## Particle-in-cell simulations

## Part I: Numerical methods

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## Plan of the lectures

- Wednesday:
- Morning: The PIC method, numerical schemes and main algorithms.
- Afternoon: Coding practice of the Boris push and the Yee algorithm.
- Thursday:
- Morning: Implementation of Zeltron, structure and methods.
- Afternoon: Zeltron hands on relativistic reconnection simulations
- Evening: Seminar applications of PIC to relativistic magnetospheres.
- Friday:
- Morning: Boundary conditions and parallelization in Zeltron.
- Afternoon: Zeltron Hands on relativistic collisionless shocks simulations


## The Holy book for PIC simulations!



## Astrophysical context

Planetary magnetospheres


Solar corona \& wind, heliosphere

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## 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, magnatars, pulsars, jets, GRBs

Hands on session II on Tuesday afternoon

## Shocks

Flow kinetic energy => Particles


GRBs, SNRs, PWNe, jets...

## Collisionless plasmas

Collisions thermalizes efficiently the particle distribution, not good for nonthermal 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 $v=\frac{V}{l_{C}}$
Collisionless plasma if the plasma frequency $\omega_{\text {pe }} \gg v$

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:

$$
f(\boldsymbol{r}, \boldsymbol{p}, t)=\frac{d N}{d \boldsymbol{r} d \boldsymbol{p}}
$$

6 D in phase space +1 D in time

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

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

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

## The Vlasov equation

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

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

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

$$
\boldsymbol{F}=q\left(\boldsymbol{E}+\frac{\boldsymbol{v} \times \boldsymbol{B}}{c}\right)
$$

We obtain the Vlasov equation:

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

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

## Two numerical approaches to solve Vlasov

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

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!


## Indirectlity 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


## The particle approach

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

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

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):

$$
\begin{aligned}
\frac{d \boldsymbol{p}}{d t} & =q\left(\boldsymbol{E}+\frac{\boldsymbol{v} \times \boldsymbol{B}}{c}\right) \quad \text { Lorentz-Newton equation } \\
\frac{d \boldsymbol{r}}{d t} & =\boldsymbol{v}
\end{aligned}
$$

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

Dirac delta function


Weight particle $\mathrm{k} \quad$ 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 $(\mathrm{q} / \mathrm{m})$ ratio.

Simulation particles => "Macroparticles"
Then we have:

$$
N \approx \sum_{k=1}^{N_{p}} w_{k} \quad \rho \approx \sum_{k=1}^{N_{p}} q_{k} w_{k} \delta\left(\boldsymbol{r}-\boldsymbol{r}_{\boldsymbol{k}}(t)\right) \quad \boldsymbol{J}=\sum_{k=1}^{N_{p}} q_{k} w_{k} \boldsymbol{v}_{\boldsymbol{k}} \delta\left(\boldsymbol{r}-\boldsymbol{r}_{\boldsymbol{k}}(t)\right)
$$

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## The Particle-In-Cell (PIC) approach

Computational domain


## 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?!


Much cheaper! Propagation of light naturally present via CFL condition

## Computation procedure per timestep in PIC



## Computation procedure per timestep in PIC



## Step 1: Particle push

$$
\begin{aligned}
\frac{d \boldsymbol{p}}{d t}=q\left(\boldsymbol{E}+\frac{\boldsymbol{v} \times \boldsymbol{B}}{c}\right) \longmapsto \frac{d \boldsymbol{u}}{d t} & =\frac{q}{m c}\left(\boldsymbol{E}+\frac{\boldsymbol{u} \times \boldsymbol{B}}{\gamma}\right) \quad \text { where }\left\{\begin{array}{l}
\gamma=\frac{1}{\sqrt{1-(v / c)^{2}}} \\
\frac{d \boldsymbol{r}}{d t}
\end{array}=\frac{c \boldsymbol{u}}{\gamma}\right.
\end{aligned}
$$

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)

$\frac{d \boldsymbol{u}}{d t}=\frac{q}{m c}\left(\boldsymbol{E}+\frac{\boldsymbol{u} \times \boldsymbol{B}}{\gamma}\right) \longrightarrow \frac{\boldsymbol{u}^{n+1 / 2}-\boldsymbol{u}^{n-1 / 2}}{\Delta t}=\frac{q \boldsymbol{E}^{n}}{m c}+\frac{q}{m c} \frac{\boldsymbol{u}^{n+1 / 2}+\boldsymbol{u}^{n-1 / 2}}{2 \gamma^{n}} \times \boldsymbol{B}^{n}$
Let's define (Half acceleration): $\left\{\begin{array}{l}\boldsymbol{u}^{n+1 / 2}=\boldsymbol{u}^{+}+\frac{q \boldsymbol{E}^{n} \Delta t}{2 m c} \\ \boldsymbol{u}^{n-1 / 2}=\boldsymbol{u}^{-}-\frac{q \boldsymbol{E}^{n} \Delta t}{2 m c}\end{array}\right.$

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

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

Where $\quad \boldsymbol{w}=\frac{q \boldsymbol{B}^{n} \Delta t}{2 m c \gamma^{n}} \quad$ and $\quad \boldsymbol{s}=\frac{2 \boldsymbol{w}}{1+w^{2}}$
Hands-on I: Code your own Boris push!

More readings: Qin+2013: Why is Boris algorithm so good?
B. Cerutti Ripperda+2018: A Comprehensive Comparison of Relativistic Particle Integrators

## 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 $\mathbf{P}(\mathbf{x}, \mathbf{y})$

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

## Computation procedure per timestep in PIC



## Step 2: Charge and current deposition

In continuous space: $\rho \approx \sum_{k=1}^{N_{p}} q_{k} w_{k} \delta\left(\boldsymbol{r}-\boldsymbol{r}_{\boldsymbol{k}}(t)\right) \quad \boldsymbol{J}=\sum_{k=1}^{N_{p}} q_{k} w_{k} \boldsymbol{v}_{\boldsymbol{k}} \delta\left(\boldsymbol{r}-\boldsymbol{r}_{\boldsymbol{k}}(t)\right)$
On the grid: $\rho_{i, j} \approx \sum_{k=1}^{N_{\text {cen }}} q_{k} w_{k} S\left(\boldsymbol{r}-\boldsymbol{r}_{\boldsymbol{k}}(t)\right)$, where $S$ is a "shape" function
2D Example: Bilinear interpolation ("area weighting", first order)


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 3: Maxwell equations

In Gaussian cgs units:

$$
\begin{array}{ll}
\nabla \cdot \boldsymbol{E}=4 \pi \rho & \nabla \cdot \boldsymbol{B}=0 \\
\frac{\partial \boldsymbol{E}}{\partial t}=c \nabla \times \boldsymbol{B}-4 \pi \boldsymbol{J} & \frac{\partial \boldsymbol{B}}{\partial t}=-c \nabla \times \boldsymbol{E} \\
\hline
\end{array}
$$

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!

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

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]

$$
\nabla \cdot B=0
$$

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

## Yee algorithm

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

The fields are staggered in both space and in time!

Time


Space: staggered mesh ("Yee mesh")

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## Yee algorithm

Finite-Difference Time-Domain (FDTD) scheme: $2^{\text {nd }}$ in space and time


$$
\frac{\left(B_{z}\right)_{i+1 / 2, j+1 / 2}^{n+1 / 2}-\left(B_{z}\right)_{i+1 / 2, j+1 / 2}^{n-1 / 2}}{\Delta t}=-c \frac{\left(E_{y}\right)_{i+1, j+1 / 2}^{n}-\left(E_{y}\right)_{i, j+1 / 2}^{n}}{\Delta x}+\frac{\left(E_{x}\right)_{i+1 / 2, j+1}^{n}-\left(E_{x}\right)_{i+1 / 2, j}^{n}}{\Delta y}
$$

Very robust and stable if the Courant-Friedrichs-Lewy (CFL) condition is fulfilled:
1D: $\left(\frac{c \Delta t}{\Delta x}\right)^{2}<1 \quad$ 2D: $(c \Delta t)^{2}\left(\frac{1}{\Delta x^{2}}+\frac{1}{\Delta y^{2}}\right)<1 \quad$ 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
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$$
\frac{\Delta x}{\Lambda_{D}}<1 \quad \omega_{p e} \Delta t<1
$$

## Numerical dispersion of the Yee solver

We are looking for plane waves solutions

$$
\begin{aligned}
& (F)_{i, j}^{n}=F_{0} \exp I\left(n \omega t-i k_{x} \Delta x-j k_{y} \Delta y\right) \\
& \left(\partial_{t} E_{x}\right)_{i+1 / 2, j}^{n+1 / 2}=\frac{2 I\left(E_{x}\right)_{i+1 / 2, j}^{n+1 / 2}}{\Delta t} \sin \frac{\omega \Delta t}{2} \\
& \left(\partial_{y} E_{x}\right)_{i+1 / 2, j+1 / 2}^{n}=\frac{2 I\left(E_{x}\right)_{i+1 / 2, j+1 / 2}^{n}}{\Delta y} \sin \frac{\omega \Delta y}{2}
\end{aligned}
$$

Dispersion relation

$$
\left[\frac{1}{c \Delta t} \sin \left(\frac{\omega \Delta t}{2}\right)\right]^{2}=\left[\frac{1}{\Delta x} \sin \left(\frac{k_{x} \Delta x}{2}\right)\right]^{2}+\left[\frac{1}{\Delta y} \sin \left(\frac{k_{y} \Delta y}{2}\right)\right]^{2}
$$

Instead of:

$$
\frac{\omega^{2}}{c^{2}}=k_{x}^{2}+k_{y}^{2}
$$

FDTD leads to numerical dispersion (last lecture)

## 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


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: $\omega_{\text {syn }} \propto \gamma^{2}(q B / m c)=\gamma^{3} \omega_{c} \gg 1 / \Delta t$
Hence, photons must be added as a separate species.
Also, the radiation reaction force must be added in the equation of motion explicitly:

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



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

$$
\boldsymbol{g} \approx \frac{2}{3} r_{e}^{2}[(\boldsymbol{E}+\boldsymbol{\beta} \times \boldsymbol{B}) \times \boldsymbol{B}+(\boldsymbol{\beta} \cdot \boldsymbol{E}) \boldsymbol{E}]-\frac{2}{3} r_{e}^{2} \gamma^{2}\left[(\boldsymbol{E}+\boldsymbol{\beta} \times \boldsymbol{B})^{2}-(\boldsymbol{\beta} \cdot \boldsymbol{E})^{2}\right] \boldsymbol{\beta}
$$

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

$$
\boldsymbol{g}=-\frac{4}{3} \sigma_{T} \gamma^{2} U_{r a d} \boldsymbol{\beta}
$$

Applications to e.g., PWN, AGN jets [See Cerutti+2013, 2016]
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## Beyond the standard electromagnetic PIC code <br> Pair creation, QED effects

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

$$
E_{Q E D}=\frac{m_{e}^{2} c^{3}}{e \hbar} \approx 4.4 \times 10^{13} \quad G
$$



Regime relevant to pulsars, magnetars ( $\mathrm{B}>\mathrm{B}_{\mathrm{QED}}$ ), 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 metricApplication to e.g., black hole magnetospheres and pulsars. " $3+1$ " space-time foliation: Equations are solved on local inertial frames ("FIDO" observers)


Maxwell:
Metric term

Equation of motion:

$$
\begin{aligned}
\frac{\mathrm{d} x^{i}}{\mathrm{~d} t} & =v^{i}=\frac{\alpha}{\Gamma} \gamma^{i j} u_{j}-\beta^{i} \\
\frac{\mathrm{~d} u_{i}}{\mathrm{~d} t} & =\underbrace{-\Gamma \partial_{i} \alpha+u_{j} \partial_{i} \beta^{j}-\frac{\alpha}{2 \Gamma} \partial_{i}\left(\gamma^{l m}\right) u_{l} u_{m}}_{\text {Metric induced terms }}
\end{aligned}
$$

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## 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/ions plasmas with realistic mass ratio Plasma frequency $\omega_{p} \propto 1 / \sqrt{m} \rightarrow \omega_{p e} / \omega_{p i}=\sqrt{m_{i} / m_{e}} \approx 43$

Hence, ion acceleration is hard to capture with PIC (except in the ultrarelativistic limit).

Hybrid code: [e.g., see Winske+2003]
Ions are PIC particles: $m_{i} \frac{d \boldsymbol{v}_{i}}{d t}=q\left(\boldsymbol{E}+\frac{\boldsymbol{v}_{\boldsymbol{i}} \times \boldsymbol{B}}{c}\right)$
Electrons are treated as a massless neutralizing fluid (method works for non-relativistic plasmas): $n_{e} m_{e} \frac{d \boldsymbol{V}_{e}}{d t}=0=-e n_{e} q\left(\boldsymbol{E}+\frac{\boldsymbol{V}_{e} \times \boldsymbol{B}}{c}\right)-\boldsymbol{\nabla} \cdot P_{e}$
Example: Application to non-relativistic shock acceleration. [Gargaté \&

## 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.
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