
Particle-in-cell simulations

Part I: Numerical methods

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Plan of the lectures

- **Monday:**

- *Morning*: The PIC method, numerical schemes and main algorithms.
- *Afternoon*: Coding practice of the Boris push and the Yee algorithm.

- **Tuesday:**

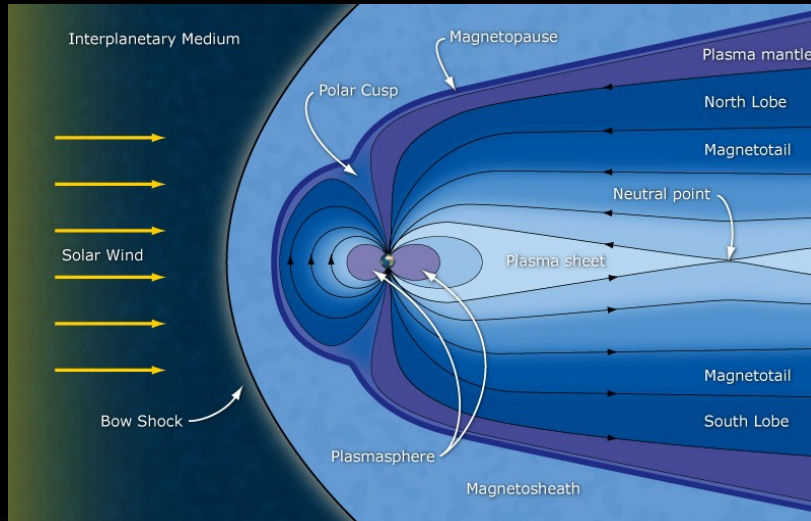
- *Morning*: Implementation of Zeltron, structure and methods.
- *Afternoon*: Zeltron hands on relativistic reconnection simulations
- *Evening*: Seminar about application of PIC to pulsar magnetospheres.

- **Wednesday:**

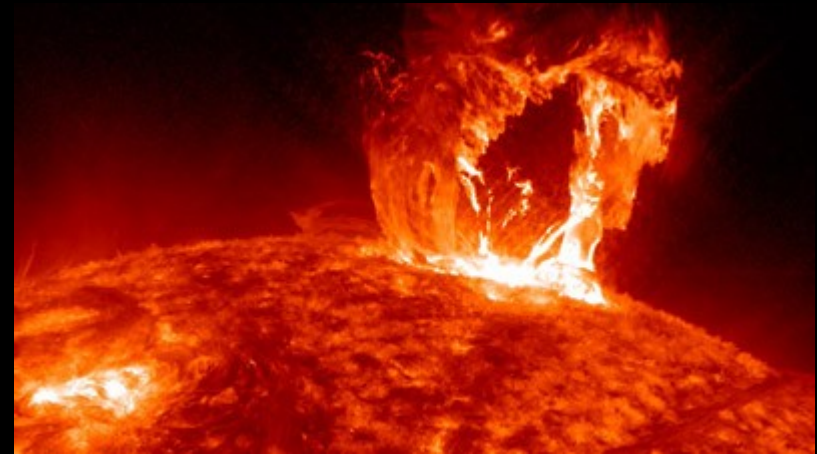
- *Morning*: Boundary conditions and parallelization in Zeltron.
- *Afternoon*: Zeltron Hands on relativistic collisionless shocks simulations

Astrophysical context

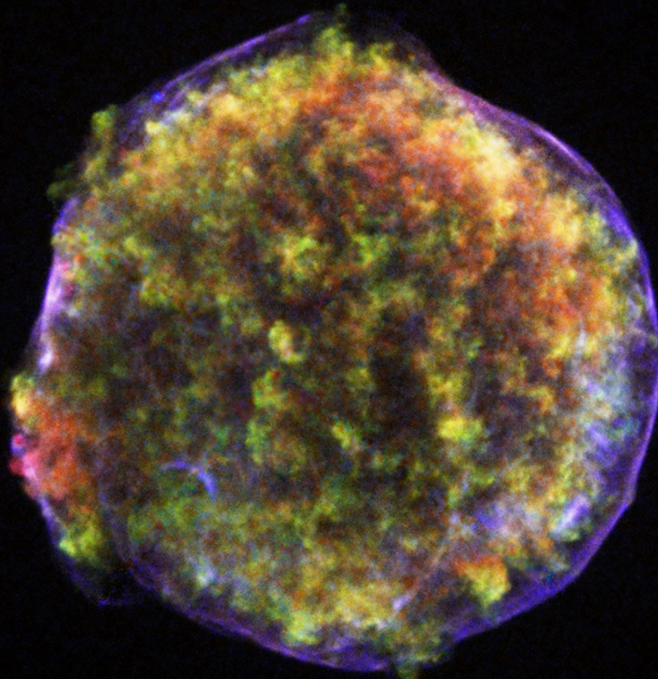
Planetary magnetospheres



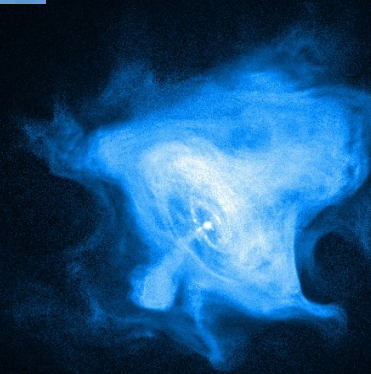
Solar corona & wind, heliosphere



Supernova Remnants



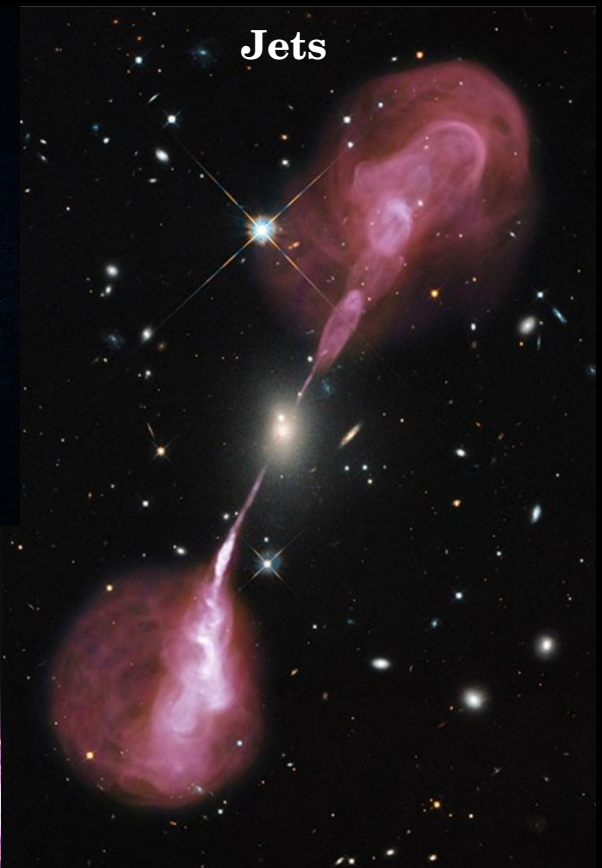
Pulsar Wind Nebulae



Gamma-ray bursts

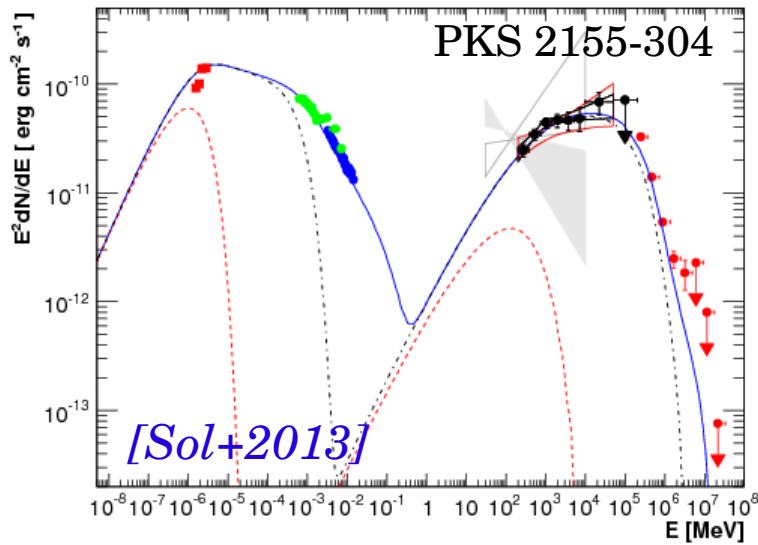


Jets

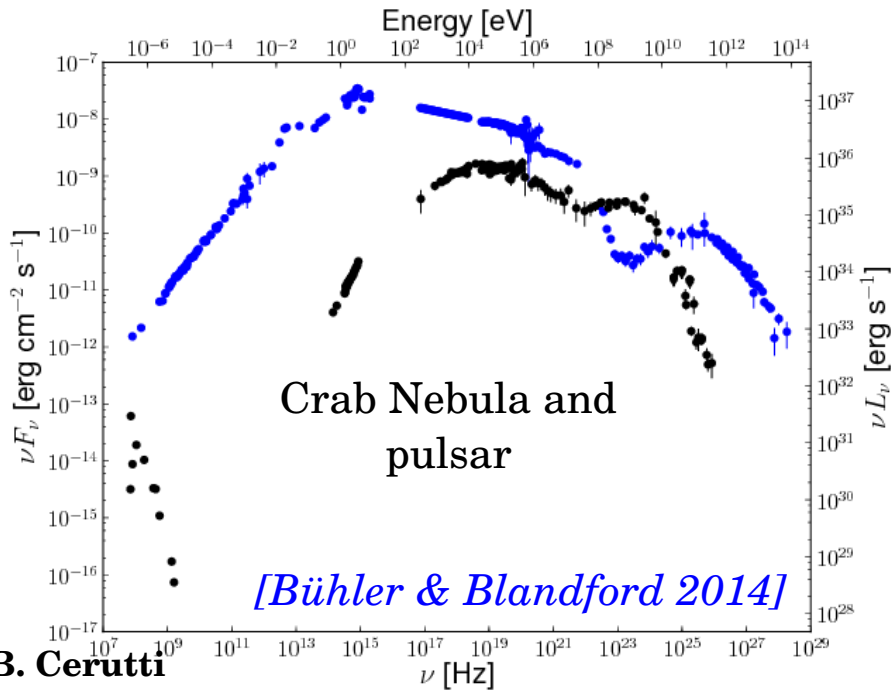


Broad non-thermal distributions

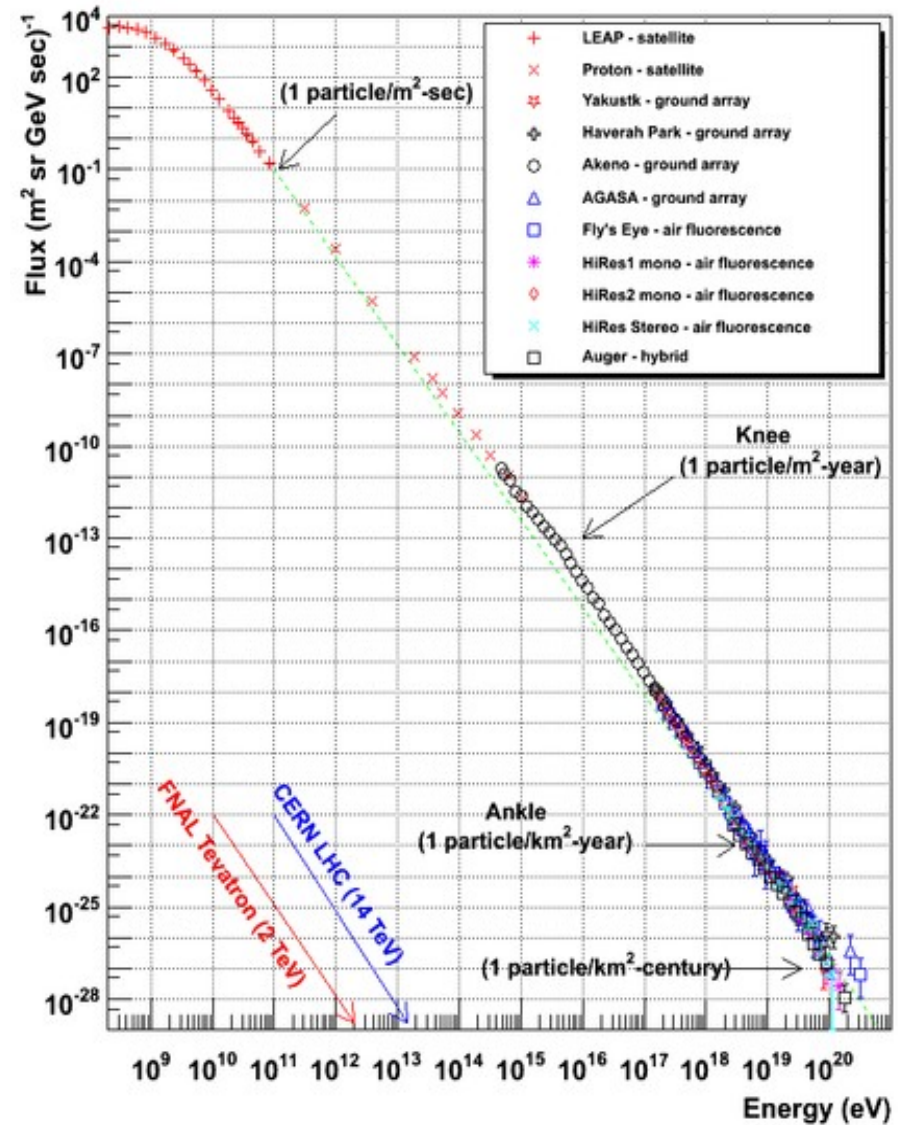
Blazars



Pulsars & Pulsar Wind Nebulae



Cosmic Ray Spectra of Various Experiments

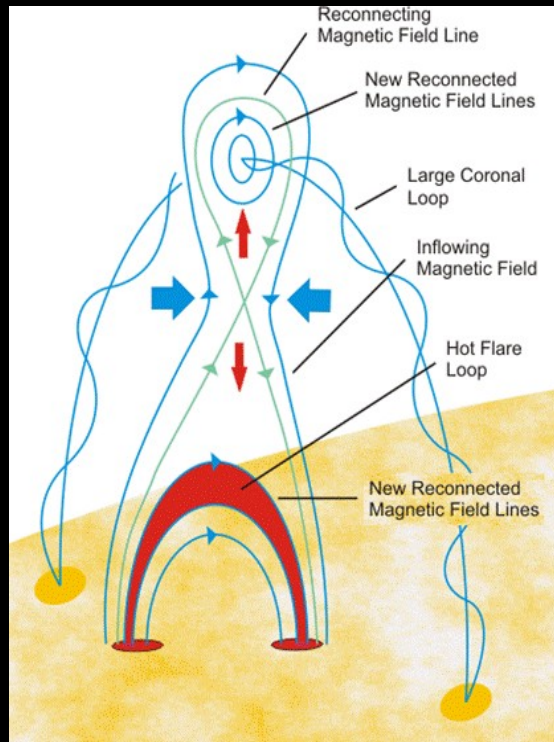


[<http://www.physics.utah.edu/~whanlon/spectrum.html>]

Particle acceleration processes

Magnetic reconnection

Magnetic energy => Particles

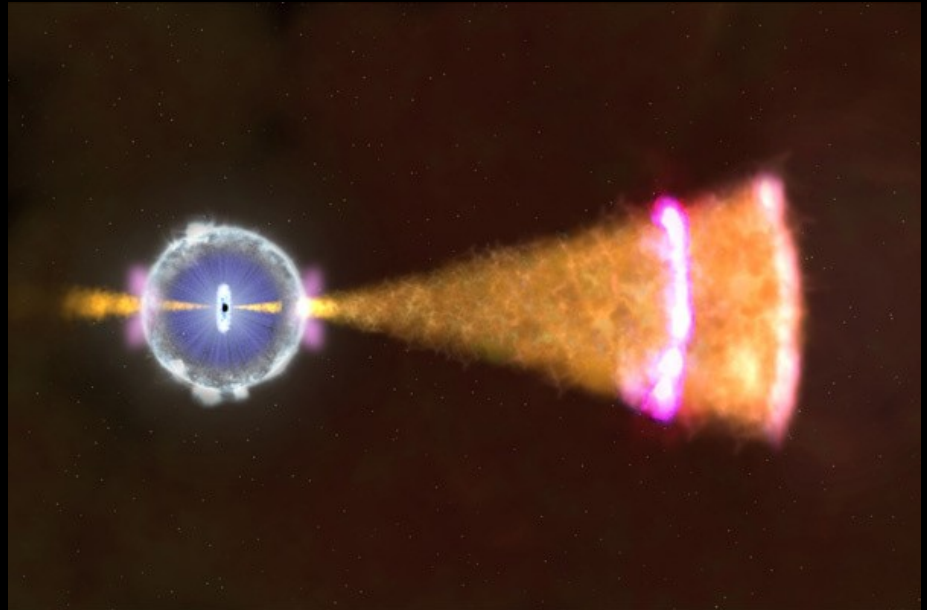


Accretion disk coronae,
magnetars, pulsars, jets, GRBs

Hands on **session II** on
Tuesday afternoon

Shocks

Flow kinetic energy => Particles



GRBs, SNRs, PWNe, jets...

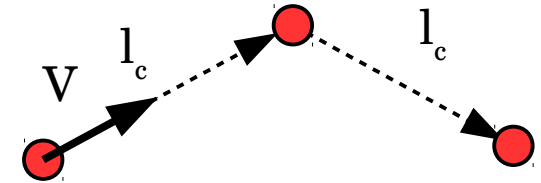
Hands on **session III** on
Wednesday afternoon

Collisionless plasmas

Collisions thermalizes efficiently the particle distribution, **not good for non-thermal** distributions. In most astrophysical environments, plasmas are **very dilute** so that they are effectively “**collisionless**”.

Coulomb collisions **mean free path**: $l_C = \frac{1}{n\sigma_C}$

Frequency of collisions $\nu = \frac{V}{l_C}$



Collisionless plasma if the plasma frequency $\omega_{pe} \gg \nu$

It also implies that there is a large number of particles per **Debye sphere**:

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

Particles sensitive to **collective plasma phenomena** over binary collisions, particularly important on the **sub-Debye length** and **plasma frequency scales** (plasma frequency and gyroradius).

These microscopic scales are involved in particle acceleration process. **Need to resolve kinetic scales** (\neq MHD approach), and system size $L \gg \lambda_D$

The particle distribution function

Let's start by defining the particle distribution function:

$$f(\mathbf{r}, \mathbf{p}, t) = \frac{dN}{d\mathbf{r} d\mathbf{p}} \quad \mathbf{6D} \text{ in phase space} + \mathbf{1D} \text{ in time}$$

The **total number** of particles is given by: $N = \iint_{\mathbf{r}, \mathbf{p}} f(\mathbf{r}, \mathbf{p}, t) d\mathbf{r} d\mathbf{p}$

The plasma **charge density** by: $\rho = q \int_{\mathbf{p}} f(\mathbf{r}, \mathbf{p}, t) d\mathbf{p}$

The plasma **current density** by: $\mathbf{J} = q \int_{\mathbf{p}} \mathbf{v} f(\mathbf{r}, \mathbf{p}, t) d\mathbf{p}$

The Vlasov equation

The evolution of distribution function is given by the **Boltzmann equation**:

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{\gamma m} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left(\frac{\partial f}{\partial t} \right)_{\text{Collisions}}$$

For a **collisionless** plasma: $\left(\frac{\partial f}{\partial t} \right)_{\text{Collisions}} = 0$

And if the fluid feels only the **electromagnetic force**: $\mathbf{F} = q \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right)$

We obtain the **Vlasov equation**:

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{\gamma m} \cdot \frac{\partial f}{\partial \mathbf{r}} + q \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$$

Along with **Maxwell equations**, we have all equations to model collisionless plasmas.

Two numerical approaches to solve Vlasov

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{\gamma m} \cdot \frac{\partial f}{\partial \mathbf{r}} + q \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$$

Ab-initio model, no approximations

Directly with a Vlasov-code

Treat phase space as a continuum fluid

Advantages:

- **No noise**, good if tail of f is important dynamically (steep power-law).
- No issue if plasma very **inhomogeneous**.
- **Weak** phenomena can be captured

Limitations:

- Problem **(6+1)D**, hard to fit in the memory, limited resolution.
- Filamentation of the phase space
But becoming more competitive, new development to come, stay tuned!

Not covered here

Indirectly with a PIC code

Sample phase space with particles

Advantages:

- Conceptually **simple**
- **Robust** and **easy to implement**.
- Easily **scalable** to large number of cores

Limitations:

- **Shot noise**, difficult to sample uniformly f ,
- Artificial collisions, requires many particles
- Hard to capture weak/subtle phenomenas
- Load-balancing issues

Main focus of this lecture

The particle approach

The Vlasov equation can be written in the form of **an advection equation**:

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{\gamma m} \cdot \frac{\partial f}{\partial \mathbf{r}} + q \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \cdot \frac{\partial f}{\partial \mathbf{p}} = 0 \quad \rightarrow \quad \frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{U}) = 0$$

Vlasov equation can be solved along **characteristics curves** along which it has the form of a set of ordinary differential equations (the method of characteristics):

$$\frac{d\mathbf{p}}{dt} = q \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \quad \text{Lorentz-Newton equation}$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}$$

The **characteristics curves** corresponds to the **trajectory** of individual particles!

Hence, we can **probe Vlasov equation by solving for the motion of particles**, the larger number, the better!

The particle approach

The particle approach consists in approximating the distribution function by an ensemble of discrete particles in phase space

$$f(\mathbf{r}, \mathbf{p}, t) \approx \sum_{k=1}^{N_p} w_k \delta(\mathbf{r} - \mathbf{r}_k(t)) \delta(\mathbf{p} - \mathbf{p}_k(t))$$

Dirac delta function

Weight particle k

Position and **momentum** particle k at time t

It is impossible to have as many particles as real plasmas
=> **Simulation particles are not physical particles.**

Instead, **they represent a large number of physical particles** which would all follow the same trajectory in phase space, with the same (q/m) ratio.

Simulation particles => **“Macroparticles”**

Then we have:

$$N \approx \sum_{k=1}^{N_p} w_k \quad \rho \approx \sum_{k=1}^{N_p} q_k w_k \delta(\mathbf{r} - \mathbf{r}_k(t)) \quad \mathbf{J} = \sum_{k=1}^{N_p} q_k w_k \mathbf{v}_k \delta(\mathbf{r} - \mathbf{r}_k(t))$$

The Particle-In-Cell (PIC) approach

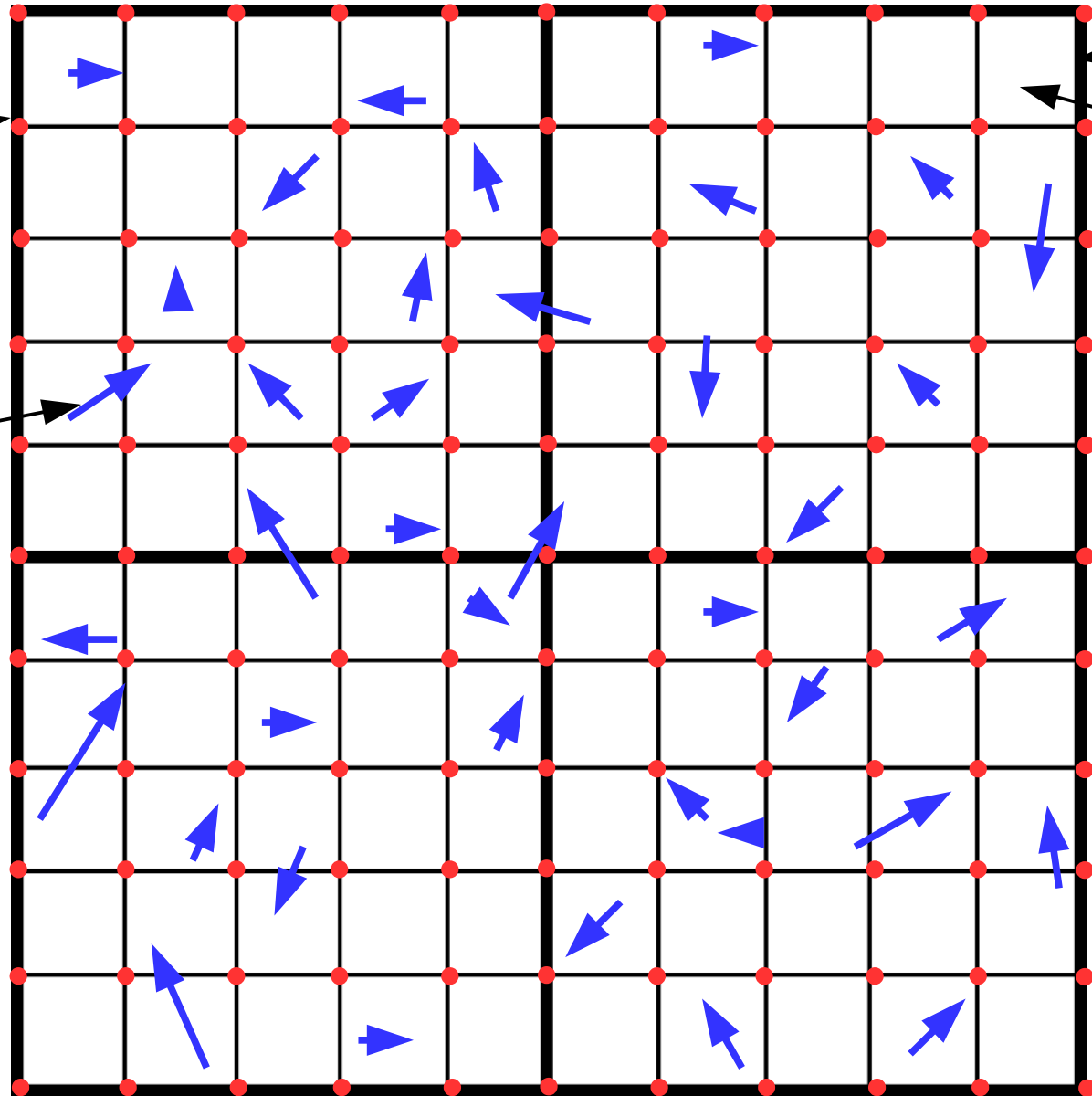
Computational domain

y

(E,B) fields known
on the grid
(Eulerian approach)

Particles evolve in
continuous space
(Lagrangian approach)

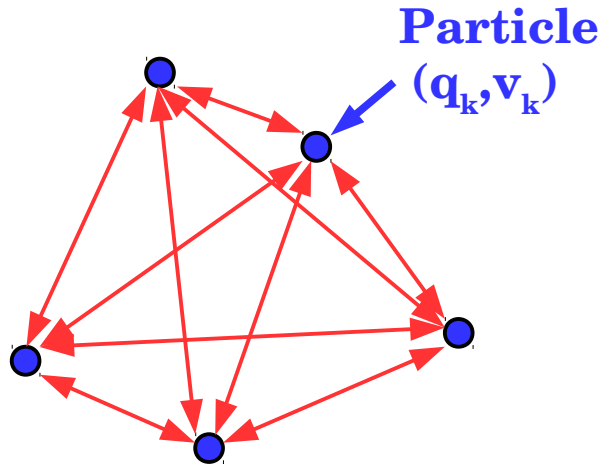
Grid
Cell



The Particle-In-Cell (PIC) approach

In the PIC approach, the particles do not feel the fields of all the other particles directly. **The particles feel each other through the grid**, via their contribution to the current and charge densities that is deposited on the grid.

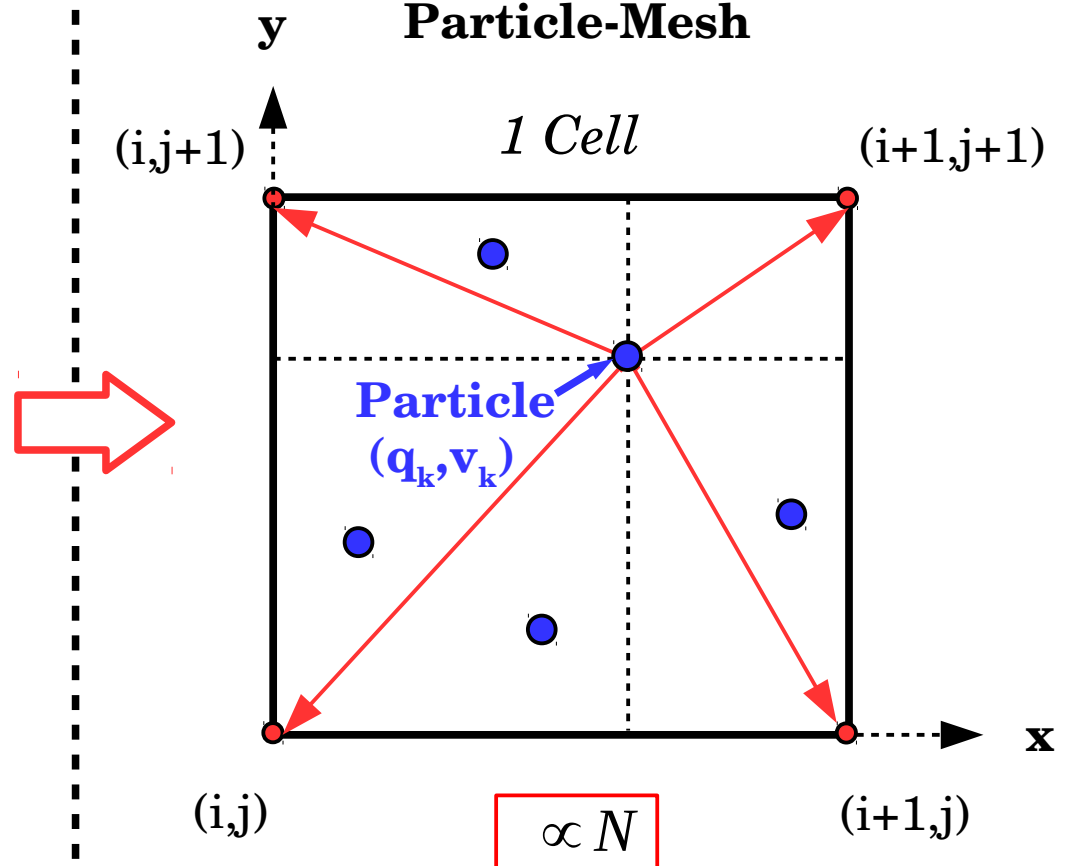
Particle-Particle



Number of pairs: $\frac{N(N-1)}{2} \propto N^2$

Caveats: **Very expansive**, long-range
Instantaneous interaction?!

Particle-Mesh



Much cheaper! Propagation of light
naturally present via CFL condition

Computation procedure per timestep in PIC

Step 1

Solve Newton's equation

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

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

$$\frac{\partial \mathbf{E}}{\partial t} = c \nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

$\Delta \mathbf{t}$

Solve Maxwell's equations (E,B)

Step 3

Deposit Charge and current densities (ρ, \mathbf{J})

Step 2

Computation procedure per timestep in PIC

Step 1

Solve Newton's equation

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

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

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Step 3

Solve Maxwell's equations (E,B)

Δt

Deposit
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Step 2

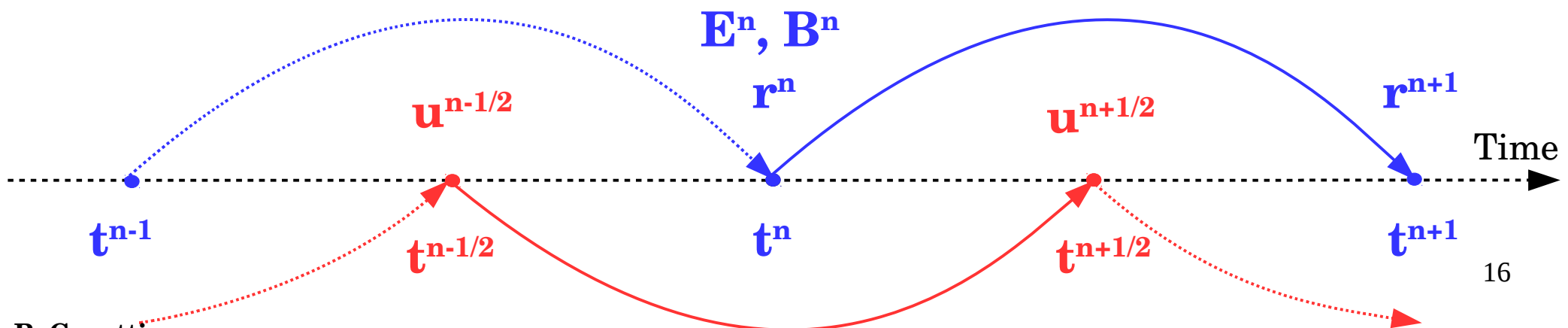
Step 1: Particle push

$$\frac{d\mathbf{p}}{dt} = q \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \longrightarrow \frac{d\mathbf{u}}{dt} = \frac{q}{mc} \left(\mathbf{E} + \frac{\mathbf{u} \times \mathbf{B}}{\gamma} \right) \quad \text{Where } \begin{cases} \gamma = \frac{1}{\sqrt{1 - (\mathbf{v}/c)^2}} \\ \mathbf{u} = \frac{\gamma \mathbf{v}}{c} \quad (\text{4-velocity}) \end{cases}$$

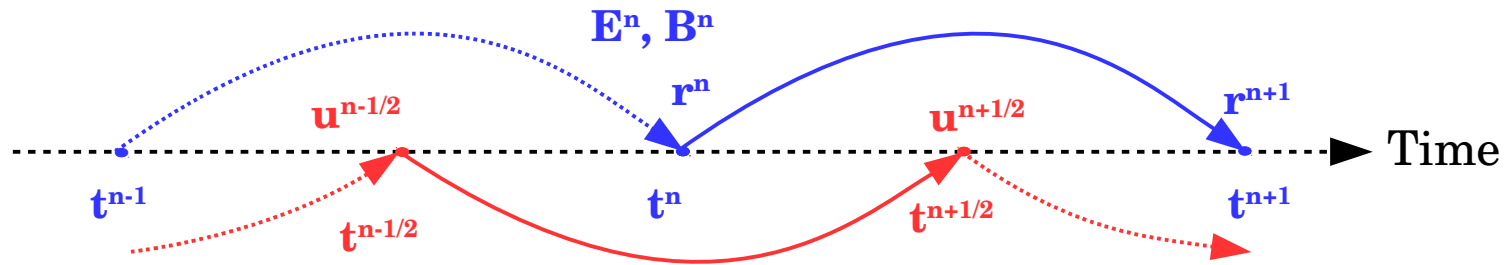
$$\frac{d\mathbf{r}}{dt} = \frac{c\mathbf{u}}{\gamma}$$

Explicit **time-centered**, finite-difference scheme (leapfrog integration method):

- \mathbf{u} and \mathbf{r} are **staggered in time** by half a time step
- **Second order** accurate but requires only to evaluate function at one time step only (fast and no extra memory needed)
- **Stable** for oscillatory motion (gyromotion) as long as $\Delta t < \Delta t_{\text{CFL}}$ (see later)
- Time-reversal and **conserves well energy**
- Implicit methods also exist



The Boris push (Boris 1970)



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

Let's define (Half acceleration):

$$\begin{cases} \mathbf{u}^{n+1/2} = \mathbf{u}^+ + \frac{q \mathbf{E}^n \Delta t}{2mc} \\ \mathbf{u}^{n-1/2} = \mathbf{u}^- - \frac{q \mathbf{E}^n \Delta t}{2mc} \end{cases}$$

Replacing \mathbf{u}^+ and \mathbf{u}^- in Newton's equation gives:

$$\mathbf{u}^+ = \mathbf{u}^- + \mathbf{u}^- \times \mathbf{s} + (\mathbf{u}^- \times \mathbf{w}) \times \mathbf{s}$$

Where $\mathbf{w} = \frac{q \mathbf{B}^n \Delta t}{2mc \gamma^n}$ and $\mathbf{s} = \frac{2\mathbf{w}}{1 + \mathbf{w}^2}$

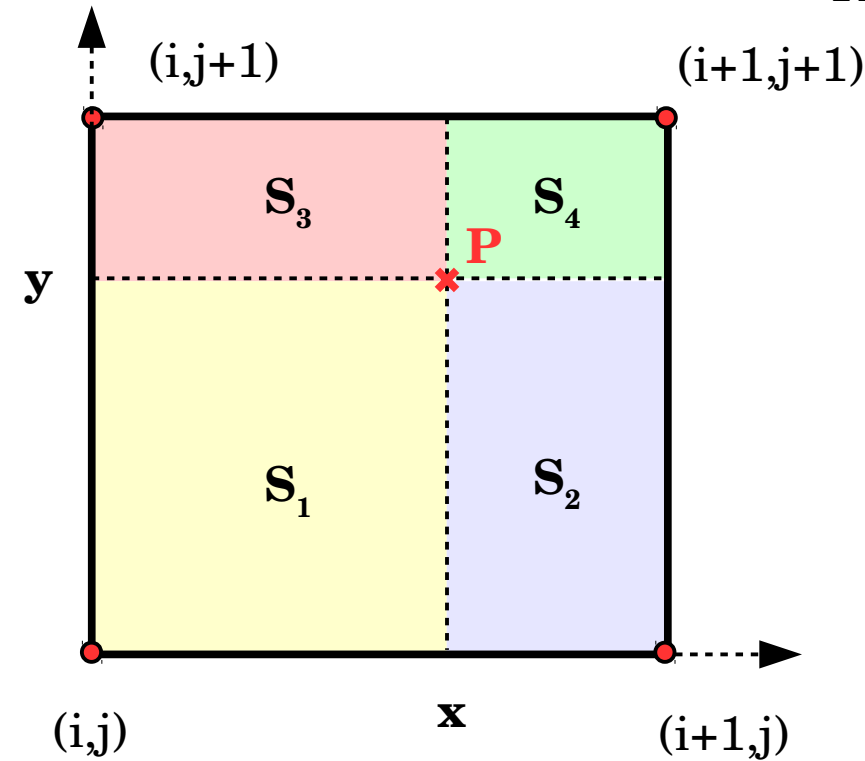
Interpolation of the fields

The fields are known on the mesh only
=> So we need to **interpolate** the fields to the **particle position**

2D Example: Bilinear interpolation (“area weighting”, first order)

Consider field F known on the grid nodes $\mathbf{F}(\mathbf{i},\mathbf{j})$, and a particle located in $\mathbf{P}(\mathbf{x},\mathbf{y})$

Then, the contribution to the field felt by the particle is:



$$W_1 = \frac{S_4}{S_{tot}} F_{i,j} = (1-p)(1-q) F_{i,j}$$

$$p = (x - x_i) / dx$$

$$W_2 = \frac{S_3}{S_{tot}} F_{i+1,j} = p(1-q) F_{i+1,j}$$

$$q = (y - y_i) / dy$$

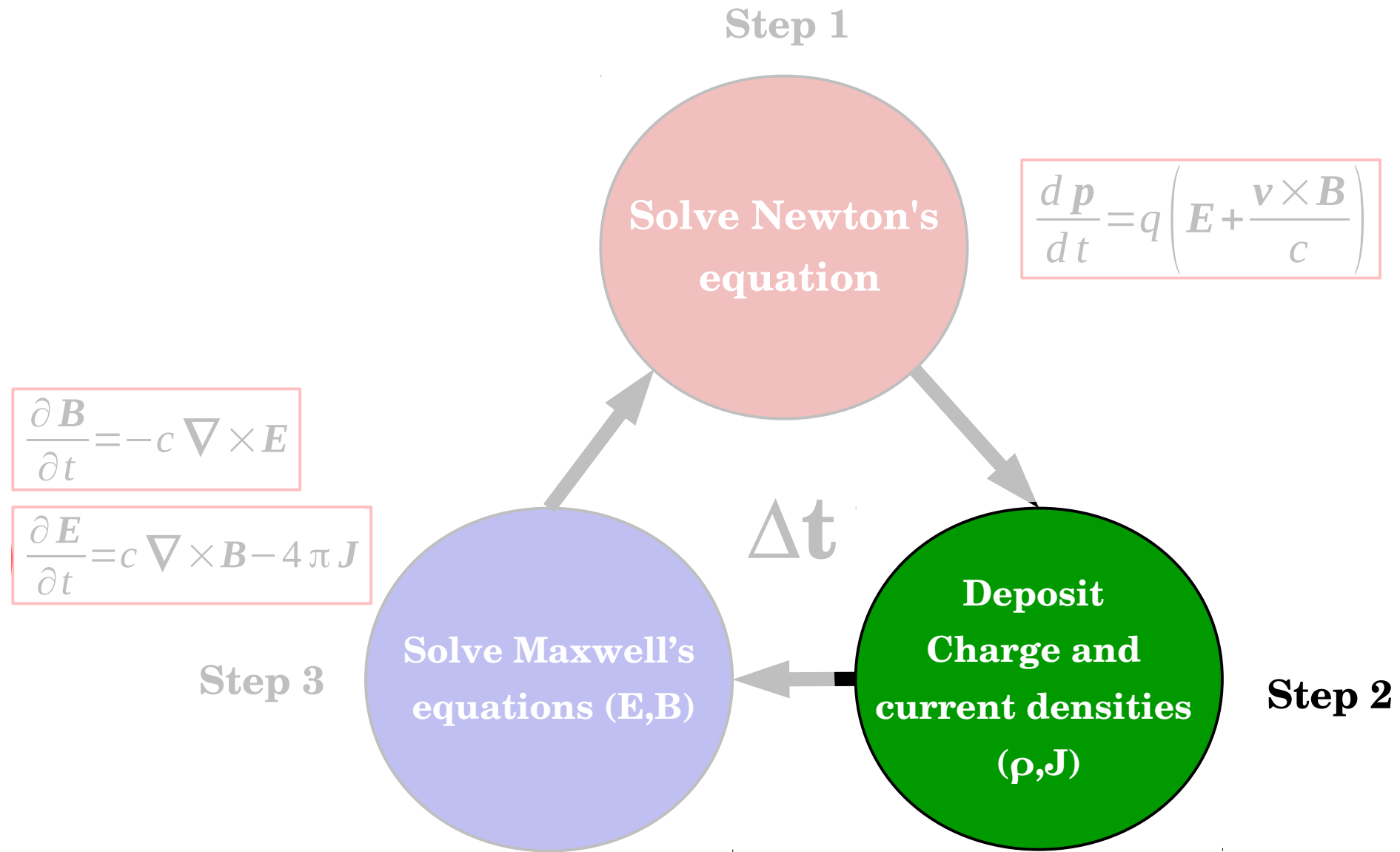
$$W_3 = \frac{S_2}{S_{tot}} F_{i,j+1} = (1-p)q F_{i,j+1}$$

$$W_4 = \frac{S_1}{S_{tot}} F_{i+1,j+1} = pq F_{i+1,j+1}$$

$$F(x, y) = W_1 + W_2 + W_3 + W_4$$

... But we can also imagine higher-order scheme. 18

Computation procedure per timestep in PIC

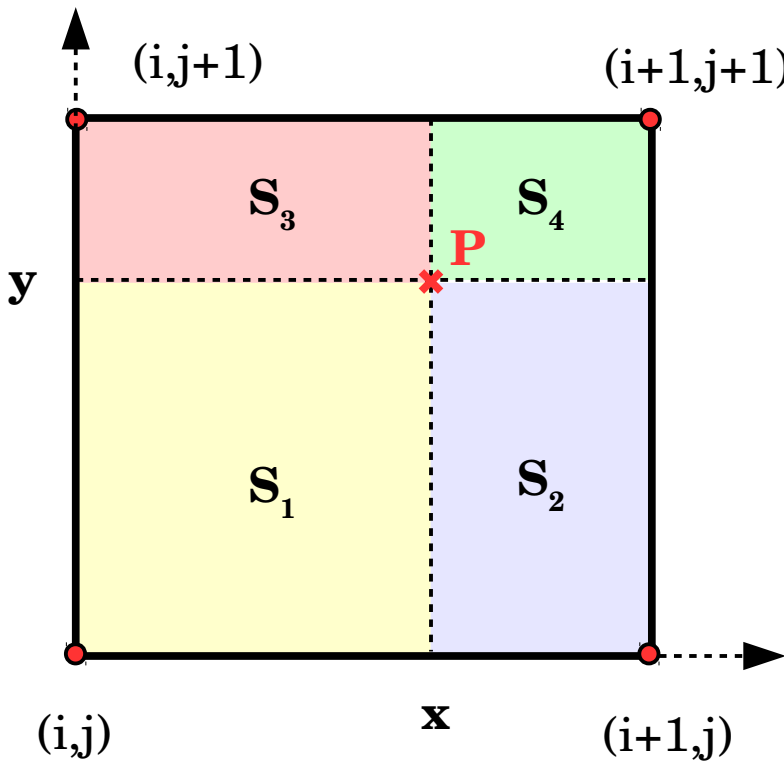


Step 2: Charge and current deposition

In **continuous** space: $\rho \approx \sum_{k=1}^{N_p} q_k w_k \delta(\mathbf{r} - \mathbf{r}_k(t))$ $\mathbf{J} = \sum_{k=1}^{N_p} q_k w_k \mathbf{v}_k \delta(\mathbf{r} - \mathbf{r}_k(t))$

On the **grid**: $\rho_{i,j} \approx \sum_{k=1}^{N_{cell}} q_k w_k S(\mathbf{r} - \mathbf{r}_k(t))$, where S is a “**shape**” function

2D Example: Bilinear interpolation (“area weighting”, first order)



Then, the contributions of all particles to the current is:

$$\mathbf{J}_{i,j} = \sum_{k=1}^{N_{cell}} q_k w_k (1-p_k)(1-q_k) \mathbf{v}_k$$

$$p_k = (x_k - x_i) / dx$$

$$\mathbf{J}_{i+1,j} = \sum_{k=1}^{N_{cell}} q_k w_k p_k (1-q_k) \mathbf{v}_k$$

$$q_k = (y_k - y_i) / dy$$

$$\mathbf{J}_{i,j+1} = \sum_{k=1}^{N_{cell}} q_k w_k (1-p_k) q_k \mathbf{v}_k$$

$$\mathbf{J}_{i+1,j+1} = \sum_{k=1}^{N_{cell}} q_k w_k p_k q_k \mathbf{v}_k$$

Even though the particles are point-like, they have an **effective size** that is felt through the deposition of currents on the grid. In this case, their effective shape is triangular.

Computation procedure per timestep in PIC

Step 1

Solve Newton's equation

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

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

$$\frac{\partial \mathbf{E}}{\partial t} = c \nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

Step 3

Solve Maxwell's equations (E,B)

Δt

Deposit
Charge and
current densities
(ρ, \mathbf{J})

Step 2

Step 3: Maxwell equations

In Gaussian cgs units:

$$\nabla \cdot \mathbf{E} = 4\pi\rho$$

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

$$\frac{\partial \mathbf{E}}{\partial t} = c \nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

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

In principle, need to solve for the **time-dependent equations only**, then the other two should be **automatically satisfied**, but this is not necessarily true due to **truncation errors**.

The total particle charge is conserved, but not necessarily the charge deposited on the grid!

$$\nabla \cdot \mathbf{E} \neq 4\pi\rho$$

Option 1: Correct the E field and solve Poisson equation

Option 2: Parabolic/Hyperbolic divergence cleaning [*Marder 1987, Munz+2000*]

Option 3: Charge conserving deposition scheme [*Esirkepov 2001, Villasenor & Buneman 1992*]

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

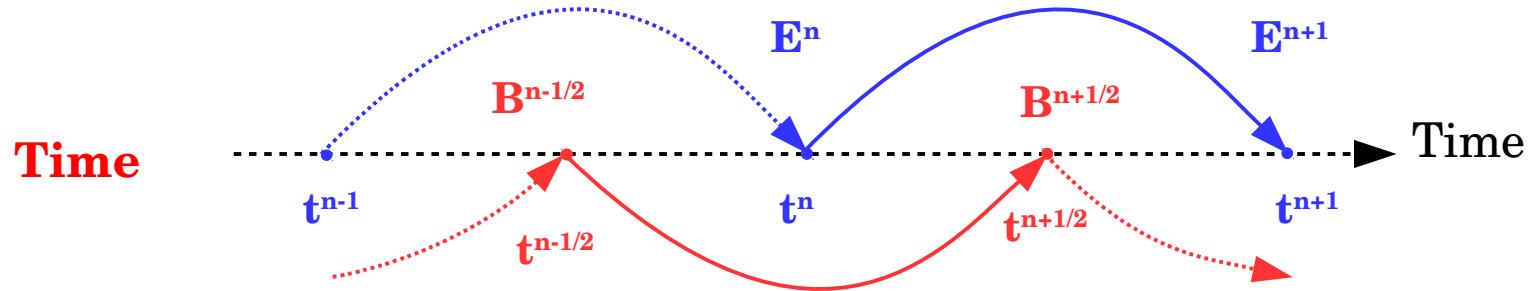
Automatically satisfied to machine roundoff precision with the Yee Algorithm! [*Yee 1966*]

Yee algorithm

$$\frac{\partial \mathbf{E}}{\partial t} = c \nabla \times \mathbf{B} - 4\pi \mathbf{J}$$

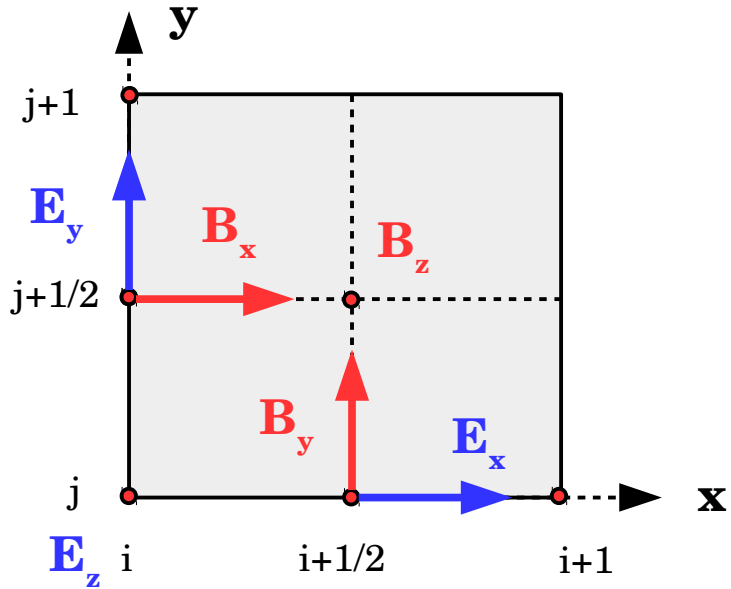
$$\frac{\partial \mathbf{B}}{\partial t} = -c \nabla \times \mathbf{E}$$

The fields are **staggered in both space and in time!**

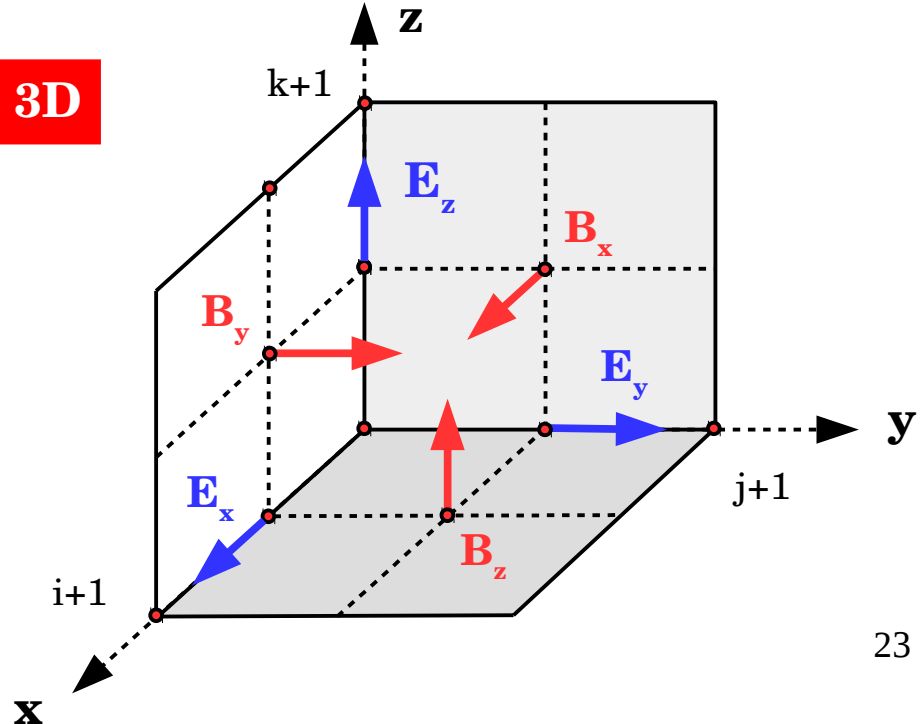


Space: staggered mesh (“Yee mesh”)

2D

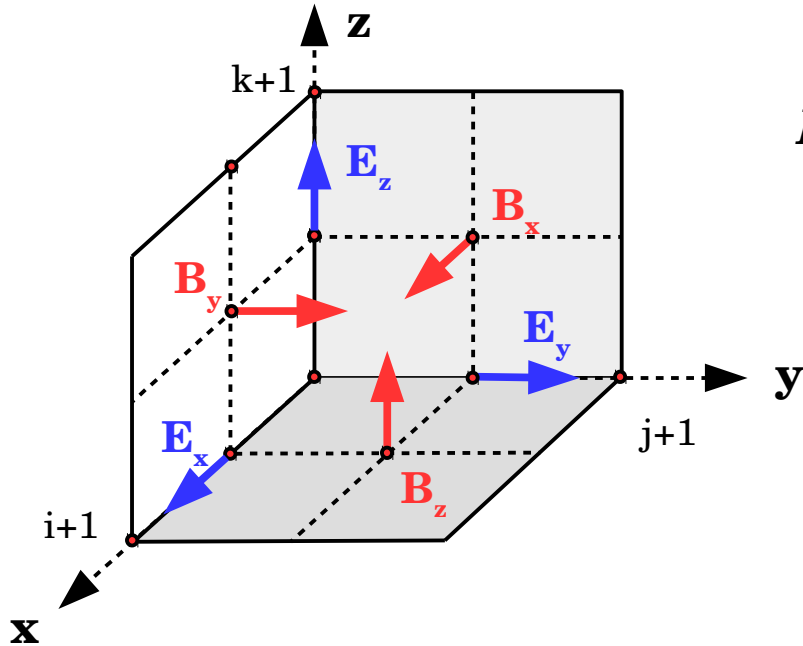


3D



Yee algorithm

Finite-Difference Time-Domain (FDTD) scheme: 2nd in space and time



Example: z-component of $\frac{\partial \mathbf{B}}{\partial t} = -c \nabla \times \mathbf{E}$

$$\frac{(B_z)_{i+1/2, j+1/2, k}^{n+1/2} - (B_z)_{i+1/2, j+1/2, k}^{n-1/2}}{\Delta t} = -c \frac{(E_y)_{i+1, j+1/2, k}^n - (E_y)_{i, j+1/2, k}^n}{\Delta x} + c \frac{(E_x)_{i+1/2, j+1, k}^n - (E_x)_{i+1/2, j, k}^n}{\Delta y}$$

Very **robust** and **stable** if the **Courant-Friedrichs-Lewy (CFL)** condition is fulfilled:

$$\mathbf{1D:} \left(\frac{c \Delta t}{\Delta x} \right)^2 < 1 \quad \mathbf{2D:} (c \Delta t)^2 \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) < 1 \quad \mathbf{3D:} (c \Delta t)^2 \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right) < 1$$

Physics: The **Debye length** and the **plasma frequency** must be resolved in PIC

$$\frac{\Delta x}{\Lambda_D} < 1 \quad \omega_{pe} \Delta t < 1$$

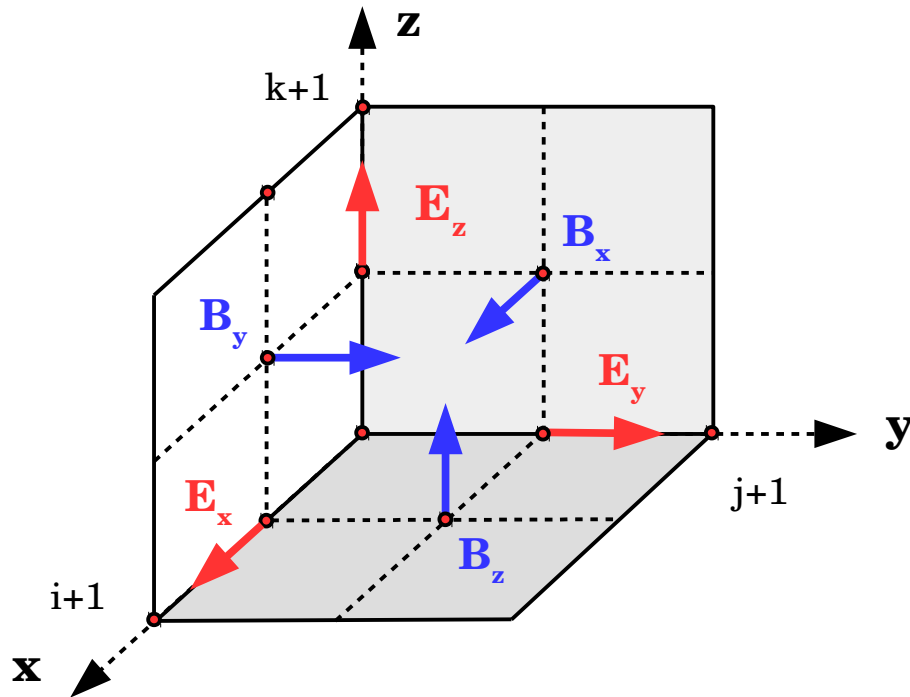
Beyond the standard electromagnetic PIC code

Non-Cartesian grid

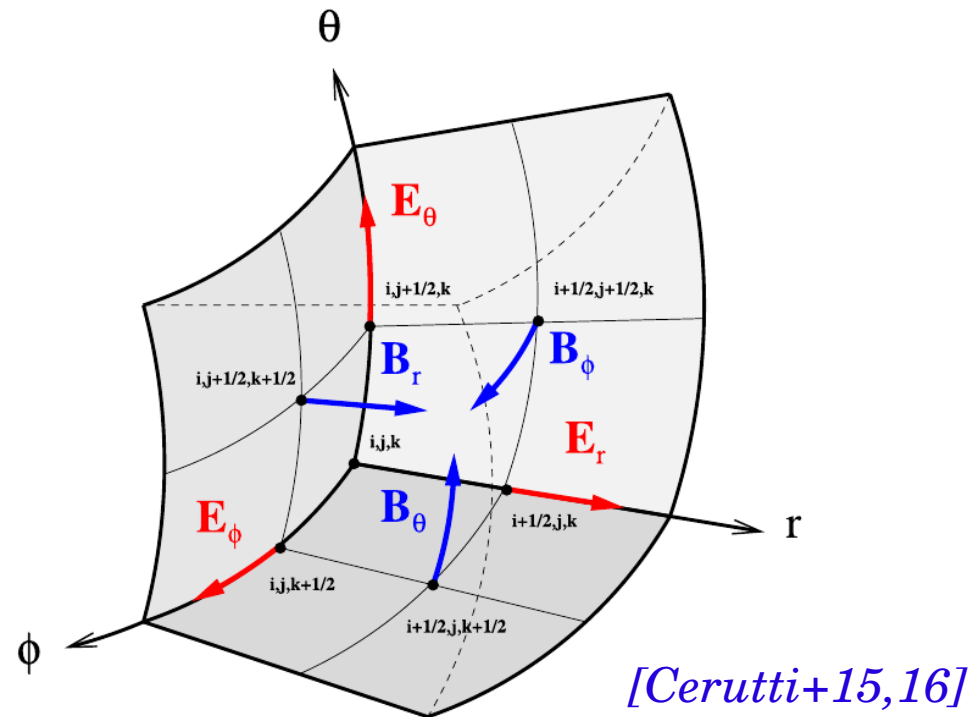
Sometimes, it can be more interesting to use **non-cartesian** grid to take advantage of the symmetries of the system.

=> **Simplifies the initial setup load balancing and boundary conditions**

Cartesian Yee-mesh



Spherical Yee-mesh



Applications to plasmas around a central object.

Examples: pulsar magnetospheres, accreting systems (see tomorrow's seminar)

Beyond the standard electromagnetic PIC code

Emission of non-thermal radiation

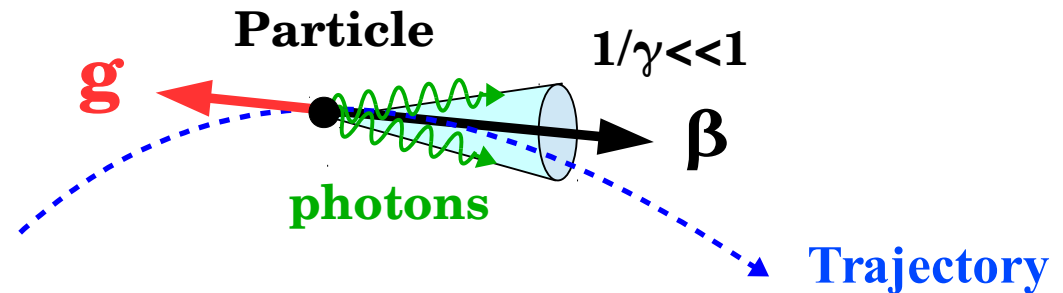
The frequency of the energetic radiation is often not resolved by the grid!

Example: Synchrotron radiation critical frequency: $\omega_{\text{syn}} \propto \gamma^2 (qB/mc) = \gamma^3 \omega_c \gg 1/\Delta t$

Hence, photons must be added as a **separate species**.

Also, the radiation reaction force must be added in the equation of motion explicitly:

$$\frac{d\mathbf{p}}{dt} = q \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) + \mathbf{g}$$



The radiation reaction force is then given by the **Landau-Lifshitz formula** (classical electrodynamics):

$$\mathbf{g} \approx \frac{2}{3} r_e^2 [(\mathbf{E} + \boldsymbol{\beta} \times \mathbf{B}) \times \mathbf{B} + (\boldsymbol{\beta} \cdot \mathbf{E}) \mathbf{E}] - \frac{2}{3} r_e^2 \gamma^2 [(\mathbf{E} + \boldsymbol{\beta} \times \mathbf{B})^2 - (\boldsymbol{\beta} \cdot \mathbf{E})^2] \boldsymbol{\beta}$$

For **inverse Compton** scattering (isotropic external source in the Thomson regime):

$$\mathbf{g} = -\frac{4}{3} \sigma_T \gamma^2 U_{\text{rad}} \boldsymbol{\beta}$$

Applications to e.g., PWN, AGN jets

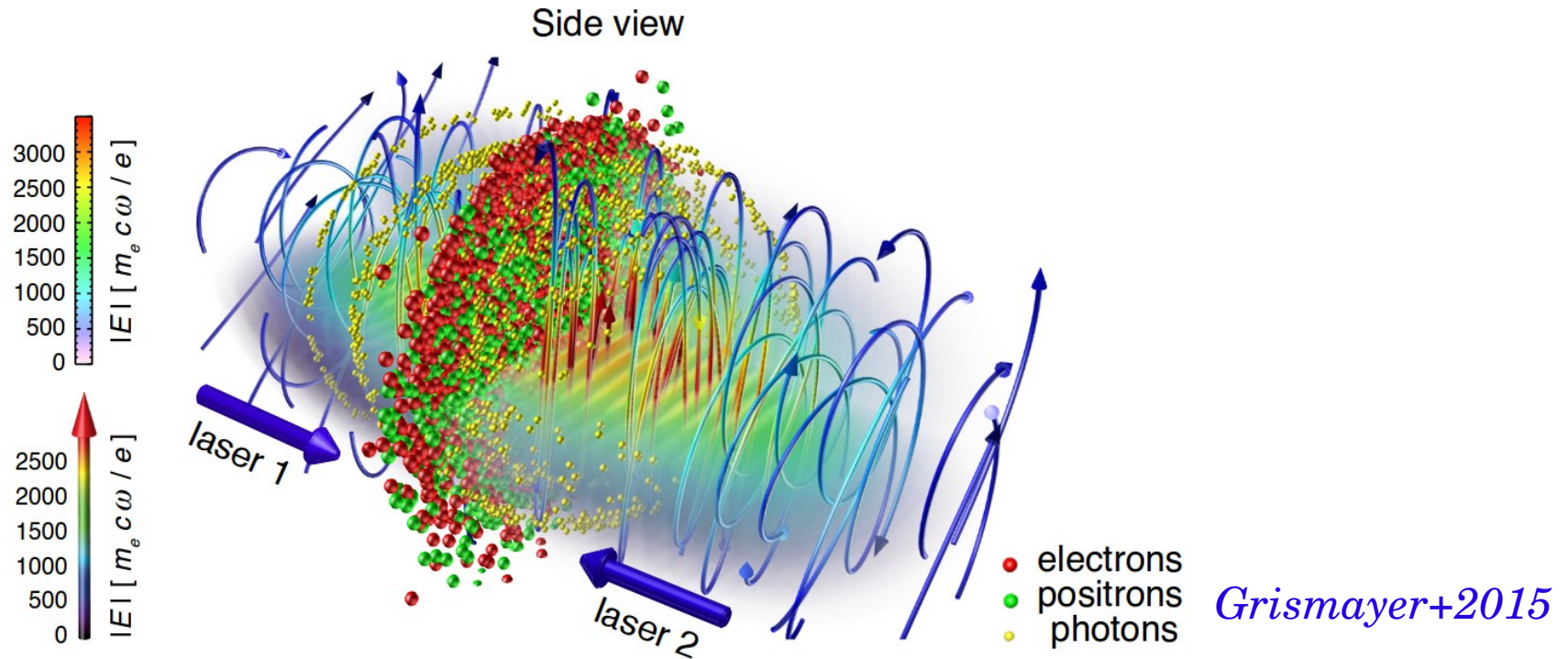
[See Cerutti+2013, 2016]

Beyond the standard electromagnetic PIC code

Pair creation, QED effects

The laser-plasma community is adding extra physics for the next generation of **high-intensity laser** that will reach a fraction of the **critical field** => **QED** effects and **pair creation** important

$$E_{QED} = \frac{m_e^2 c^3}{e \hbar} \approx 4.4 \times 10^{13} \text{ G}$$



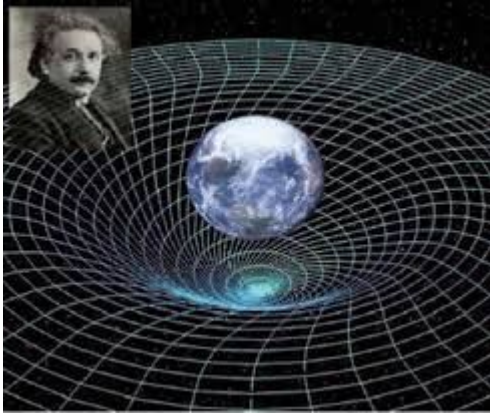
Regime relevant to **pulsars**, **magnetars** ($B > B_{QED}$), and **black hole** magnetospheres.

PIC with pair creation start being used in astrophysics: *Timokhin 2010, Chen & Beloborodov 2014, Philippov + 2015a,b.*

Beyond the standard electromagnetic PIC code

Non-Euclidian metric

Application to e.g., **black hole** magnetospheres and **pulsars**.



The metric changes Maxwell equations, the effective size of the particles (current deposition), and the equation of motion.

Example: For a Schwarzschild metric

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -\alpha^2 dt^2 + dr^2 / \alpha^2 + r^2 (d\theta^2 + \sin^2\theta d\varphi^2)$$

Where $\alpha = \sqrt{1 - \frac{r_g}{r}}$ is the “lapse function”

Maxwell equation as seen in a local frame (“FIDO” observers):
[Thorne+1986]

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

See PIC implementation in *EZeltron* by *Philippov + 2015* for details.

A few words about hybrid PIC codes

An important limitation of full PIC methods is the **limited separation of scales**. Only microscopic systems can be modelled.

In particular, it's hard to model electron/ion plasmas with realistic mass ratio

Plasma frequency $\omega_p \propto 1/\sqrt{m} \rightarrow \omega_{pe}/\omega_{pi} = \sqrt{m_i/m_e} \approx 43$

Hence, **ion acceleration is hard to capture with PIC** (except in the ultra-relativistic limit).

Hybrid code: *[e.g., see Winske+2003]*

Ions are PIC particles:
$$m_i \frac{d\mathbf{v}_i}{dt} = q \left(\mathbf{E} + \frac{\mathbf{v}_i \times \mathbf{B}}{c} \right)$$

Electrons are treated as a massless neutralizing **fluid** (method works for **non-relativistic plasmas**):

$$n_e m_e \frac{d\mathbf{V}_e}{dt} = 0 = -e n_e q \left(\mathbf{E} + \frac{\mathbf{V}_e \times \mathbf{B}}{c} \right) - \nabla \cdot \mathbf{P}_e$$

Example: *Application to non-relativistic shock acceleration. [Gargaté & Spitkovsky 2011, Caprioli & Spitkovsky 2014]*

Summary Part I

- PIC methods appropriate to model particle acceleration in **relativistic collisionless** outflows.
- Main algorithms for explicit PIC codes:
 - Evolving particles: **Boris push**
 - Evolving the fields: **FDTD Yee method**
- **PIC** is very **robust**, **scalable**, and **versatile** to various setup.

A few useful references:

- C.K. Birdsall, A.B. Langdon, “*Plasma Physics via Computer Simulation*”, Series in Plasma Physics
- R.W. Hockney, J.W. Eastwood, “*Computer Simulation Using Particles*”
- Philip L. Pritchett, “*Particle-in-Cell Simulation of Plasmas – A Tutorial*”, J. Büchner, C.T. Dum, M. Scholer (Eds.): LNP 615, pp. 1–24, 2003.
- J. Büchner, “*Vlasov-code simulation*”, Advanced Methods for Space Simulations, edited by H. Usui and Y. Omura, pp. 23–46, 2007.