Smilei) workshop 2023

PIC basics

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What is a PIC code supposed to do?

- Simulate a plasma with kinetic effects (not hydrodynamics)
- Neglect particle-particle interactions (collisions)
- Electromagnetic effects

Distribution function $f_s(t, \mathbf{x}, \mathbf{p})$

Boltzmann Vlasov equation

$$\partial_t f_s + \mathbf{v} \cdot \nabla f_s + \overset{\text{Mean force}}{\mathbf{F}} \cdot \nabla_p \overset{\text{Mean distribution}}{f_s} = \cancel{(\partial_t f_s)_{\text{collisions}}}$$

Maxwell equations

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \qquad \partial_t \mathbf{E} = -\frac{1}{\epsilon_0}\mathbf{J} + c^2 \nabla \times \mathbf{B}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

The Maxwell-Vlasov system

Particles (Vlasov)

$$\partial_t f_s + \mathbf{v} \cdot \nabla f_s + \mathbf{F} \cdot \nabla_p f_s = 0$$

Current & density

$$\rho(t, \mathbf{x}) = \int d^3\mathbf{p} \; f_s(t, \mathbf{x}, \mathbf{p})$$

$$\mathbf{J}(t, \mathbf{x}) = q_s \int d^3\mathbf{p} \;\; \mathbf{v} \; f_s(t, \mathbf{x}, \mathbf{p})$$

Fields (Maxwell)

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \qquad \partial_t \mathbf{E} = -\frac{1}{\epsilon_0}\mathbf{J} + c^2 \nabla \times \mathbf{B}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Lorentz Force

$$\mathbf{F}_L = q_s \left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)$$

Units

There is a natural set of units

Velocity	c
Charge	e
Mass	m_e
Momentum	$m_e c$
Energy, Temperature	$m_e c^2$

ω_r is the **reference angular frequency.**
The code does not need to know its value.
Results of the simulation can be scaled *a posteriori.*

Maxwell equations

$$\nabla \cdot \mathbf{E} = \rho \qquad \partial_t \mathbf{E} = -\mathbf{J} + \nabla \times \mathbf{B}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

The units of density n_r
is not equal to $(c/\omega_r)^{-3}$

How to choose ω_r ?

ω_r is generally an important frequency of the problem

- laser frequency (in this case, $n_r = n_c$)
- plasma frequency (in this case, $n_r = n$)
- cyclotron frequency (in this case, $B_r = B/\gamma$)

Again, the code does not need to know its value

(unless you need collisions, ionization, …)

The Maxwell-Vlasov system

Particles (Vlasov)

$$\partial_t f_s + \mathbf{v}\cdot\nabla f_s + \mathbf{F}\cdot\nabla_p f_s = 0$$

Current & density

$$\rho(t,\mathbf{x}) = \int d^3\mathbf{p}\ f_s(t,\mathbf{x},\mathbf{p})$$

$$\mathbf{J}(t,\mathbf{x}) = q_s \int d^3\mathbf{p}\ \ \mathbf{v}\ f_s(t,\mathbf{x},\mathbf{p})$$

Fields (Maxwell)

$$\nabla\cdot\mathbf{E} = \rho \qquad \partial_t\mathbf{E} = -\mathbf{J} + \nabla\times\mathbf{B}$$

$$\nabla\cdot\mathbf{B} = 0 \qquad \partial_t\mathbf{B} = -\nabla\times\mathbf{E}$$

Lorentz Force

$$\mathbf{F}_L = q_s\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right)$$

Solving Maxwell

We need only 2 of Maxwell's equations

Maxwell-Ampere

$$\partial_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}$$

divergence

$$\partial_t \, \nabla \cdot \mathbf{E} + \nabla \cdot \mathbf{J} = 0$$

Conservation of charge $\partial_t \rho + \nabla \cdot \mathbf{J} = 0$

$$\partial_t \left(\nabla \cdot \mathbf{E} - \rho \right) = 0$$

Maxwell-Poisson is conserved

Maxwell-Faraday

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

divergence

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

Maxwell-Gauss is conserved

We do not need to solve Maxwell-Poisson and Maxwell-Gauss,
(provided they are satisfied initially)

Towards the PIC loop

Particles (Vlasov)

$$\partial_t f_s + \mathbf{v} \cdot \nabla f_s + \mathbf{F} \cdot \nabla_p f_s = 0$$

Current

$$\mathbf{J}(t, \mathbf{x}) = q_s \int d^3\mathbf{p} \;\; \mathbf{v} \; f_s(t, \mathbf{x}, \mathbf{p})$$

Fields (Maxwell)

$$\partial_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Lorentz Force

$$\mathbf{F}_L = q_s \left(\mathbf{E} + \mathbf{v} \times \mathbf{B} \right)$$

The fields are defined on a grid

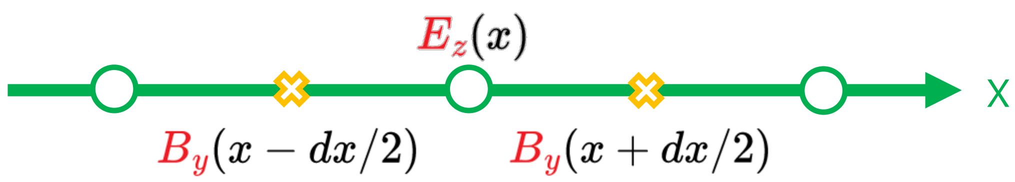
There are several ways to solve Maxwell on a grid.
Let us illustrate with the most common technique
"*Finite Difference Time Domain*" (FDTD)

Maxwell-Ampere in 1D:

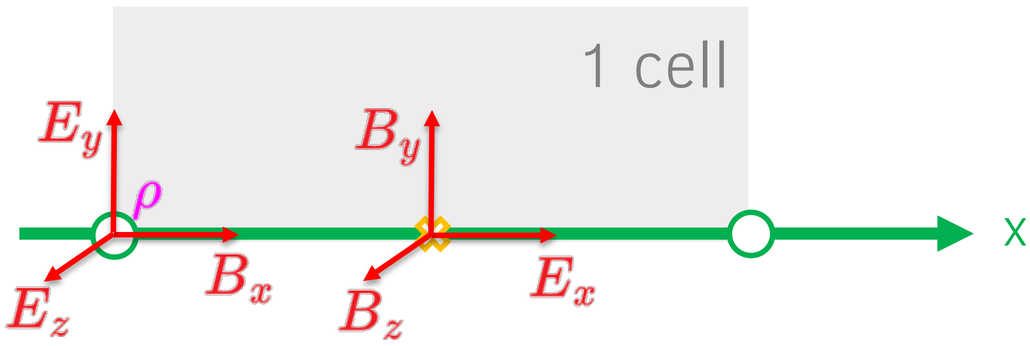
$$\partial_t E_z = \partial_x B_y - J_z \Rightarrow (\partial_t E_z)(x) = (\partial_x B_y)(x) - J_z(x)$$

$$\Rightarrow \partial_t \, E_z(x) = \frac{B_y(x+\Delta x/2) - B_y(x-\Delta x/2)}{\Delta x} - J_z(x)$$

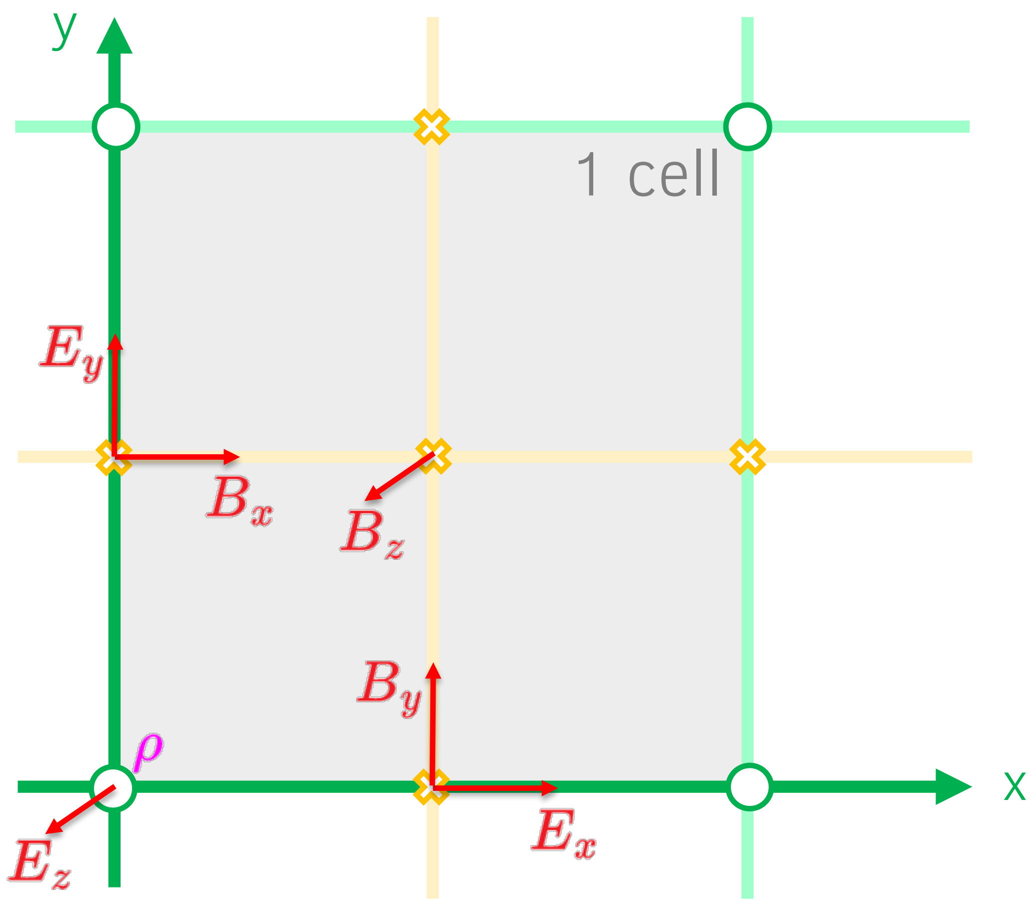
offset in space



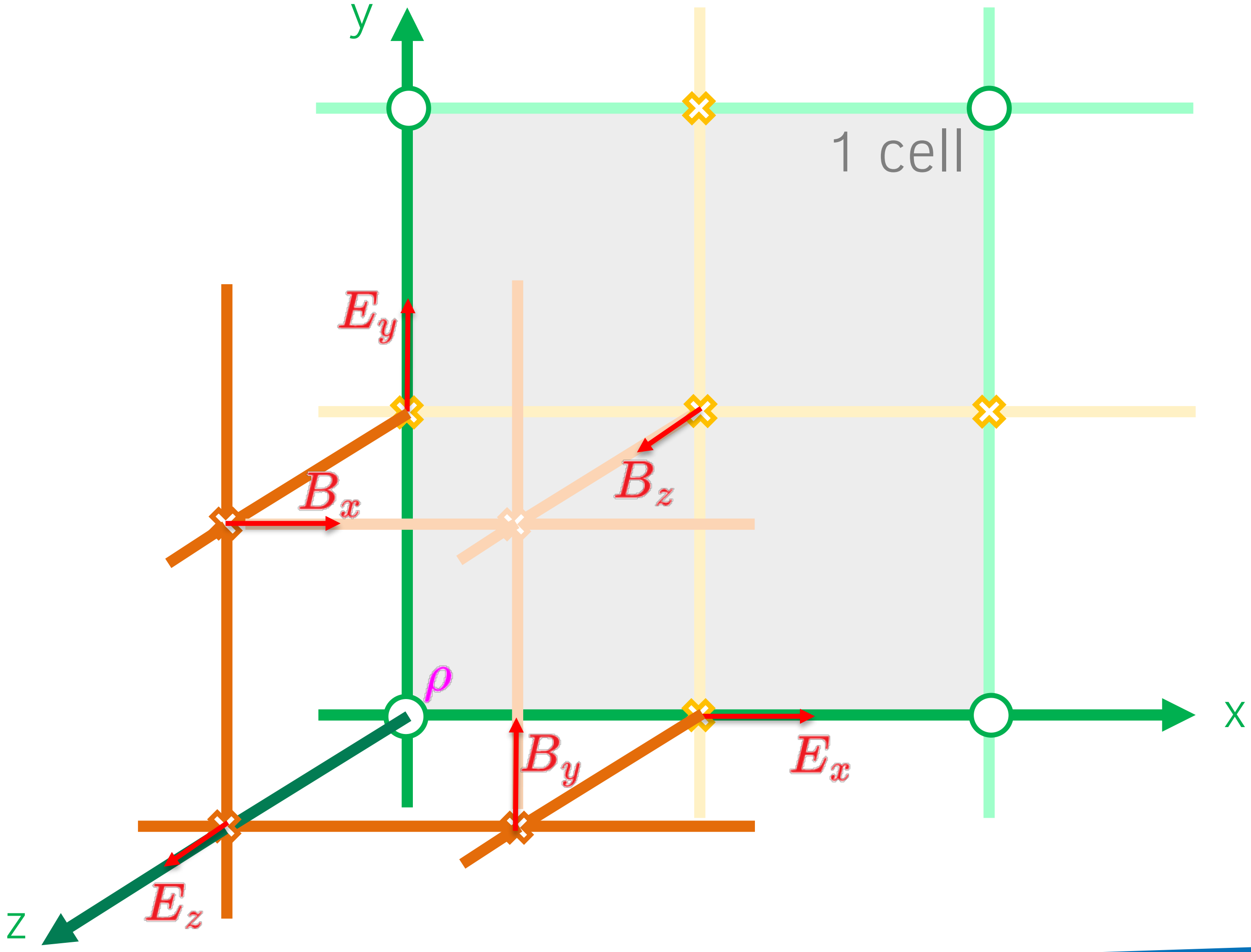
The grid is “staggered”: *Yee’s grid*



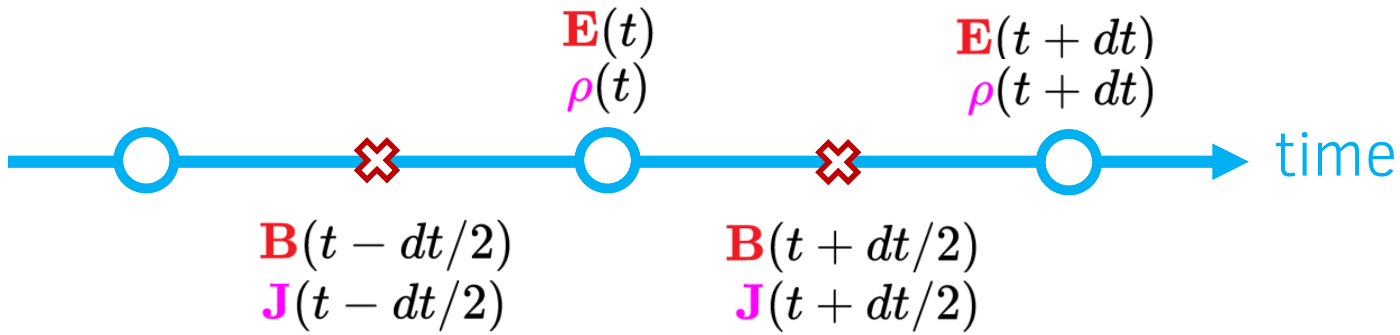
The grid is "staggered": *Yee's grid*



The grid is "staggered": *Yee's grid*



The grid is also staggered in time!



"Leap-frog" scheme

Towards the PIC loop

Particles (Vlasov)

$$\partial_t f_s + \mathbf{v} \cdot \nabla f_s + \mathbf{F} \cdot \nabla_p f_s = 0$$

Current

$$\mathbf{J}(t, \mathbf{x}) = q_s \int d^3\mathbf{p} \;\; \mathbf{v} \; f_s(t, \mathbf{x}, \mathbf{p})$$

Fields (Maxwell)

$$\partial_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Lorentz Force

$$\mathbf{F}_L = q_s \left(\mathbf{E} + \mathbf{v} \times \mathbf{B} \right)$$

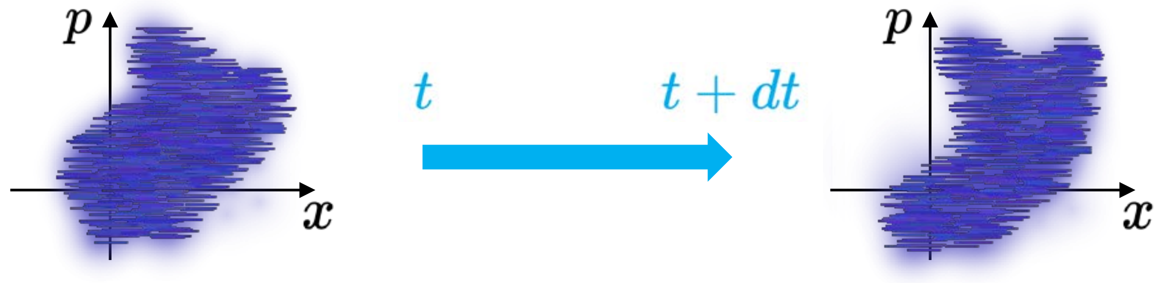
Solving Vlasov

A simplified distribution function

Vlasov = partial differential equation in a 6D space.

$$\partial_t f_s + \mathbf{v} \cdot \nabla f_s + \mathbf{F} \cdot \nabla_p f_s = 0$$

Direct integration (*Vlasov codes*) has a tremendous computational cost.



In a PIC code, the distribution function is approximated as a sum over macro-particles

$$f_s(t, \mathbf{x}, \mathbf{p}) = \sum_{p=1}^{N} w_p \, S(\mathbf{x} - \mathbf{x}_p(t)) \, \delta(\mathbf{p} - \mathbf{p}_p(t))$$

Statistical weight

Shape function

From Vlasov to the macro-particle motion

$$f_s(t,\mathbf{x},\mathbf{p}) = \sum_{p=1}^{N} w_p\, S(\mathbf{x}-\mathbf{x}_p(t))\,\delta(\mathbf{p}-\mathbf{p}_p(t)) \qquad \& \qquad \partial_t f_s + \mathbf{v}\cdot\nabla f_s + \mathbf{F}\cdot\nabla_p f_s = 0$$

Integrate over $\boldsymbol{p}$ $\rightarrow$ $\partial_t \mathbf{x}_p = \mathbf{v}_p$

Multiply by $\boldsymbol{p}$ then integrate over $\boldsymbol{p}$ and $\boldsymbol{x}$ $\rightarrow$ $\partial_t \mathbf{p}_p = q_s\,\mathbf{E}_p + q_s\,\mathbf{v}_p \times \mathbf{B}_p$

The movement of macro-particles is essentially that of real particles

But …
$$\begin{cases} \mathbf{E}_p = \int \mathbf{E}(\mathbf{x})\, S(\mathbf{x}-\mathbf{x}_p)\, d^3\mathbf{x} \\ \mathbf{B}_p = \int \mathbf{B}(\mathbf{x})\, S(\mathbf{x}-\mathbf{x}_p)\, d^3\mathbf{x} \end{cases}$$

The fields are “averaged” around the particle position.

We have discovered pusher & interpolation !

Pusher

= macro-particle motion

$$\begin{cases} \partial_t \mathbf{x}_p = \mathbf{v}_p \\ \partial_t \mathbf{p}_p = q_s\, \mathbf{E}_p + q_s\, \mathbf{v}_p \times \mathbf{B}_p \end{cases}$$

Field interpolation

= calculate fields at macro-particle location

$$\begin{cases} \mathbf{E}_p = \int \mathbf{E}(\mathbf{x})\, S(\mathbf{x} - \mathbf{x}_p)\, d^3\mathbf{x} \\ \mathbf{B}_p = \int \mathbf{B}(\mathbf{x})\, S(\mathbf{x} - \mathbf{x}_p)\, d^3\mathbf{x} \end{cases}$$

Towards the PIC loop

Particle pusher

$$\partial_t \mathbf{x}_p = \mathbf{v}_p$$

$$\partial_t \mathbf{p}_p = q_s\, \mathbf{E}_p + q_s\, \mathbf{v}_p \times \mathbf{B}_p$$

Current

$$\mathbf{J}(t,\mathbf{x}) = q_s \int d^3\mathbf{p}\ \ \mathbf{v}\ f_s(t,\mathbf{x},\mathbf{p})$$

Fields (Maxwell)

$$\partial_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Field interpolation

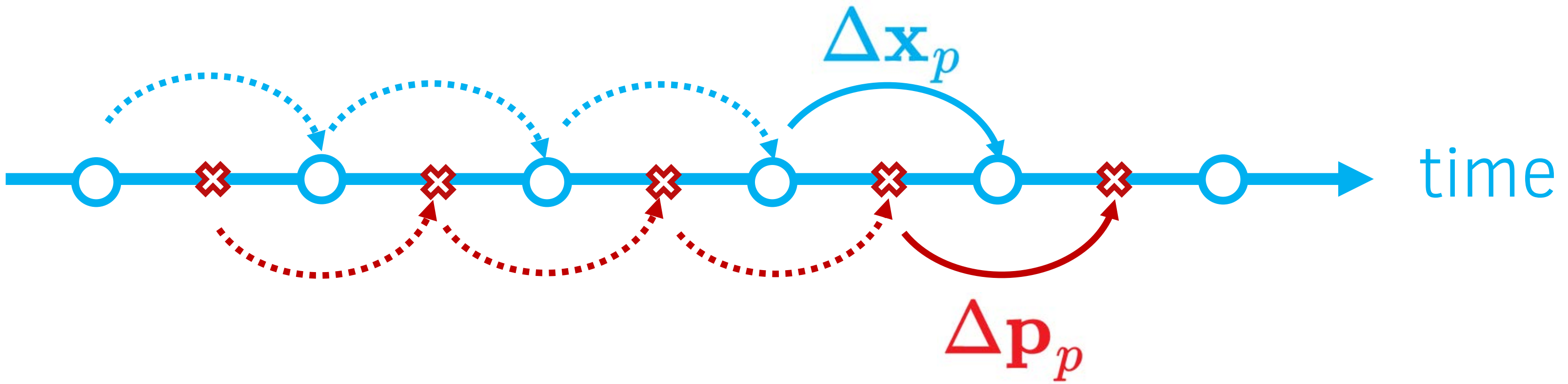
$$\mathbf{E}_p = \int \mathbf{E}(\mathbf{x})\, S(\mathbf{x}-\mathbf{x}_p)\, d^3\mathbf{x}$$

$$\mathbf{B}_p = \int \mathbf{B}(\mathbf{x})\, S(\mathbf{x}-\mathbf{x}_p)\, d^3\mathbf{x}$$

A few details about the **pusher**

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p \quad \Longrightarrow \quad \mathbf{x}_p^{n+1} - \mathbf{x}_p^{n} = \mathbf{v}_p^{n+1/2}\Delta t$$

$$\frac{d\mathbf{p}_p}{dt} = \mathbf{F}_p \quad \Longrightarrow \quad \mathbf{p}_p^{n+1/2} - \mathbf{p}_p^{n-1/2} = \mathbf{F}_p^{n}\Delta t$$

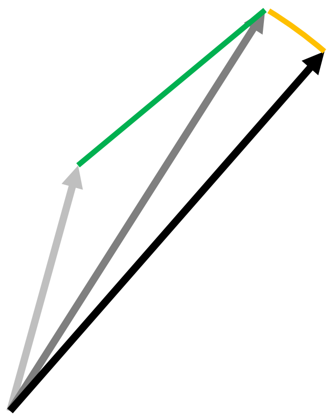


“Leap-frog” scheme

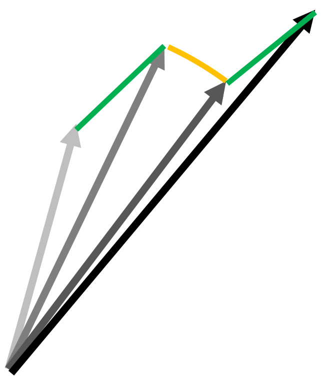
A few details about the pusher

$$\frac{d\mathbf{p}_p}{dt} = q_s \mathbf{E}_p + q_s \mathbf{v}_p \times \mathbf{B}_p$$

addition + rotation



Naïve method

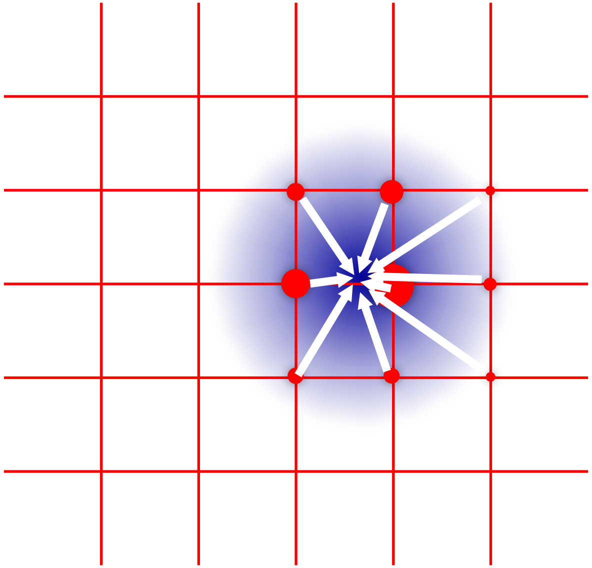


Boris’ method
(more accurate)

A few details about the **interpolation**

Fields have values on grid points

$$\begin{cases} \mathbf{E}_p = \int \mathbf{E}(\mathbf{x}) S^{(m)}(\mathbf{x}_i - \mathbf{x}_p) \\ \mathbf{B}_p = \int \mathbf{B}(\mathbf{x}) S^{(m)}(\mathbf{x}_i - \mathbf{x}_p) \end{cases} \Rightarrow \begin{cases} \mathbf{E}_p = \sum_{i \in S} \mathbf{E}(\mathbf{x}_i) S^{(m+1)}(\mathbf{x}_i - \mathbf{x}_p) \\ \mathbf{B}_p = \sum_{i \in S} \mathbf{B}(\mathbf{x}_i) S^{(m+1)}(\mathbf{x}_i - \mathbf{x}_p) \end{cases}$$



Each grid point surrounding the macro-particle contributes to the field it sees

Towards the PIC loop

Particle pusher

$$\partial_t \mathbf{x}_p = \mathbf{v}_p$$

$$\partial_t \mathbf{p}_p = q_s\, \mathbf{E}_p + q_s\, \mathbf{v}_p \times \mathbf{B}_p$$

Current

$$\mathbf{J}(t, \mathbf{x}) = q_s \int d^3\mathbf{p} \;\; \mathbf{v} \;\; f_s(t, \mathbf{x}, \mathbf{p})$$

Fields (Maxwell)

$$\partial_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Field interpolation

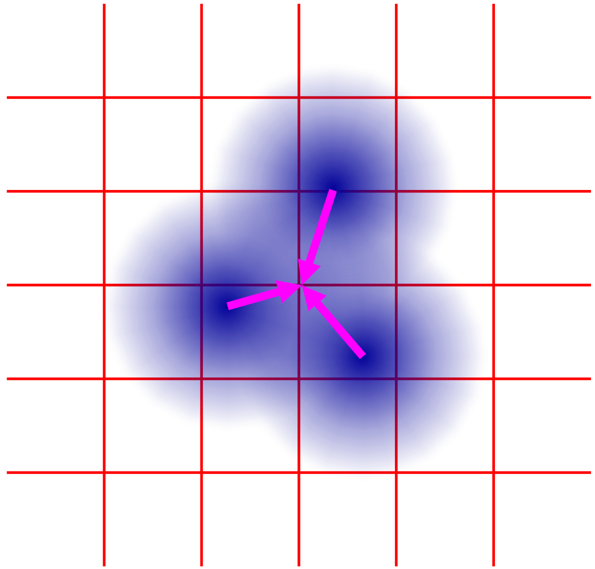
$$\mathbf{E}_p = \sum_{i \in S} \mathbf{E}(\mathbf{x}_i)\; S(\mathbf{x}_i - \mathbf{x}_p)$$

$$\mathbf{B}_p = \sum_{i \in S} \mathbf{B}(\mathbf{x}_i)\; S(\mathbf{x}_i - \mathbf{x}_p)$$

Calculate the current

Calculate the current "directly"

$$\begin{cases} f_s(t,\mathbf{x},\mathbf{p}) = \sum_{p=1}^{N} w_p\, S(\mathbf{x}-\mathbf{x}_p(t))\,\delta(\mathbf{p}-\mathbf{p}_p(t)) \\ \mathbf{J}(t,\mathbf{x}) = q_s \int d^3\mathbf{p}\;\; \mathbf{v}\; f_s(t,\mathbf{x},\mathbf{p}) \end{cases} \Rightarrow \quad \mathbf{J}(\mathbf{x}_i) = \sum_{\text{particles}} q_s w_p\; \mathbf{v}_p\; S(\mathbf{x}_i - \mathbf{x}_p)$$



macro-particles surrounding a grid point "deposit" their current

Unfortunately, this does not satisfy the charge-conservation equation

Forcing charge conservation

$$
\begin{cases}
f_s(t,\mathbf{x},\mathbf{p}) = \sum_{p=1}^{N} w_p\, S(\mathbf{x}-\mathbf{x}_p(t))\,\delta(\mathbf{p}-\mathbf{p}_p(t)) \\
\rho(t,\mathbf{x}) = \int d^3\mathbf{p}\ f_s(t,\mathbf{x},\mathbf{p}) \\
\partial_t\rho + \nabla\cdot\mathbf{J} = 0
\end{cases}
$$

$$\Rightarrow \quad \mathbf{J}(\mathbf{x}_i + d\mathbf{x}/2) - \mathbf{J}(\mathbf{x}_i - d\mathbf{x}/2) = \ \ldots$$

Esirkepov's method

The PIC loop … at last !

Particle pusher

$$\partial_t \mathbf{x}_p = \mathbf{v}_p$$

$$\partial_t \mathbf{p}_p = q_s\, \mathbf{E}_p + q_s\, \mathbf{v}_p \times \mathbf{B}_p$$

Current deposition

$$\mathbf{J}(\mathbf{x}_i + d\mathbf{x}/2) - \mathbf{J}(\mathbf{x}_i - d\mathbf{x}/2) = \ \ldots$$

Fields (Maxwell)

$$\partial_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Field interpolation

$$\mathbf{E}_p = \sum_{i \in S} \mathbf{E}(\mathbf{x}_i)\ S(\mathbf{x}_i - \mathbf{x}_p)$$

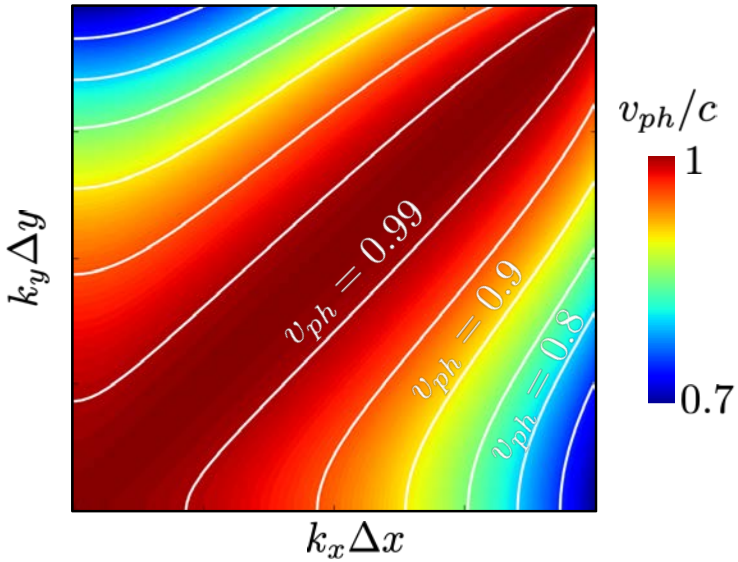
$$\mathbf{B}_p = \sum_{i \in S} \mathbf{B}(\mathbf{x}_i)\ S(\mathbf{x}_i - \mathbf{x}_p)$$

Limitations

The numerical vacuum is dispersive and anisotropic !

FDTD equations + search for wave-like solutions

Dispersion relation $\Delta t^{-2} \sin^2(\omega \Delta t/2) = \sum_{a=x,y,z} \Delta a^{-2} \sin^2(k_a \Delta a/2)$



Dispersive

Numerical Cherenkov radiation

The timestep cannot be too large

From the dispersion relation, one can show that **stability requires**:

$$\Delta t^{-2} > \sum_{a=x,y,z} \Delta a^{-2}$$

$$\Delta t < \left(\sum_{a=x,y,z} \Delta a^{-2} \right)^{-1/2}$$

Courant-Friedrich-Levy (CFL) condition

The cell size cannot be too large either

Depending on the situation you may need to resolve:

- ✓ The **Debye length** (or the simulation will have numerical heating)
- ✓ The **laser wavelength** (or it won't propagate)
- ✓ The **skin depth**

Often, a PIC simulation won't crash when the results are meaningless.
Users must understand the limitations and test.

Thank you for your attention!

Particle pusher

$$\partial_t \mathbf{x}_p = \mathbf{v}_p$$

$$\partial_t \mathbf{p}_p = q_s\, \mathbf{E}_p + q_s\, \mathbf{v}_p \times \mathbf{B}_p$$

Current deposition

$$\mathbf{J}(\mathbf{x}_i + d\mathbf{x}/2) - \mathbf{J}(\mathbf{x}_i - d\mathbf{x}/2) = \ \dots$$

Fields (Maxwell)

$$\partial_t \mathbf{E} = \nabla \times \mathbf{B} - \mathbf{J}$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

Field interpolation

$$\mathbf{E}_p = \sum_{i \in S} \mathbf{E}(\mathbf{x}_i)\ S(\mathbf{x}_i - \mathbf{x}_p)$$

$$\mathbf{B}_p = \sum_{i \in S} \mathbf{B}(\mathbf{x}_i)\ S(\mathbf{x}_i - \mathbf{x}_p)$$

Thanks & Keep Smileing!

Thanks for supporting this event

Contributing labs, institutions & funding agencies