Electromagnetic Particle-In-Cell codes

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Self-Consistent Simulations of Beam and Plasma Systems

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Electromagnetic Particle-In-Cell codes: Outline

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 $\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$ and $\boldsymbol{\nabla} \cdot \boldsymbol{E} = \rho/\epsilon_0$
3. Current deposition and continuity equation
   - Direct current deposition and continuity equation
   - Boris correction
   - Charge-conserving deposition

When to use ES-PIC or EM-PIC

Electrostatics

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

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

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

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

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

Full set of equations:

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

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**

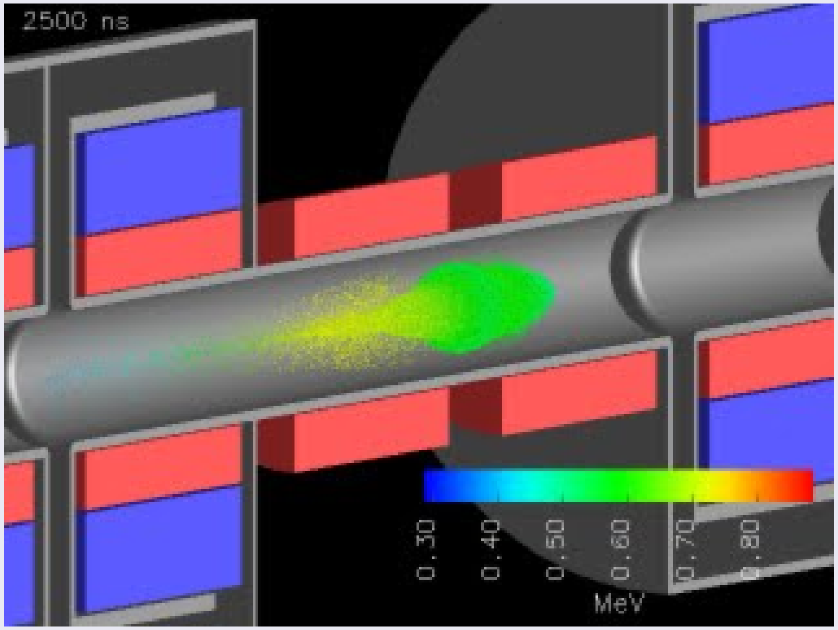
- The particles move **close to** c, and accelerate abruptly.
- The fields depend on the **history** of the particles (radiation effects)

→ **Electromagnetic PIC is needed**

When to use ES-PIC or EM-PIC

Example using electrostatic PIC:

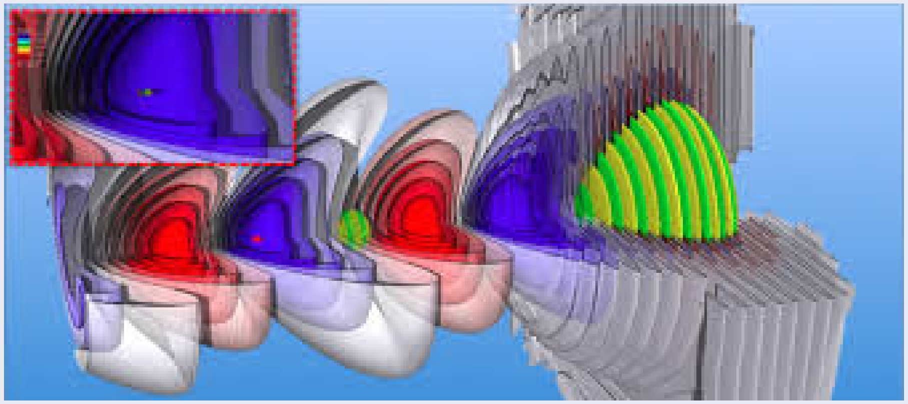
Sub-GeV acceleration of ions in conventional accelerators



- The ions are slower than c.

Example using electromagnetic PIC:

Laser-driven acceleration of electrons in plasmas



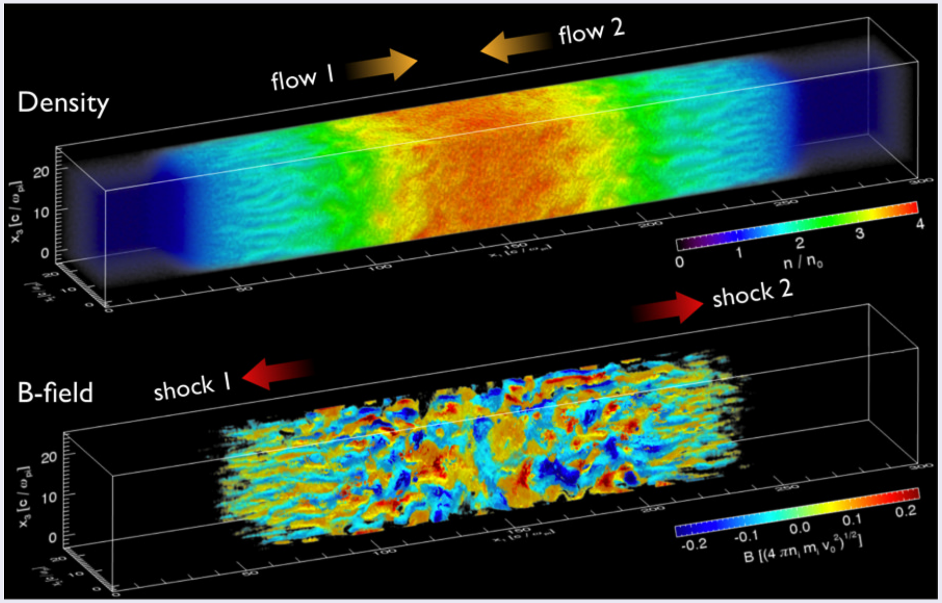
- Presence of radiation (the laser)
- The electrons move close to c.

When to use ES-PIC or EM-PIC

Other examples using **electromagnetic PIC**

Electromagnetic plasma instabilities

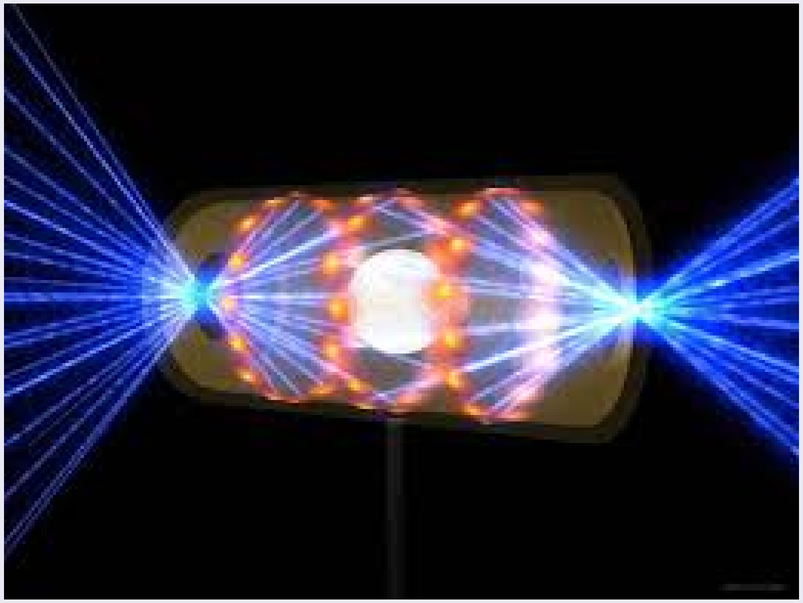
e.g. collisionless astrophysical shocks



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

Interaction of intense lasers with plasmas

e.g. inertial fusion



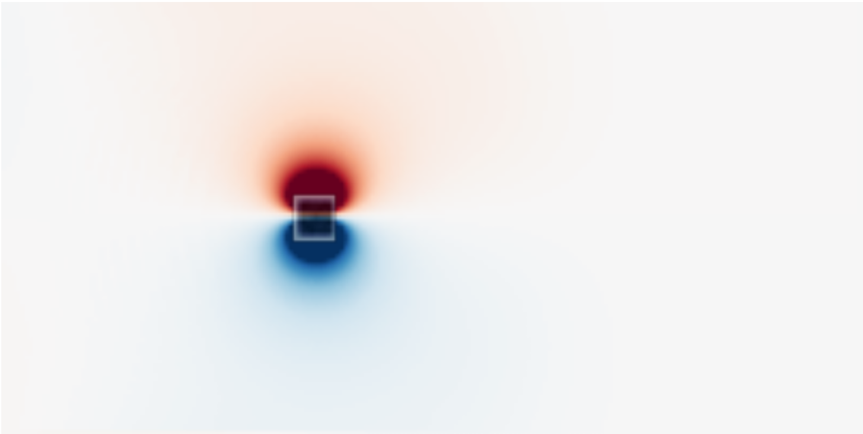
- Presence of radiation (lasers)

Field solver in ES-PIC and EM-PIC

Electrostatic field solver

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0} \qquad \boldsymbol{E} = -\nabla \phi$$

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

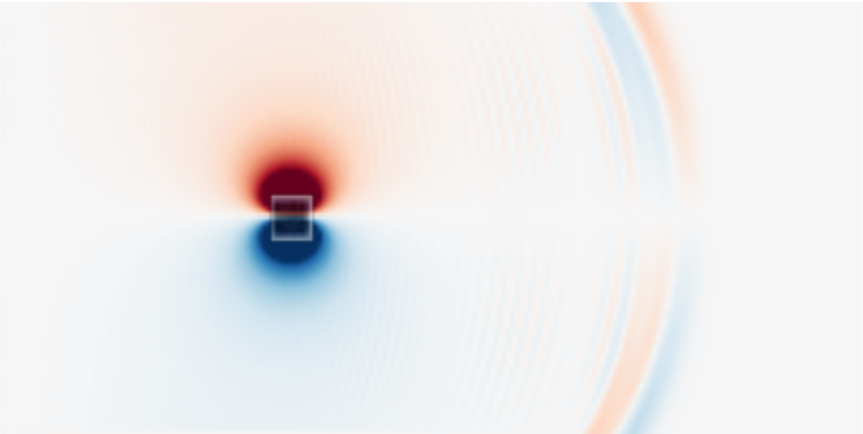


Electromagnetic field solver

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

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

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



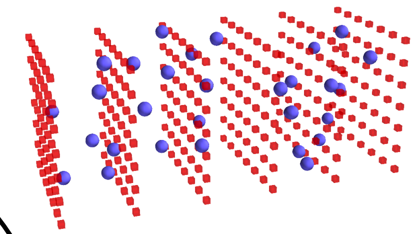
The PIC loop in Electrostatic-PIC

Particle push

Update $\boldsymbol{x}_i$ and $\boldsymbol{p}_i$

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

$$\frac{d\boldsymbol{p}_i}{dt} = q\left(\boldsymbol{E} + \boldsymbol{v}_i \times \boldsymbol{B}\right)$$



Charge deposition

Calculate ρ from the $\boldsymbol{x}_i$

Field solver

Calculate $\boldsymbol{E}$ from ρ

$$\boldsymbol{\nabla}^2\phi = -\frac{\rho}{\epsilon_0} \qquad \boldsymbol{E} = -\boldsymbol{\nabla}\phi$$

Field gathering

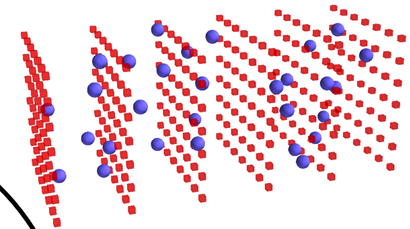
Interpolate $\boldsymbol{E}$ on the $\boldsymbol{x}_i$

The PIC loop in Electromagnetic-PIC

Particle push

Update $\boldsymbol{x}_i$ and $\boldsymbol{p}_i$

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$$
$$\frac{d\boldsymbol{p}_i}{dt} = q\left(\boldsymbol{E} + \boldsymbol{v}_i \times \boldsymbol{B}\right)$$



Charge/current deposition

Calculate $\rho, \boldsymbol{j}$ from the $\boldsymbol{x}_i, \boldsymbol{v}_i$

Field solver

Update $\boldsymbol{E}, \boldsymbol{B}$ using $\boldsymbol{j}$

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

Field gathering

Interpolate $\boldsymbol{E}, \boldsymbol{B}$ on the $\boldsymbol{x}_i$

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Staggering in time

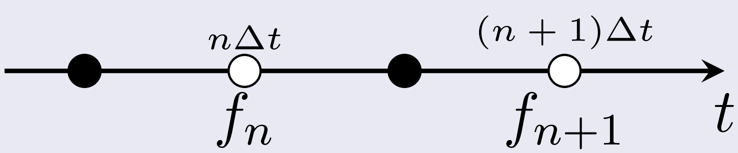
Reminder: (Monday's *Overview of Basic Numerical Methods*)

Centered discretization of derivatives is more accurate

Non-centered discretization

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

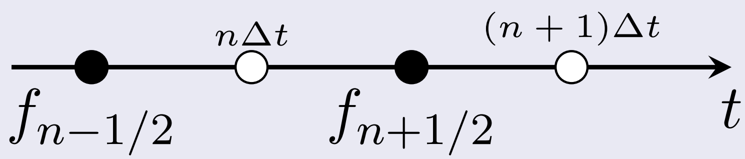
$$\left.\frac{\partial f}{\partial t}\right|_n$$



Centered discretization

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

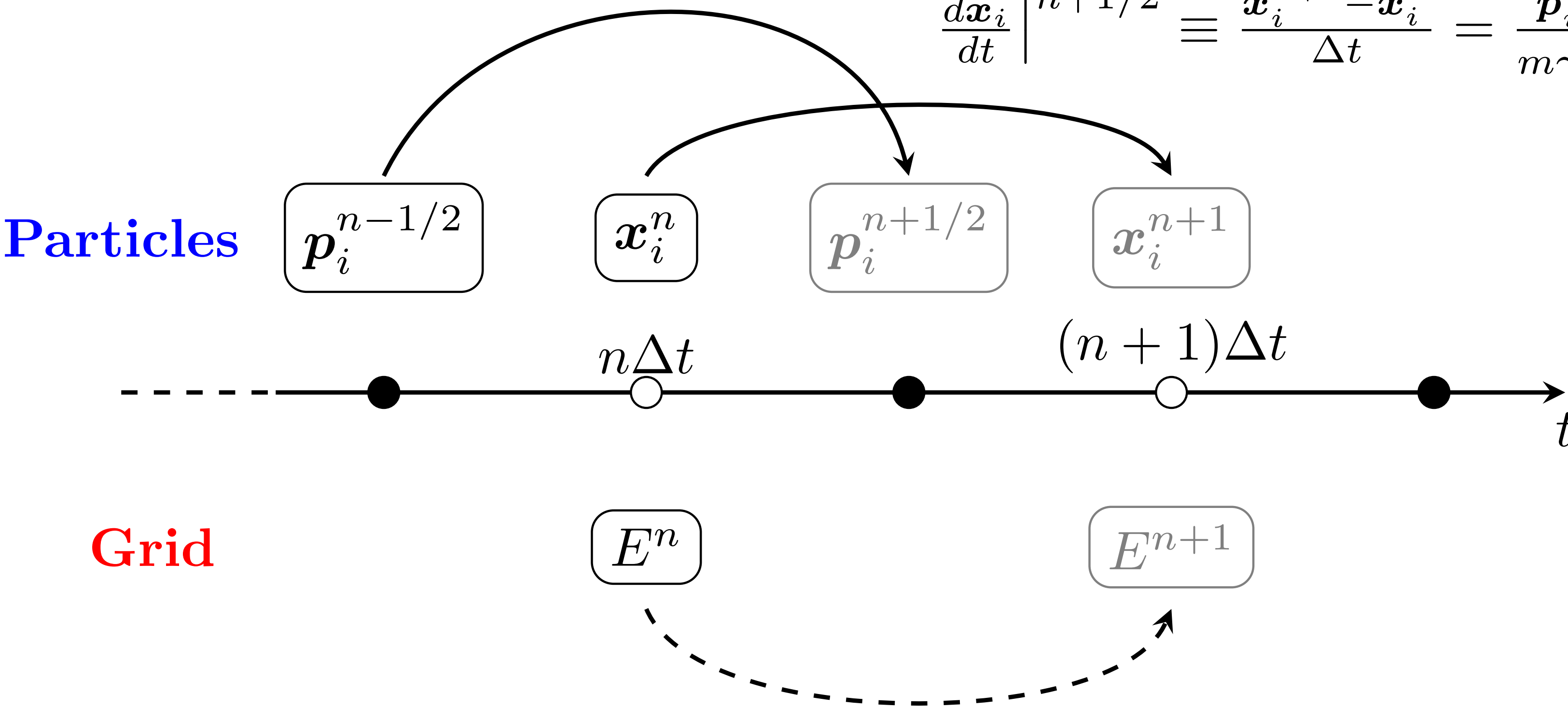
$$\left.\frac{\partial f}{\partial t}\right|_n$$



Staggering in time

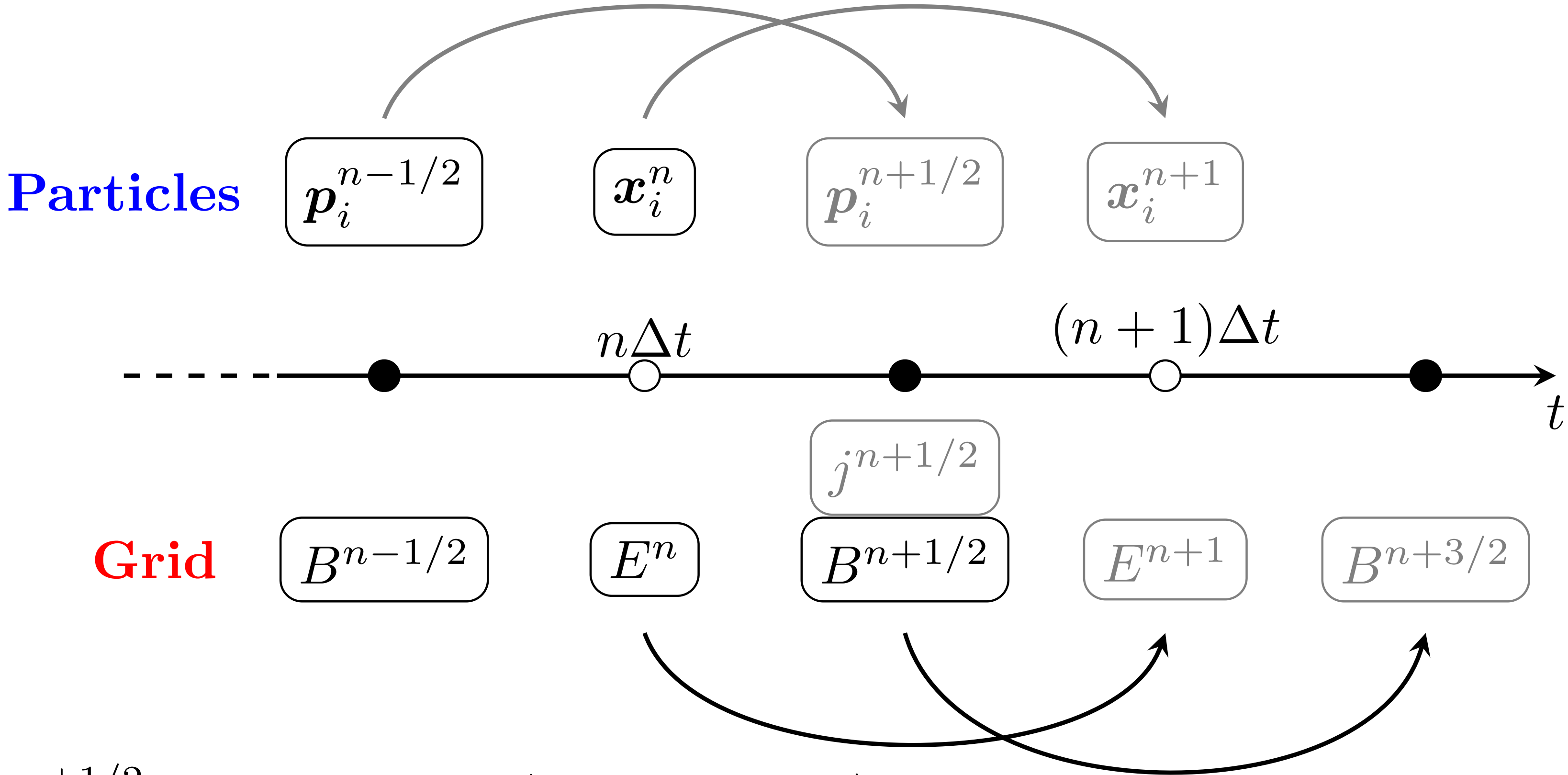
$$\left.\frac{d\boldsymbol{p}_i}{dt}\right|^n \equiv \frac{\boldsymbol{p}_i^{n+1/2}-\boldsymbol{p}_i^{n-1/2}}{\Delta t} = q\left(\boldsymbol{E}(\boldsymbol{x}_i^n) + \boldsymbol{v}_i \times \boldsymbol{B}(\boldsymbol{x}_i^n)\right)$$

$$\left.\frac{d\boldsymbol{x}_i}{dt}\right|^{n+1/2} \equiv \frac{\boldsymbol{x}_i^{n+1}-\boldsymbol{x}_i^n}{\Delta t} = \frac{\boldsymbol{p}_i^{n+1/2}}{m\gamma_i^{n+1/2}}$$



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

Staggering in time



$$\left.\frac{\partial \boldsymbol{E}}{\partial t}\right|^{n+1/2} = c^2 \boldsymbol{\nabla} \times \boldsymbol{B}^{n+1/2} - \mu_0 c^2 \boldsymbol{j}^{n+1/2} \qquad \left.\frac{\partial \boldsymbol{B}}{\partial t}\right|^{n+1} = -\boldsymbol{\nabla} \times \boldsymbol{E}^{n+1}$$

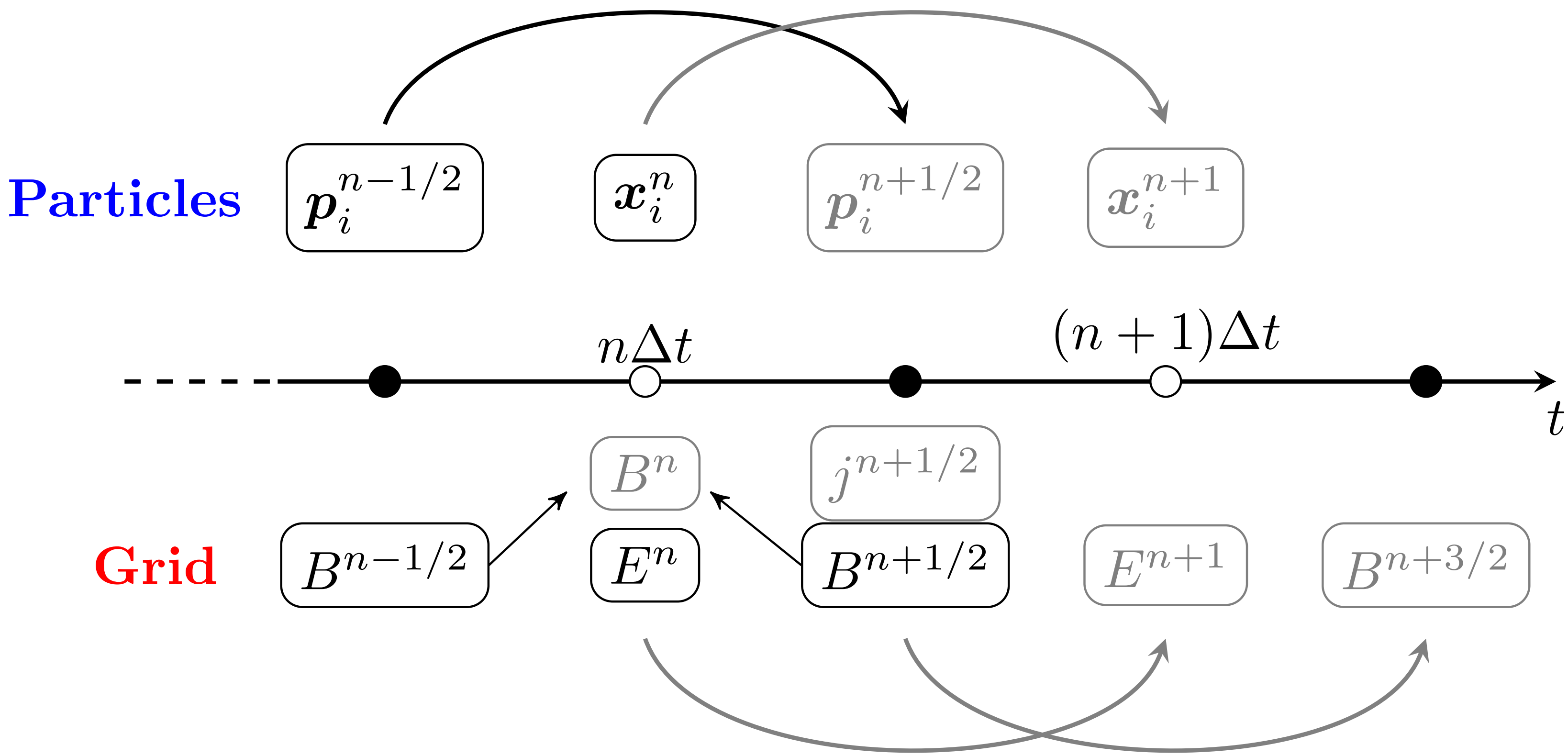
- $\boldsymbol{E}$ is defined at integer timestep.
- $\boldsymbol{B}$ and $\boldsymbol{j}$ are defined at half-integer timestep.

Staggering in time

Implication for **field gathering**

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

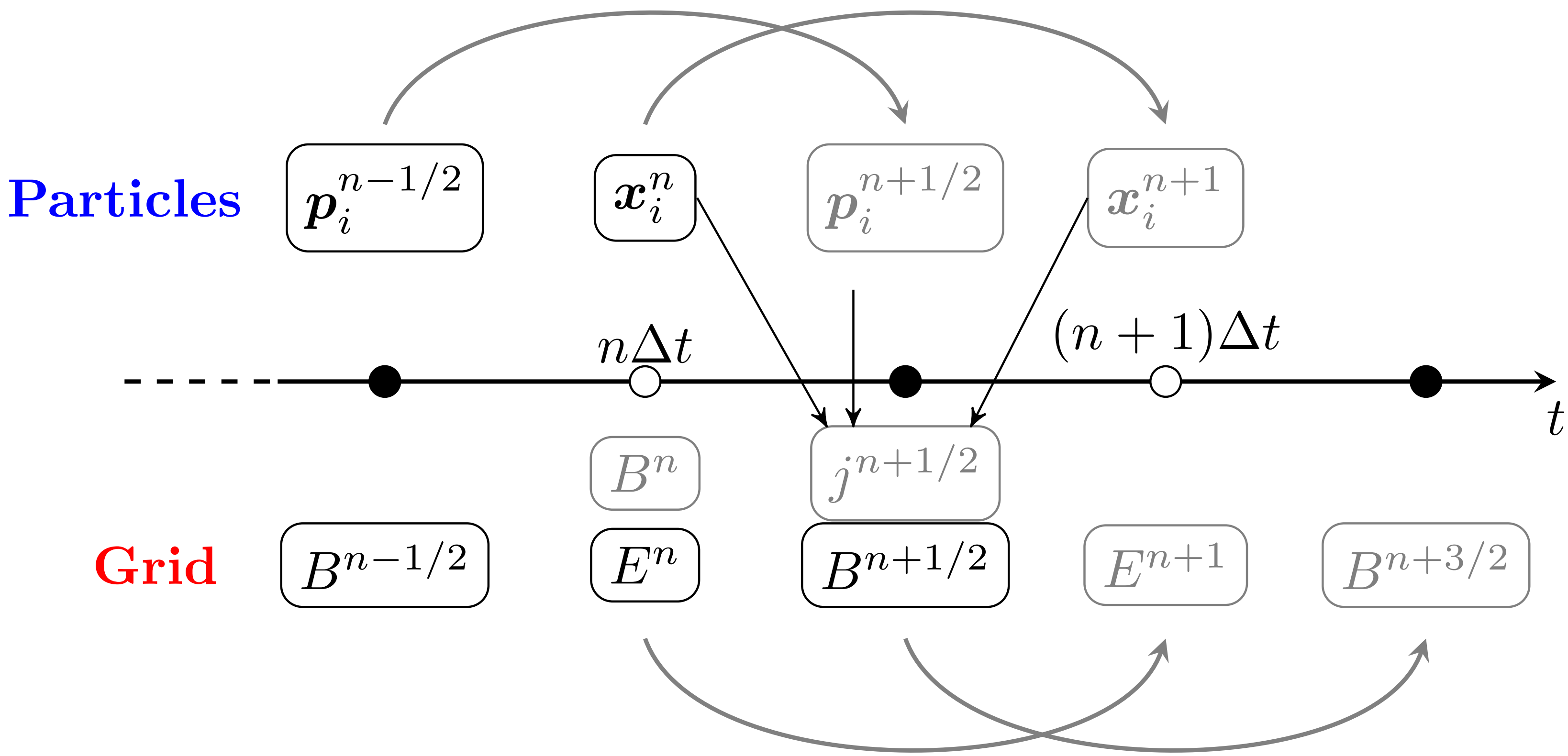
$$\left.\frac{d\boldsymbol{p}_i}{dt}\right|^n = q\left(\boldsymbol{E}^n(\boldsymbol{x}_i^n) + \boldsymbol{v}\times\boldsymbol{B}^n(\boldsymbol{x}_i^n)\right)$$



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 $\boldsymbol{v}_i^{n+1/2}$ and **some combination** of $\boldsymbol{x}_i^n$ and $\boldsymbol{x}_i^{n+1}$. (See Section 3)

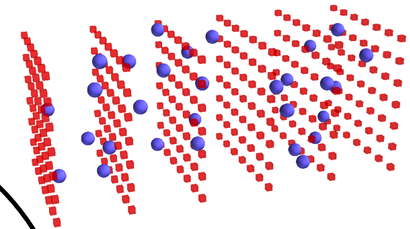


Staggering in time: the full EM-PIC cycle

Particle push

Update $\boldsymbol{x}_i$ and $\boldsymbol{p}_i$

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$$
$$\frac{d\boldsymbol{p}_i}{dt} = q\left(\boldsymbol{E} + \boldsymbol{v}_i \times \boldsymbol{B}\right)$$



Charge/current deposition

Calculate $\rho, \boldsymbol{j}$ from the $\boldsymbol{x}_i, \boldsymbol{v}_i$

Field solver

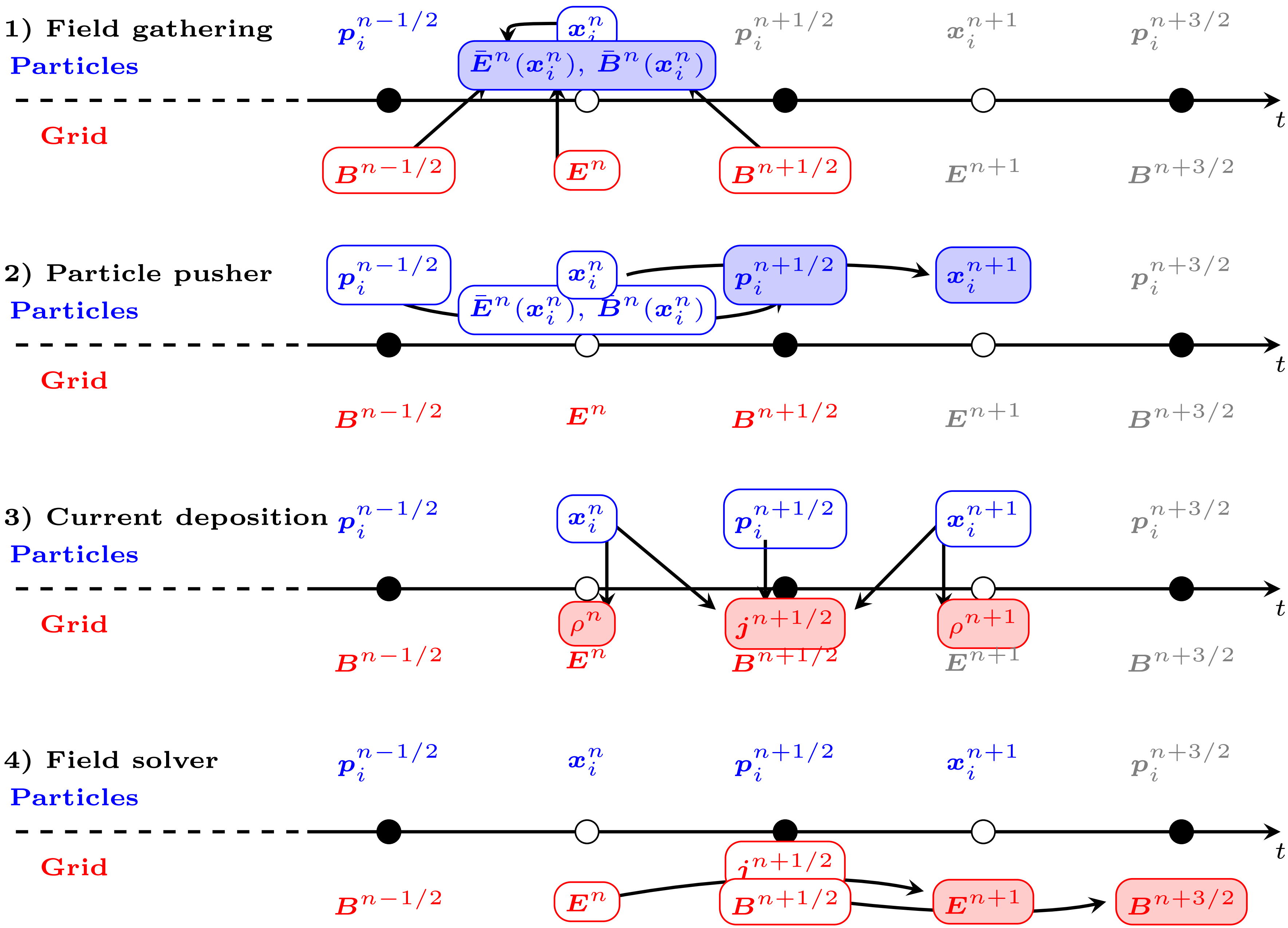
Update $\boldsymbol{E}, \boldsymbol{B}$ using $\boldsymbol{j}$

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

Field gathering

Interpolate $\boldsymbol{E}, \boldsymbol{B}$ on the $\boldsymbol{x}_i$

Staggering in time: the full EM-PIC cycle



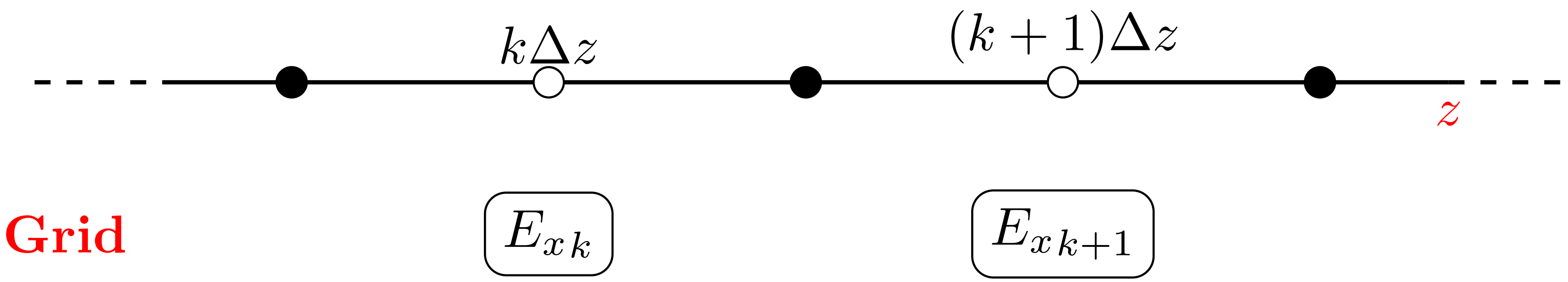
Staggering in space (1D)

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

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

(demonstration on the white board)



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

Staggering in space (1D)

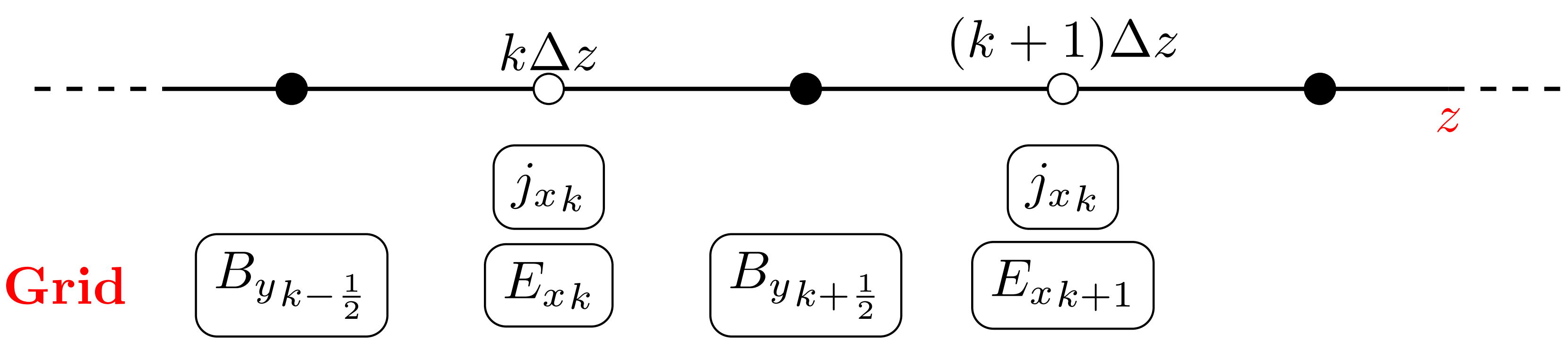
1D **discretized** Maxwell equations for E_x and B_y

$$\partial_t B_y|^n_{k+\frac{1}{2}} = -\partial_z E_x|^n_{k+\frac{1}{2}}$$

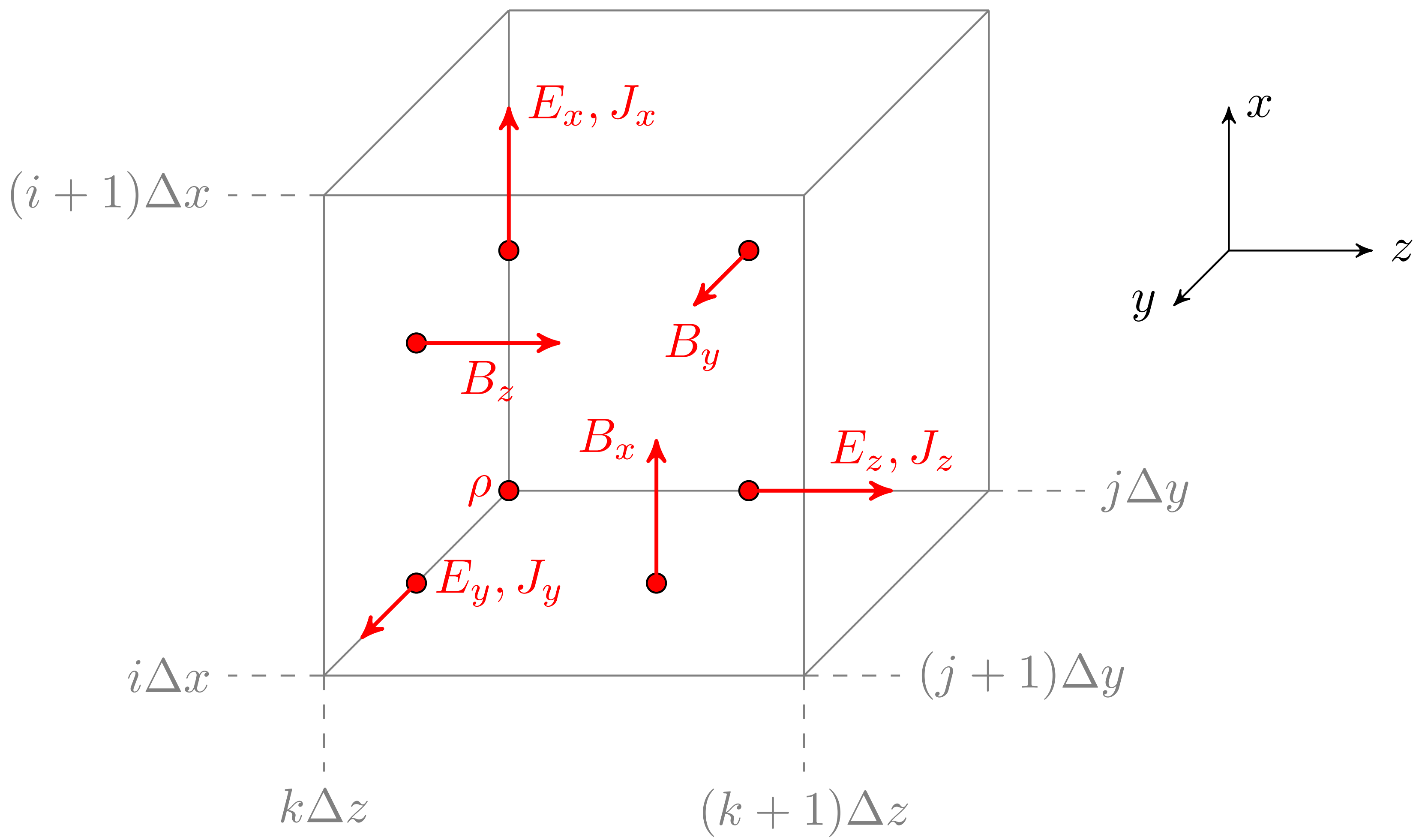
$$i.e. \quad \frac{{B_y}^{n+\frac{1}{2}}_{k+\frac{1}{2}} - {B_y}^{n-\frac{1}{2}}_{k+\frac{1}{2}}}{\Delta t} = -\left(\frac{{E_x}^n_{k+1} - {E_x}^n_k}{\Delta z}\right)$$

$$\partial_t E_x|^{n+\frac{1}{2}}_k = -c^2 \partial_z B_y|^{n+\frac{1}{2}}_k - \mu_0 c^2 {j_x}^{n+\frac{1}{2}}_k$$

$$i.e. \quad \frac{{E_x}^{n+1}_k - {E_x}^n_k}{\Delta t} = -c^2\left(\frac{{B_y}^{n+\frac{1}{2}}_{k+\frac{1}{2}} - {B_y}^{n+\frac{1}{2}}_{k-\frac{1}{2}}}{\Delta z}\right) - \mu_0 c^2 {j_x}^{n+\frac{1}{2}}_k$$



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	$(i+\frac{1}{2})\Delta x$	$j\Delta y$	$k\Delta z$	$n\Delta t$	${E_x}^n_{i+\frac{1}{2},j,k}$
E_y	$i\Delta x$	$(j+\frac{1}{2})\Delta y$	$k\Delta z$	$n\Delta t$	${E_y}^n_{i,j+\frac{1}{2},k}$
E_z	$i\Delta x$	$j\Delta y$	$(k+\frac{1}{2})\Delta z$	$n\Delta t$	${E_z}^n_{i,j,k+\frac{1}{2}}$
B_x	$i\Delta x$	$(j+\frac{1}{2})\Delta y$	$(k+\frac{1}{2})\Delta z$	$(n+\frac{1}{2})\Delta t$	${B_x}^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}}$
B_y	$(i+\frac{1}{2})\Delta x$	$j\Delta y$	$(k+\frac{1}{2})\Delta z$	$(n+\frac{1}{2})\Delta t$	${B_y}^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k+\frac{1}{2}}$
B_z	$(i+\frac{1}{2})\Delta x$	$(j+\frac{1}{2})\Delta y$	$k\Delta z$	$(n+\frac{1}{2})\Delta t$	${B_z}^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},k}$
ρ	$i\Delta x$	$j\Delta y$	$k\Delta z$	$n\Delta t$	$\rho^n_{i,j,k}$
j_x	$(i+\frac{1}{2})\Delta x$	$j\Delta y$	$k\Delta z$	$(n+\frac{1}{2})\Delta t$	${j_x}^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k}$
j_y	$i\Delta x$	$(j+\frac{1}{2})\Delta y$	$k\Delta z$	$(n+\frac{1}{2})\Delta t$	${j_y}^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k}$
j_z	$i\Delta x$	$j\Delta y$	$(k+\frac{1}{2})\Delta z$	$(n+\frac{1}{2})\Delta t$	${j_z}^{n+\frac{1}{2}}_{i,j,k+\frac{1}{2}}$

Staggering in space (3D): the Maxwell equations

Maxwell-Ampère

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

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

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

Maxwell-Faraday

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

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

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

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

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

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

Gauss law for magnetic field

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

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

Gauss law

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

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

These equations are not used during the PIC loop!
(Since we use only $\partial_t \boldsymbol{E} = c^2 \nabla \times \boldsymbol{B} - \mu_0 c^2 \boldsymbol{j}$ and $\partial_t \boldsymbol{B} = \nabla \times \boldsymbol{E}$ to update the fields.)
$\rightarrow$ Are $\nabla \cdot \boldsymbol{B} = 0$ and $\nabla \cdot \boldsymbol{E} = \rho/\epsilon_0$ actually satisfied?

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

Provided that:

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

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

$$i.e. \quad \nabla \cdot \boldsymbol{B} = 0 \quad \text{at all time}$$

This remains true for the discretized operators.

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

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

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

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

Provided that:

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

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

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

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

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

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

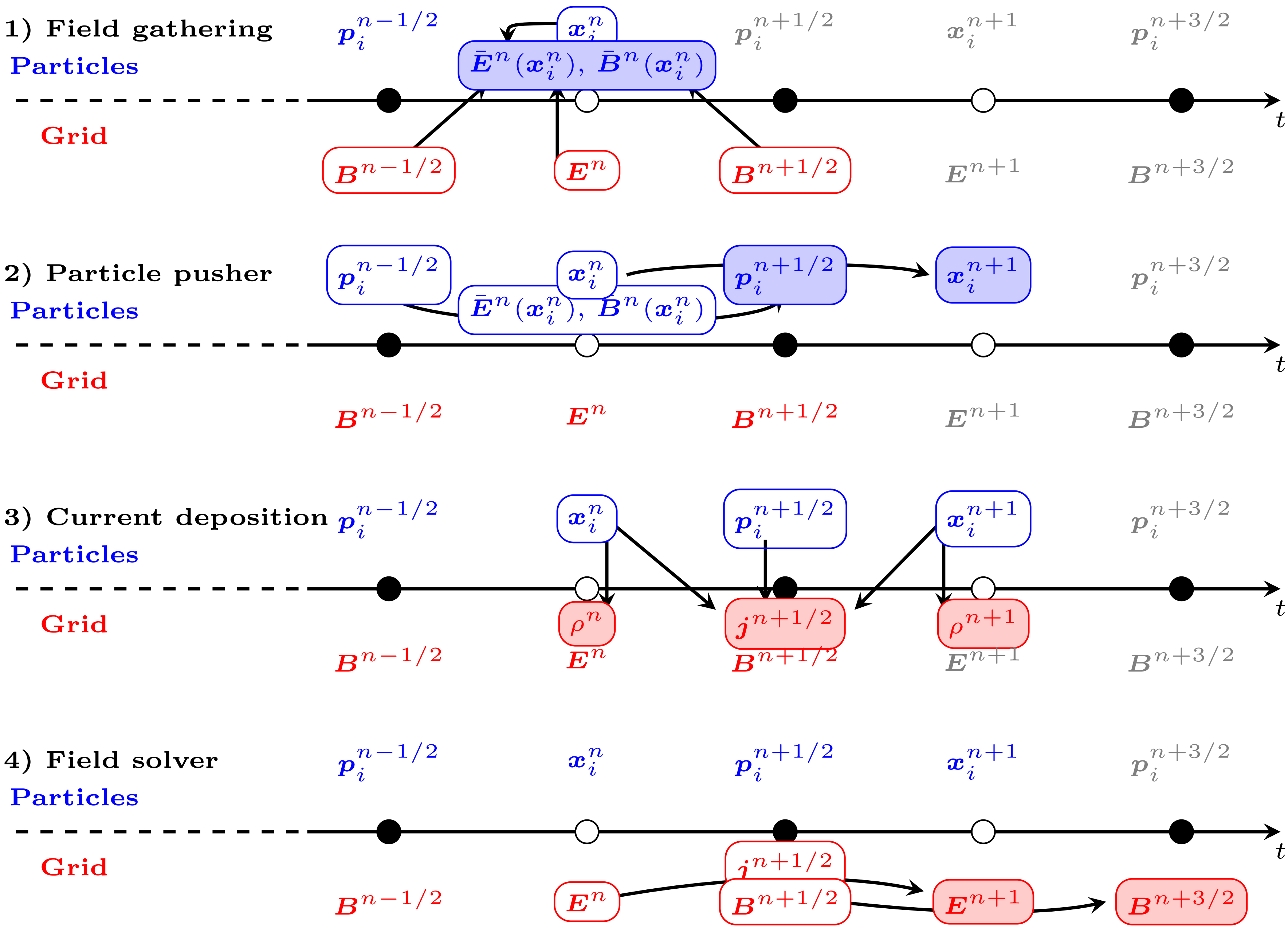
provided that the continuity equation is satisfied at each iteration:

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

Electromagnetic Particle-In-Cell codes: Outline

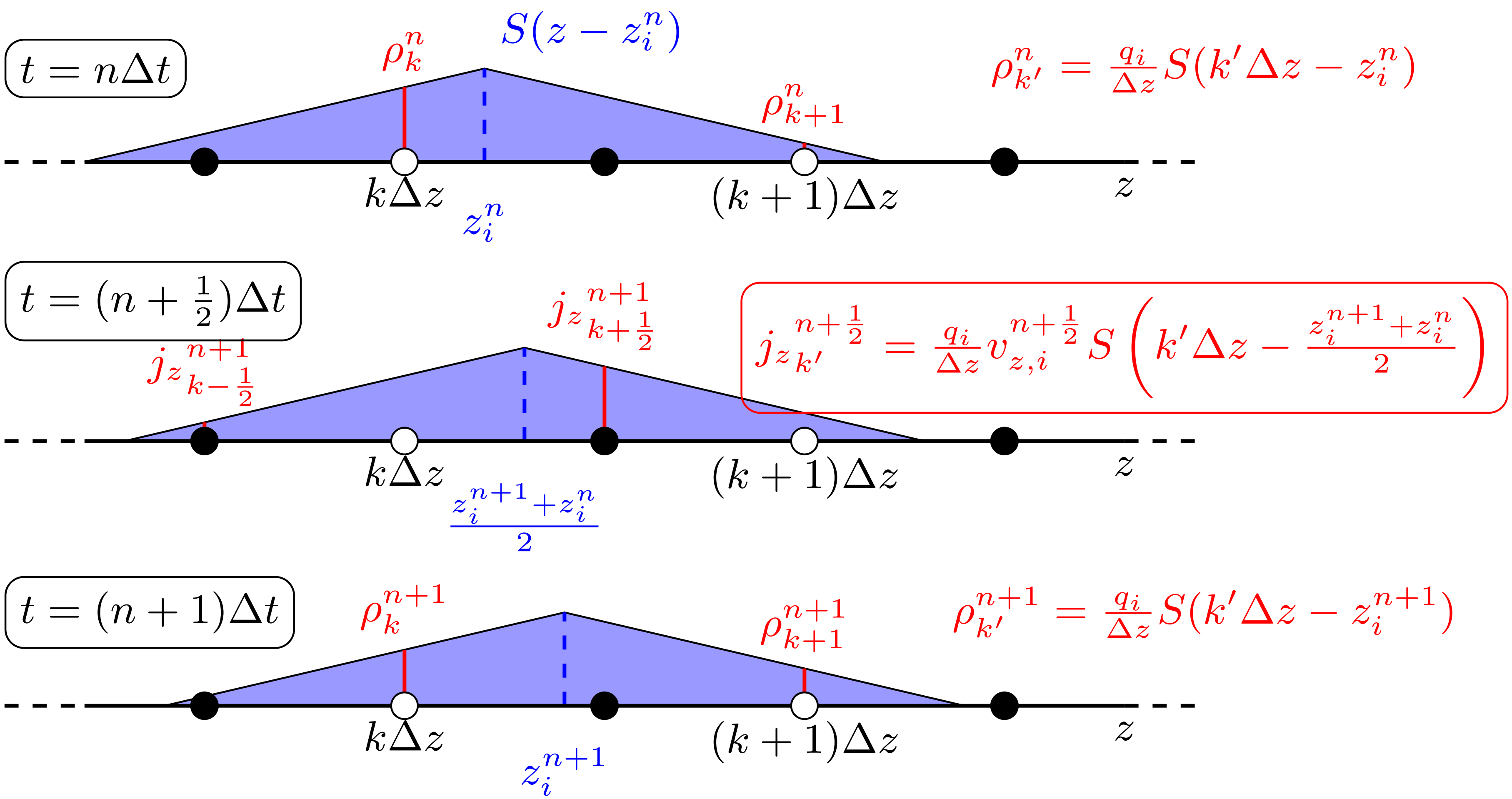
1. Electromagnetic PIC vs. electrostatic PIC
   - When to use electrostatic or electromagnetic PIC
   - The PIC loop in electrostatic and electromagnetic PIC
2. Finite-difference electromagnetic field solvers
   - Staggering in time
   - Staggering in space
   - The equations $\boldsymbol{\nabla} \cdot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

Charge/current deposition: reminder



Direct current deposition: 1D example

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



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

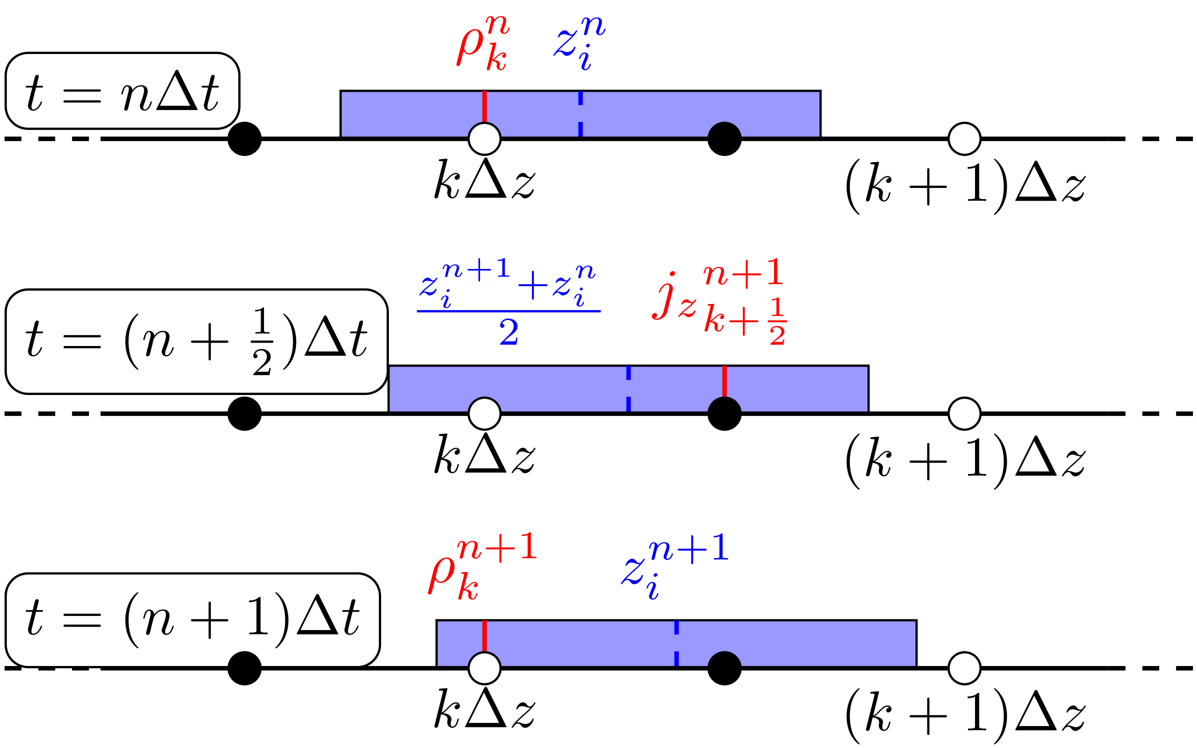
Direct current deposition and continuity equation

1D continuity equation

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

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:

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

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

Direct current deposition and continuity equation

Direct current deposition does not satisfy the continuity equation.

Reminder:
Updating $\boldsymbol{E}$ with the discretized Maxwell-Ampère equation preserves

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

provided that the continuity equation is satisfied at each iteration.

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

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

Two alternative solutions:

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

Boris correction

Boris correction

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

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

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

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

Practical implementation

The discretized version of

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

needs to be solved on the grid at each iteration, so as to obtain $\delta\phi$.
$\rightarrow$ Can be done using techniques from electrostatic PIC (see previous lecture), e.g. direct matrix, spectral or relaxation methods

Charge-conserving deposition

Charge-conserving deposition

The current $\boldsymbol{j}$ 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

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

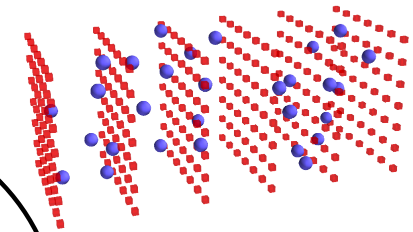
The Boris correction is not needed.

Summary

Update $\boldsymbol{x}_i$ and $\boldsymbol{p}_i$

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

$$\frac{d\boldsymbol{p}_i}{dt} = q\left(\boldsymbol{E} + \boldsymbol{v}_i \times \boldsymbol{B}\right)$$



Calculate $\rho, \boldsymbol{j}$ from the $\boldsymbol{x}_i, \boldsymbol{v}_i$ (either direct or charge-conservings)

Update $\boldsymbol{E}, \boldsymbol{B}$ using $\boldsymbol{j}$

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

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

then apply Boris correction using ρ (if needed)

Interpolate $\boldsymbol{E}, \boldsymbol{B}$ on the $\boldsymbol{x}_i$ (average $\boldsymbol{B}$ in time)

References

Esirkepov, T. (2001). Exact charge conservation scheme for particle-in-cell simulation with an arbitrary form-factor. *Computer Physics Communications*, 135(2):144 – 153.

Umeda, T., Omura, Y., Tominaga, T., and Matsumoto, H. (2003). A new charge conservation method in electromagnetic particle-in-cell simulations. *Computer Physics Communications*, 156(1):73 – 85.

Yee, K. (1966). Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media. *Antennas and Propagation, IEEE Transactions on*, 14(3):302 –307.