\Delta t$. This is obtained by averaging $B^{n+1/2}$ and $B^{n-1/2}$.



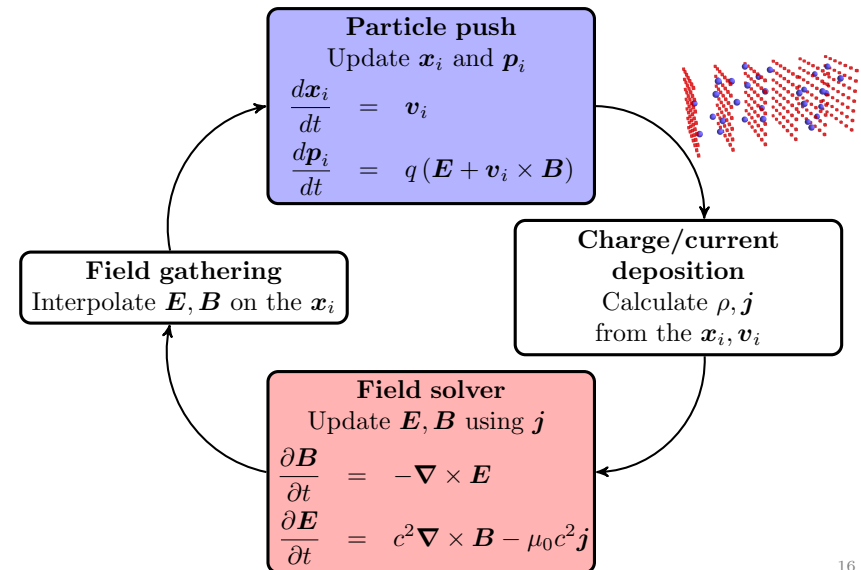
Staggering in time

Implication for current deposition

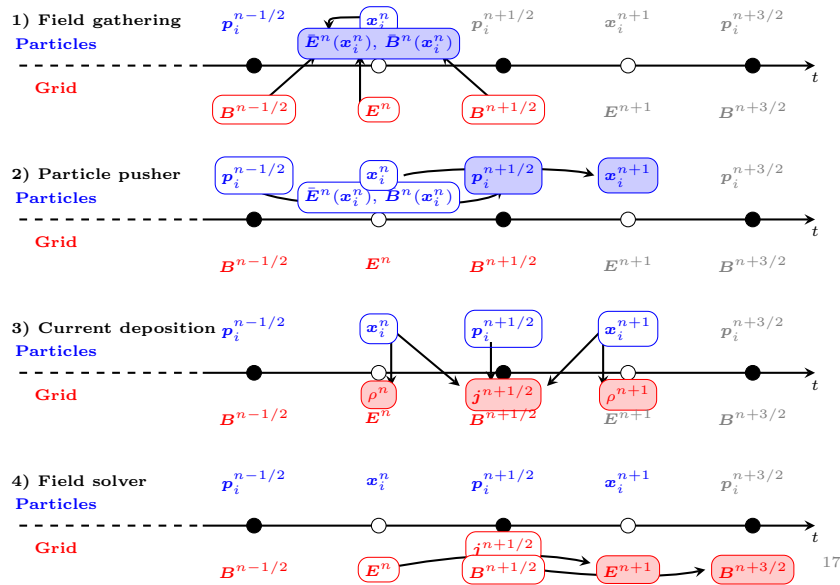
The current should be deposited at time $(n + 1/2)\Delta t$. This is done by using the particle's $v_i^{n+1/2}$ and **some combination** of x_i^n and x_i^{n+1} . (See Section 3)



Staggering in time: the full EM-PIC cycle



Staggering in time: the full EM-PIC cycle



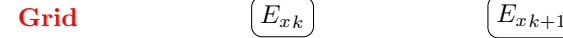
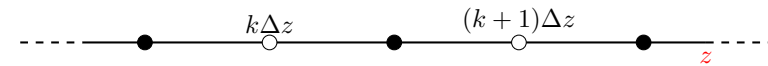
Staggering in space (1D)

To illustrate staggering in space, let us consider a **simplified case** where the fields vary only along z (1D case).

1D Maxwell equations for E_x and B_y

$$\begin{cases} \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \\ \frac{\partial \mathbf{E}}{\partial t} = c^2 \nabla \times \mathbf{B} - \mu_0 c^2 \mathbf{j} \end{cases} \rightarrow \begin{cases} \frac{\partial B_y}{\partial t} = -\frac{\partial E_x}{\partial z} \\ \frac{\partial E_x}{\partial t} = -c^2 \frac{\partial B_y}{\partial z} - \mu_0 c^2 j_x \end{cases}$$

(demonstration on the white board)

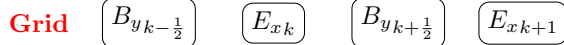


- How to discretize these equations?
- How to stagger E_x, B_y, j_x ?

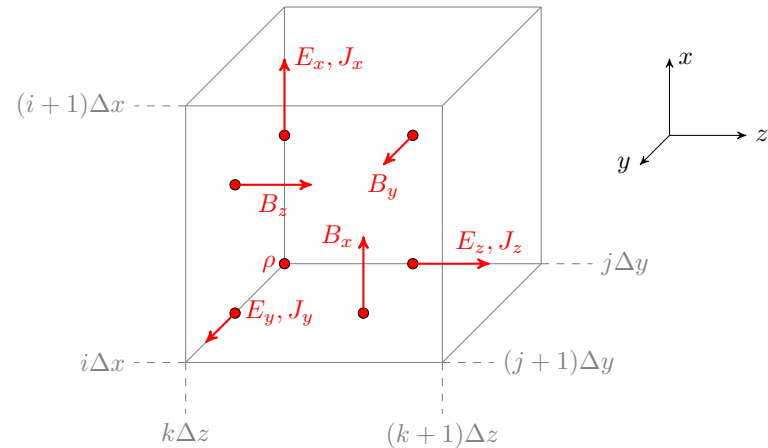
Staggering in space (1D)

1D discretized Maxwell equations for E_x and B_y

$$\begin{aligned} \frac{\partial B_y|_{k+\frac{1}{2}}}{\partial t} &= -\partial_z E_x|_{k+\frac{1}{2}} \\ \text{i.e. } \frac{B_{y_{k+\frac{1}{2}}}^{n+\frac{1}{2}} - B_{y_{k+\frac{1}{2}}}^{n-\frac{1}{2}}}{\Delta t} &= -\left(\frac{E_{x_{k+1}}^n - E_{x_k}^n}{\Delta z} \right) \\ \frac{\partial E_x|_k}{\partial t} &= -c^2 \partial_z B_y|_k^{n+\frac{1}{2}} - \mu_0 c^2 j_{x_k}^{n+\frac{1}{2}} \\ \text{i.e. } \frac{E_{x_k}^{n+1} - E_{x_k}^n}{\Delta t} &= -c^2 \left(\frac{B_{y_{k+\frac{1}{2}}}^{n+\frac{1}{2}} - B_{y_{k-\frac{1}{2}}}^{n+\frac{1}{2}}}{\Delta z} \right) - \mu_0 c^2 j_{x_k}^{n+\frac{1}{2}} \end{aligned}$$



Staggering in space (3D): the Yee grid



The different components of the different fields are staggered, so that all derivatives in the Maxwell equations are centered (Yee, 1966).

Staggering in space (3D): the Yee grid

Field	Position in space and time				Notation
	x	y	z	t	
E_x	$(i + \frac{1}{2})\Delta x$	$j\Delta y$	$k\Delta z$	$n\Delta t$	$E_{x_{i+\frac{1}{2},j,k}}^n$
E_y	$i\Delta x$	$(j + \frac{1}{2})\Delta y$	$k\Delta z$	$n\Delta t$	$E_{y_{i,j+\frac{1}{2},k}}^n$
E_z	$i\Delta x$	$j\Delta y$	$(k + \frac{1}{2})\Delta z$	$n\Delta t$	$E_{z_{i,j,k+\frac{1}{2}}}^n$
B_x	$i\Delta x$	$(j + \frac{1}{2})\Delta y$	$(k + \frac{1}{2})\Delta z$	$(n + \frac{1}{2})\Delta t$	$B_{x_{i,j+\frac{1}{2},k+\frac{1}{2}}}^{n+\frac{1}{2}}$
B_y	$(i + \frac{1}{2})\Delta x$	$j\Delta y$	$(k + \frac{1}{2})\Delta z$	$(n + \frac{1}{2})\Delta t$	$B_{y_{i+\frac{1}{2},j,k+\frac{1}{2}}}^{n+\frac{1}{2}}$
B_z	$(i + \frac{1}{2})\Delta x$	$(j + \frac{1}{2})\Delta y$	$k\Delta z$	$(n + \frac{1}{2})\Delta t$	$B_{z_{i+\frac{1}{2},j+\frac{1}{2},k}}^{n+\frac{1}{2}}$
ρ	$i\Delta x$	$j\Delta y$	$k\Delta z$	$n\Delta t$	$\rho_{i,j,k}^n$
j_x	$(i + \frac{1}{2})\Delta x$	$j\Delta y$	$k\Delta z$	$(n + \frac{1}{2})\Delta t$	$j_{x_{i+\frac{1}{2},j,k}}^{n+\frac{1}{2}}$
j_y	$i\Delta x$	$(j + \frac{1}{2})\Delta y$	$k\Delta z$	$(n + \frac{1}{2})\Delta t$	$j_{y_{i,j+\frac{1}{2},k}}^{n+\frac{1}{2}}$
j_z	$i\Delta x$	$j\Delta y$	$(k + \frac{1}{2})\Delta z$	$(n + \frac{1}{2})\Delta t$	$j_{z_{i,j,k+\frac{1}{2}}}^{n+\frac{1}{2}}$

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Staggering in space (3D): the Maxwell equations

Maxwell-Ampère

$$\partial_t E_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} = c^2 \partial_y B_z|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} - c^2 \partial_z B_y|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} - \mu_0 c^2 j_x|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}}$$

$$\partial_t E_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} = c^2 \partial_z B_x|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} - c^2 \partial_x B_z|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}} - \mu_0 c^2 j_y|_{i,j+\frac{1}{2},k}^{n+\frac{1}{2}}$$

$$\partial_t E_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} = c^2 \partial_x B_y|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - c^2 \partial_y B_x|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - \mu_0 c^2 j_z|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}}$$

Maxwell-Faraday

$$\partial_t B_x|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n = -\partial_y E_z|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n + \partial_z E_y|_{i,j+\frac{1}{2},k+\frac{1}{2}}^n$$

$$\partial_t B_y|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n = -\partial_z E_x|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n + \partial_x E_z|_{i+\frac{1}{2},j,k+\frac{1}{2}}^n$$

$$\partial_t B_z|_{i+\frac{1}{2},j+\frac{1}{2},k}^n = -\partial_x E_y|_{i+\frac{1}{2},j+\frac{1}{2},k}^n + \partial_y E_x|_{i+\frac{1}{2},j+\frac{1}{2},k}^n$$

$$\partial_t F|_{i',j',k'}^{n'} \equiv \frac{F_{i',j',k'}^{n'+\frac{1}{2}} - F_{i',j',k'}^{n'-\frac{1}{2}}}{\Delta t} \quad \partial_x F|_{i',j',k'}^{n'} \equiv \frac{F_{i'+\frac{1}{2},j',k'}^{n'} - F_{i'-\frac{1}{2},j',k'}^{n'}}{\Delta x}$$

$$\partial_y F|_{i',j',k'}^{n'} \equiv \frac{F_{i',j'+\frac{1}{2},k'}^{n'} - F_{i',j'-\frac{1}{2},k'}^{n'}}{\Delta y} \quad \partial_z F|_{i',j',k'}^{n'} \equiv \frac{F_{i',j',k'+\frac{1}{2}}^{n'} - F_{i',j',k'-\frac{1}{2}}^{n'}}{\Delta z}$$

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The equations $\nabla \cdot \mathbf{B} = 0$ and $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$

Gauss law for magnetic field

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

$$\partial_x B_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} + \partial_y B_y|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} + \partial_z B_z|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} = 0$$

Gauss law

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

$$\partial_x E_x|_{i,j,k}^n + \partial_y E_y|_{i,j,k}^n + \partial_z E_z|_{i,j,k}^n = \frac{\rho_{i,j,k}^n}{\epsilon_0}$$

These equations are not used during the PIC loop!

(Since we use only $\partial_t \mathbf{E} = c^2 \nabla \times \mathbf{B} - \mu_0 c^2 \mathbf{j}$ and $\partial_t \mathbf{B} = \nabla \times \mathbf{E}$ to update the fields.)

→ Are $\nabla \cdot \mathbf{B} = 0$ and $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$ actually satisfied?

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

Provided that:

- $\nabla \cdot \mathbf{B} = 0$ is satisfied initially
- $\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$ is satisfied at all time.

$$\text{then : } \frac{\partial(\nabla \cdot \mathbf{B})}{\partial t} = \nabla \cdot \frac{\partial \mathbf{B}}{\partial t} = \nabla \cdot (-\nabla \times \mathbf{E}) = 0$$

i.e. $\nabla \cdot \mathbf{B} = 0$ at all time

This remains true for the discretized operators.

Conservation of $\nabla \cdot \mathbf{B}$

Updating \mathbf{B} with the discretized Maxwell-Faraday equation preserves

$$\partial_x B_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} + \partial_y B_y|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} + \partial_z B_z|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} = 0$$

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The equation $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$

Provided that:

- $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$ is satisfied initially
- $\frac{\partial \mathbf{E}}{\partial t} = -c^2 \nabla \times \mathbf{B} - \mu_0 c^2 \mathbf{j}$ is satisfied at all time.

then :
$$\frac{\partial}{\partial t} \left(\nabla \cdot \mathbf{E} - \frac{\rho}{\epsilon_0} \right) = -\frac{1}{\epsilon_0} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} \right)$$

i.e. $\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$ at all time, provided that $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$

Conservation of $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$

Updating \mathbf{E} with the discretized Maxwell-Ampère equation preserves

$$\partial_x E_x|_{i,j,k}^n + \partial_y E_y|_{i,j,k}^n + \partial_z E_z|_{i,j,k}^n = \frac{\rho_{i,j,k}^n}{\epsilon_0}$$

provided that the continuity equation is satisfied at each iteration:

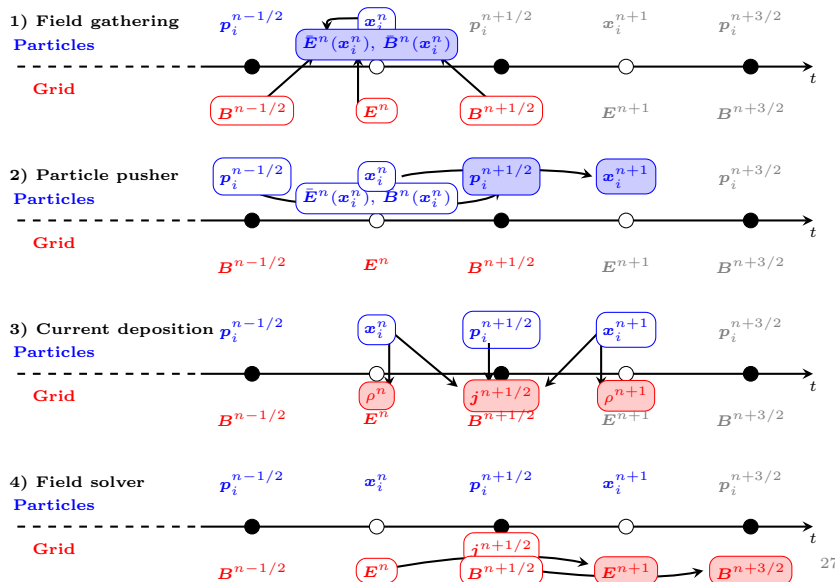
$$\partial_t \rho|_{i,j,k}^{n+\frac{1}{2}} + \partial_x j_x|_{i,j,k}^{n+\frac{1}{2}} + \partial_y j_y|_{i,j,k}^{n+\frac{1}{2}} + \partial_z j_z|_{i,j,k}^{n+\frac{1}{2}} = 0$$

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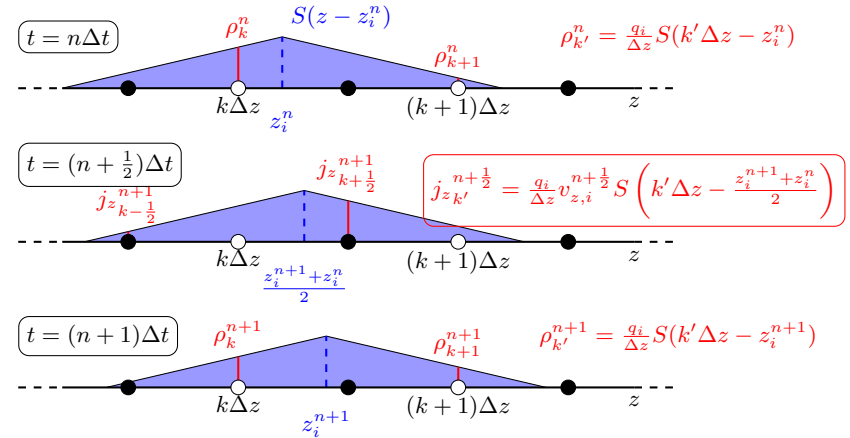
Charge/current deposition: reminder



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Direct current deposition: 1D example

Direct current deposition: The current \mathbf{j} is deposited with the same shape factor as the charge density ρ .



Here, linear weights: $S(z - z_i) = \begin{cases} 1 - |z - z_i|/\Delta z & \text{if } |z - z_i| < \Delta z \\ 0 & \text{otherwise} \end{cases}$

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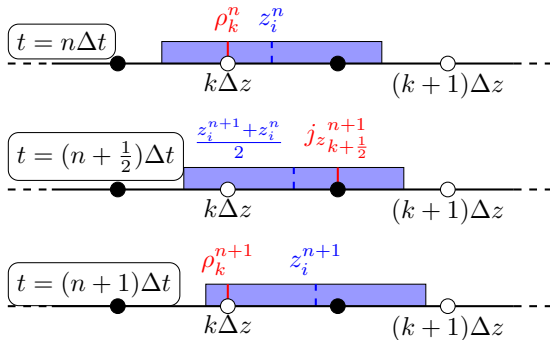
Direct current deposition and continuity equation

1D continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial j_z}{\partial z} = 0 \quad \rightarrow \quad \frac{\rho_k^{n+1} - \rho_k^n}{\Delta t} + \frac{j_{z_{k+\frac{1}{2}}}^{n+\frac{1}{2}} - j_{z_{k-\frac{1}{2}}}^{n+\frac{1}{2}}}{\Delta z} = 0$$

Does direct deposition satisfy the continuity equation?

Example with *nearest grid point*, i.e. $S(z - z_i) = 1$ if $|z - z_i| < \Delta z/2$



Here:

$$\frac{\rho_k^{n+1} - \rho_k^n}{\Delta t} = 0$$

$$\frac{j_{z_{k+\frac{1}{2}}}^{n+\frac{1}{2}} - j_{z_{k-\frac{1}{2}}}^{n+\frac{1}{2}}}{\Delta z} \neq 0$$

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Direct current deposition and continuity equation

Direct current deposition does not satisfy the continuity equation.

Reminder:

Updating \mathbf{E} with the discretized Maxwell-Ampère equation preserves

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

provided that the continuity equation is satisfied at each iteration.

The PIC loop with **direct current deposition** does not preserve

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

Two alternative solutions:

- Boris correction: correcting $\nabla \cdot \mathbf{E}$ at each iteration.
- Use a charge-conserving deposition instead of direct deposition.

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Boris correction

Boris correction

At each iteration, after updating \mathbf{E} , correct it using

$$\mathbf{E}' = \mathbf{E} - \nabla \delta \phi \quad \text{with} \quad \nabla^2 \delta \phi = \nabla \cdot \mathbf{E} - \frac{\rho}{\epsilon_0}$$

The new field \mathbf{E}' does satisfy (demonstration on the white board)

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

Practical implementation

The discretized version of

$$\nabla^2 \delta \phi = \nabla \cdot \mathbf{E} - \frac{\rho}{\epsilon_0}$$

needs to be solved on the grid at each iteration, so as to obtain $\delta \phi$.

→ Can be done using techniques from electrostatic PIC (see previous lecture), e.g. direct matrix, spectral or relaxation methods

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Charge-conserving deposition

Charge-conserving deposition

The current \mathbf{j} is deposited in such a way that it automatically satisfies the continuity equation

$$\partial_t \rho|_{i,j,k}^{n+\frac{1}{2}} + \partial_x j_x|_{i,j,k}^{n+\frac{1}{2}} + \partial_y j_y|_{i,j,k}^{n+\frac{1}{2}} + \partial_z j_z|_{i,j,k}^{n+\frac{1}{2}} = 0$$

Several algorithms exist, e.g.

- Esirkepov (Esirkepov, 2001)
- ZigZag (Umeda et al., 2003)

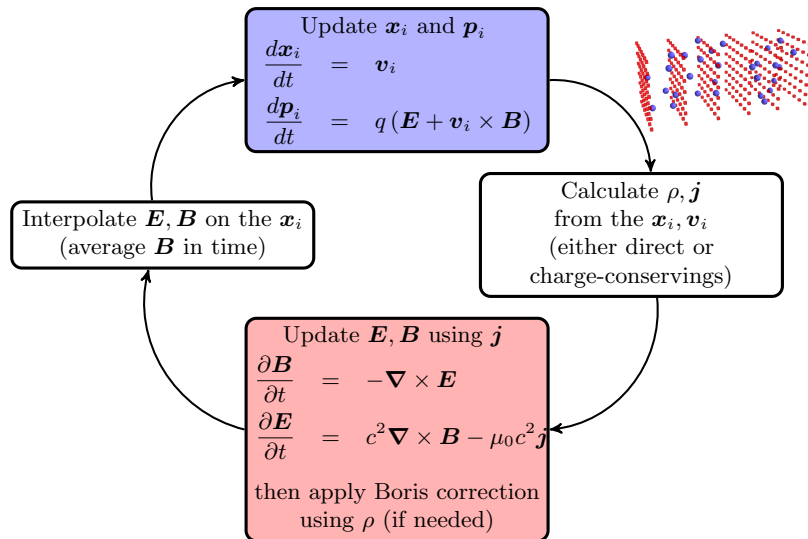
In these cases, the PIC loop automatically preserves

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

The Boris correction is not needed.

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Summary



References

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