The Particle-In-Cell method

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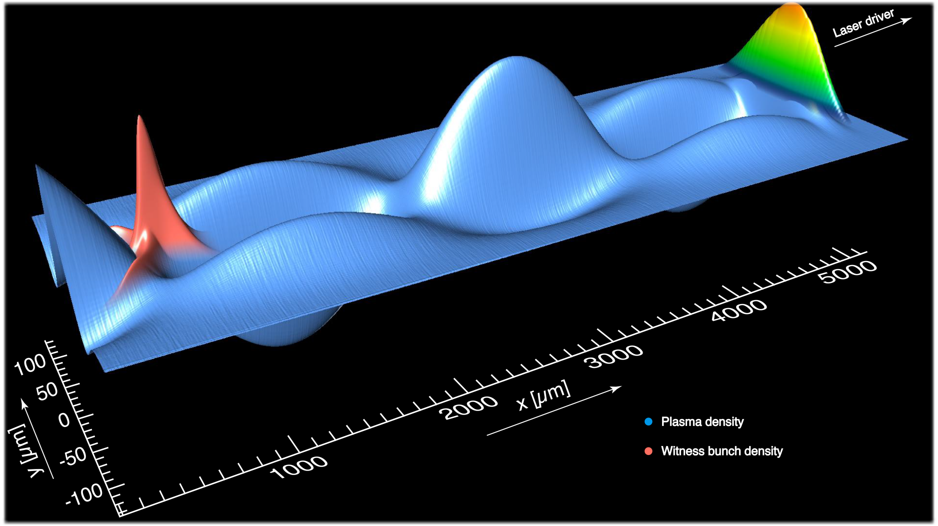

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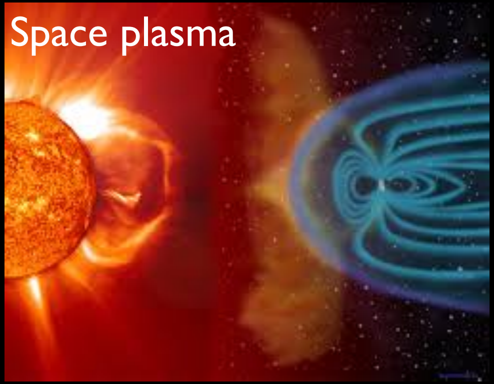
Before starting…

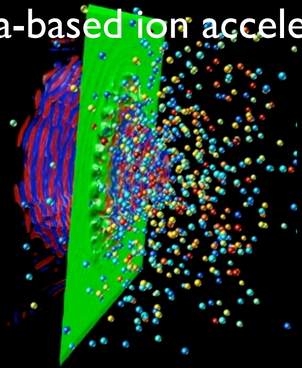
Go to https://www.menti.com/pt67fa419s

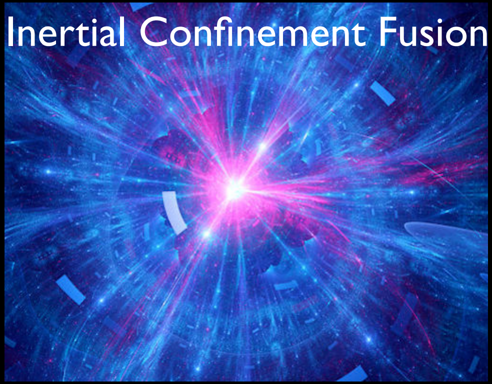
or

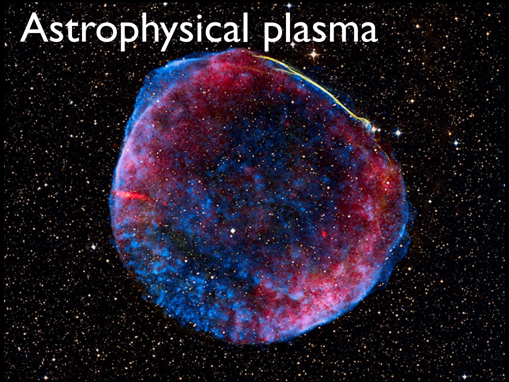
Go to menti.com and digit 94 06 35

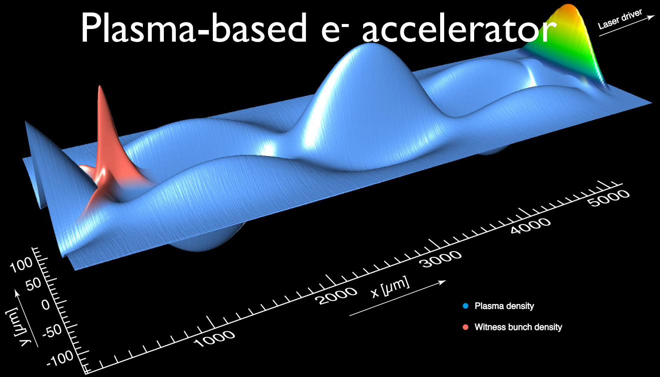
Plasma: the most abundant form of matter in the Universe

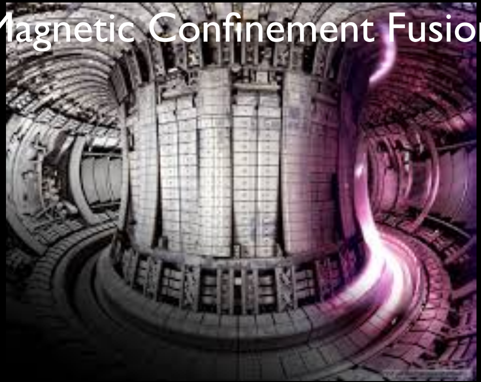




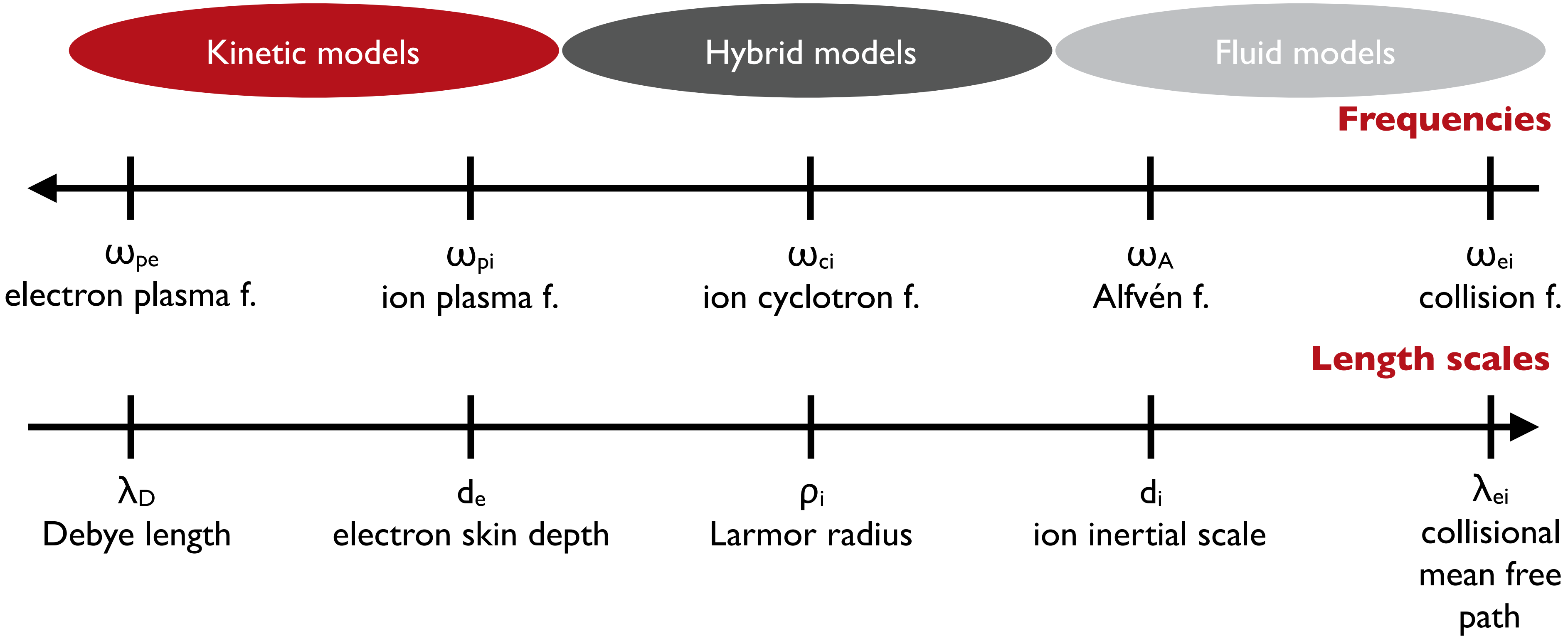








Different ways to model plasmas: the right one depends on the intrinsic plasma scales and its properties



Once determined the plasma model, we can then choose the appropriate numerical technique

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Microscopic $\xrightarrow{\text{statistical average}}$ Kinetic $\xrightarrow{\text{velocity moments}}$ Hybrid $\xrightarrow{\text{velocity moments}}$ Fluid

- Microscopic
  - non-equilibrium: Molecular dynamics codes
  - equilibrium: Monte Carlo codes
- Kinetic
  - collisionless: Vlasov codes
  - collisionless: Particle-In-Cell codes
  - collisional: Fokker-Plank codes
- Fluid
  - Hydro codes
  - + EM fields: MHD codes
  - d/dt = 0: Quasi-static codes

P. Gibbon "Short Pulse Laser Interactions with Matter" Imperial College Press (2007).

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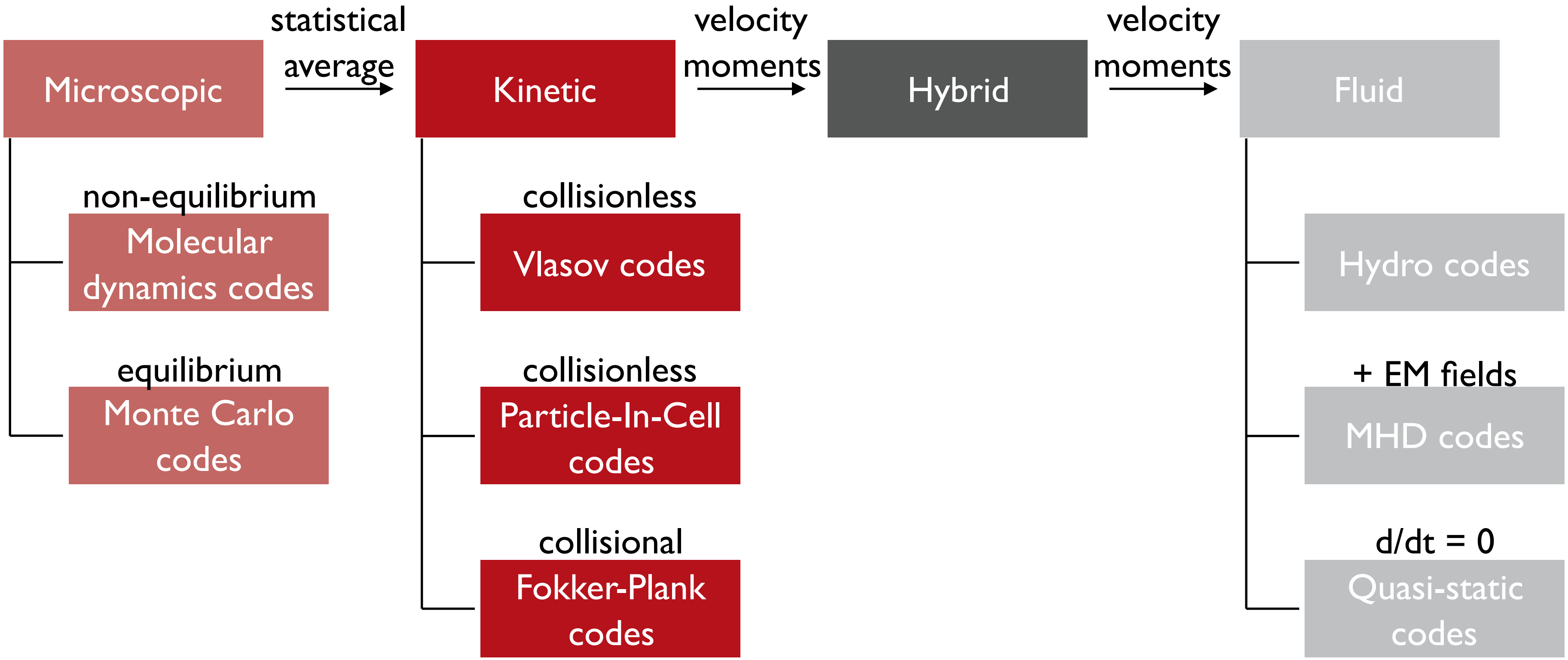


P. Gibbon "Short Pulse Laser Interactions with Matter" Imperial College Press (2007).

Are collisions important?

Parameters to consider:

- N_D: number of particles in Debye cube $N_D = n\lambda_D^3$ with $\lambda_D = \sqrt{\frac{k_B T_e}{4\pi e^2 n}}$
- Γ: coupling parameter, e.g. ratio between potential and kinetic energy $\Gamma = \frac{e^2 n^{1/3}}{k_B T_e}$
- ν/ω_p: ratio between collision and plasma frequency $\omega_p = \sqrt{\frac{4\pi e^2 n}{m_e}}$
- λ/L: ratio between particle mean free path and size of the system

Collisionless plasma	Solid density plasma	Solar corona
$N_D >> 1$	$n = 10^{20}$ pp/cm^3	$n = 10^9$ pp/cm^3
$\Gamma << 1$	$T = 100$ eV	$T = 100$ eV
$\nu/\omega_p << 1$	$N_D = 40$	$N_D = 8 * 10^6$
$\lambda/L >> 1$	$\nu/\omega_p = 3 * 10^{-2}$	$\nu/\omega_p = 3 * 10^{-8}$

The Vlasov-Maxwell system models a collisionless plasma

Vlasov equation

$$\frac{\partial f_j(\mathbf{x},\mathbf{u},t)}{\partial t} = -\mathbf{v}\cdot\frac{\partial f_j(\mathbf{x},\mathbf{u},t)}{\partial \mathbf{x}} - \frac{q_j}{m_j}\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)\cdot\frac{\partial f_j(\mathbf{x},\mathbf{u},t)}{\partial \mathbf{u}}$$

Maxwell's equations

$$\begin{aligned}
\nabla\cdot\mathbf{E} &= 4\pi\rho \\
\nabla\cdot\mathbf{B} &= 0 \\
\nabla\times\mathbf{E} &= -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} \\
\nabla\times\mathbf{B} &= \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}
\end{aligned}$$

Source terms of Maxwell's equations

$$\begin{aligned}
\rho &= \sum_j q_j \int f_j(\mathbf{x},\mathbf{u},t)\,\mathrm{d}\mathbf{u} \\
\mathbf{J} &= \sum_j q_j \int \frac{\mathbf{u}}{\gamma} f_j(\mathbf{x},\mathbf{u},t)\,\mathrm{d}\mathbf{u}
\end{aligned}$$

$$\mathbf{u} = \gamma\mathbf{v}$$

$$\gamma = \sqrt{1+\mathbf{u}^2}$$

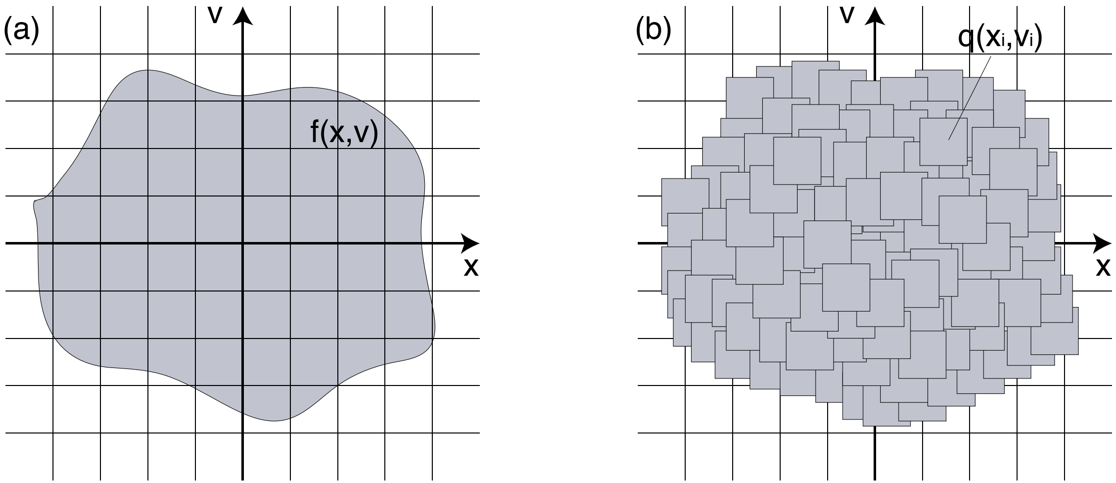
Vlasov equation is 6D: direct integration is impossible even for modern supercomputers!

Idea: use macroparticles

Macroparticles/Computational particles/Superparticles

can be seen as a cloud of many real particles or as blobs of incompressible fluid moving in the 6D phase-space

The continuum distribution function is replaced by discrete macroparticles



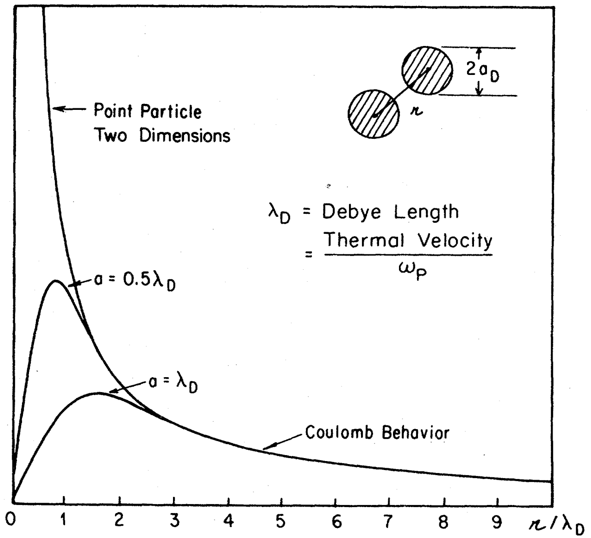
Each macroparticle has its own q and m, but q/m is that of the real plasma species

P. Gibbon "Short Pulse Laser Interactions with Matter" Imperial College Press (2007).

Macroparticles must have a finite size to reduce "close encounter" effects

Using particles introduces granularity not suitable for a collisionless plasma

Number of macro particles << Real number of particles in the plasma ⇒ stochasticity ($\delta F \propto 1/N_p^{1/2}$)



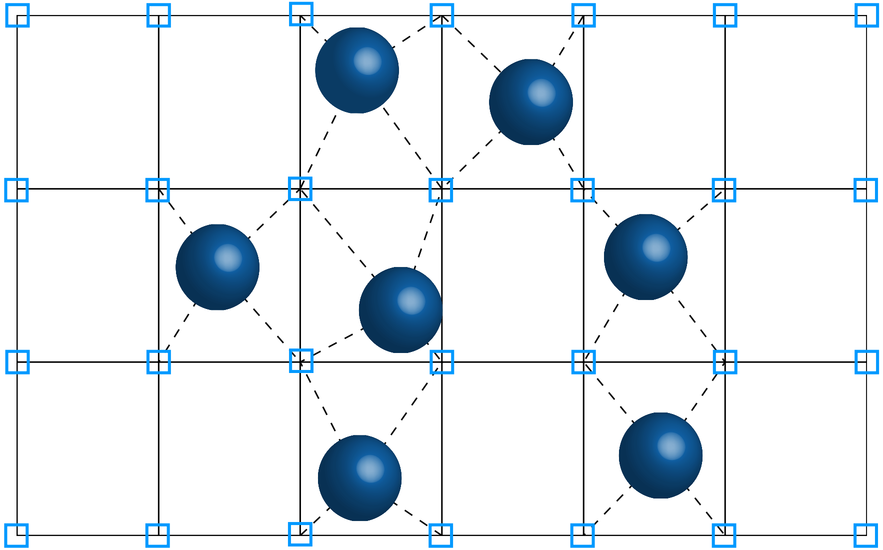
The correct coupling parameter is achieved using fewer particles that interact more weakly

Using finite size particles means that quantity variations smaller than the particle size cannot be captured!

J. M. Dawson, Rev. Mod. Phys. 55, 403 (1983).

While macroparticles are followed according to a Lagrangian fashion, fields are solved on an Eulerian grid

N_p computational particles, N_g grid cells



Number of computational operations $\propto N_p$

In EM PIC codes,
only Maxwell-Ampère & Maxwell-Faraday are solved

In the continuum, if we take the divergence of Faraday and Ampère equations we get

$$\frac{\partial}{\partial t}\nabla \cdot \mathbf{B} = -c\nabla \cdot \nabla \times \mathbf{E} = 0$$

$$\frac{\partial}{\partial t}\nabla \cdot \mathbf{E} = c\nabla \cdot \nabla \times \mathbf{B} - 4\pi\nabla \cdot \mathbf{J} \xrightarrow[\text{using } \nabla \cdot \mathbf{E} = 4\pi\rho]{} \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

Charge conservation equation

In the continuum, the divergence conditions are valid at all times
if they are valid at t = 0 and the charge continuity equation is always satisfied

In the discrete, this holds if the discretised operators retain the property $\nabla \cdot \nabla \times (\,) = 0$ and if the discrete current is computed in a way to satisfy charge conservation equation

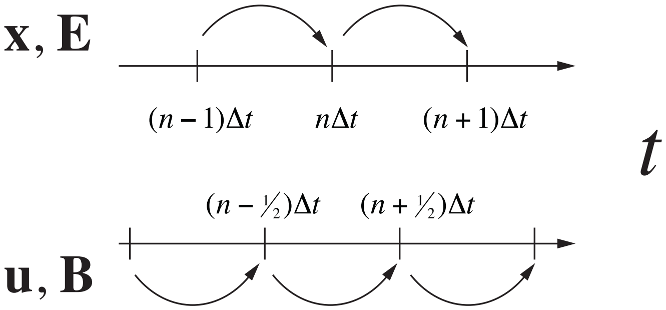
The Yee scheme: a discretisation lattice that ensures $\nabla \cdot \nabla \times (\ ) = 0$

Faraday and Ampère are discretised following the Finite Difference Time Domain algorithm using finite difference:

- **E**, **B** and **J** are staggered in time
  E is computed at t^n
  B and **J** are computed at $t^{n+1/2}$
- **E** and **B** are defined on the Yee mesh

Accuracy of the scheme is
- second order in time
- second order in space

Leapfrog scheme



A. Taflove and S. C. Hagness, Computational Electrodynamics:
B. The Finite- Difference Time-Domain Method. Artech House Publishers, 2005.

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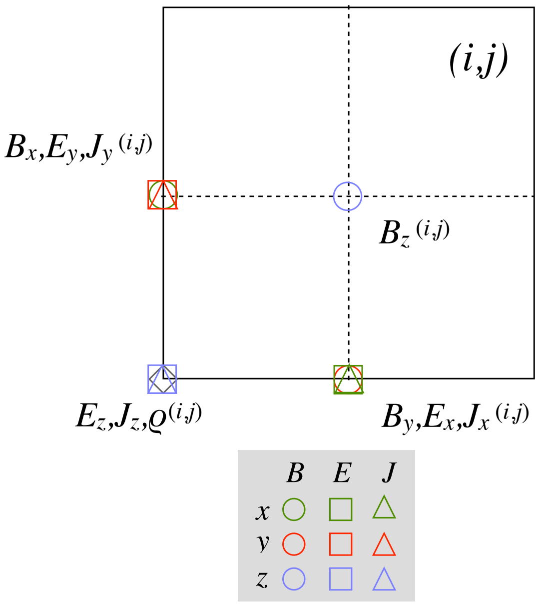
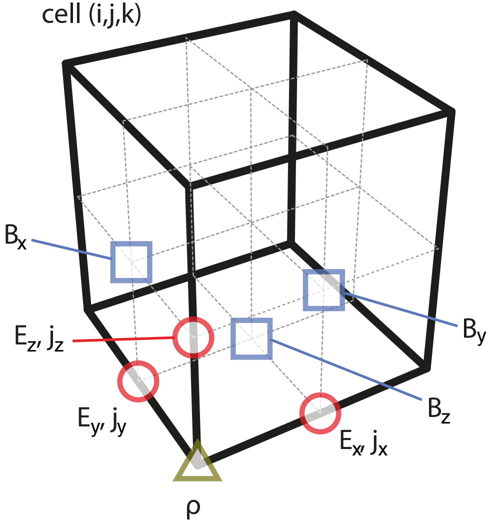
2D Yee mesh



3D Yee mesh



A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite- Difference Time-Domain Method. Artech House Publishers, 2005.

The Yee scheme:
a discretisation lattice that ensures ∇ · ∇ × ( ) = 0

Magnetic field update

$B^{(n-1/2)} \longrightarrow B^{(n+1/2)}$

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

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

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

Electric field update

$E^{(n)} \longrightarrow E^{(n+1)}$

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

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

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

Use of upwind scheme leads to a severe constraint on the choice of the time step respect to the spatial resolution

For simplicity we resort to 1D, but results can be generalised to 3D

Deriving Faraday and Ampère equations respect to t and combining them, we get the wave equation in continuum

$$\frac{1}{c}\frac{\partial^2 E}{\partial t^2} = \frac{\partial^2 E}{\partial x^2}$$

The second order derivatives in the wave equation are discretised following the same scheme that was used before

$$\frac{\partial^2 E}{\partial t^2} \simeq \frac{E_i^{n+1} - 2E_i^n + E_i^{n-1}}{\Delta t^2} \qquad \frac{\partial^2 E}{\partial x^2} \simeq \frac{E_{i+1}^n - 2E_i^n + E_{i-1}^n}{\Delta t^2}$$

Introducing the discretised derivatives into the wave equation, we get

$$E_i^{n+1} = \frac{c\Delta t^2}{\Delta x^2}\left(E_{i+1}^n - 2E_i^n + E_{i-1}^n\right) + 2E_i^n - E_i^{n-1}$$

Now we look for plane wave solutions

$$E_i^n = E_0 \mathrm{e}^{j(ki\Delta x - \omega n t)}$$

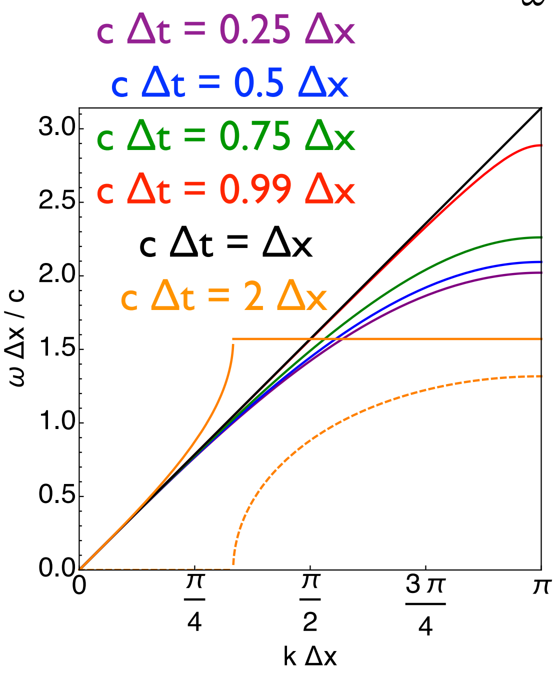
Introducing the plane wave solution into the discretised wave equation we get

$$\underbrace{\frac{e^{j\omega\Delta t} + e^{-j\omega\Delta t}}{2}}_{\cos(\omega\Delta t)} = \frac{c^2\Delta t^2}{\Delta x^2}\left(\underbrace{\frac{e^{jk\Delta x} + e^{-jk\Delta x}}{2}}_{\cos(k\Delta x)} - 1\right) + 1$$

Use of upwind scheme leads to a severe constraint on the choice of the time step respect to the spatial resolution

We can thus obtain the discretised dispersion relation of electromagnetic waves in vacuum:

$$\omega = \frac{1}{\Delta t} \arccos\left\{ \frac{c^2 \Delta t^2}{\Delta x^2} [\cos(k\Delta x) - 1] + 1 \right\}$$



- If $\Delta t, \Delta x \rightarrow 0$, the continuum dispersion relation for EM waves ($\omega = ck$) is retrieved
- For $c\,\Delta t = \Delta x$, the continuum dispersion relation for EM waves is also retrieved
- For $c\,\Delta t > \Delta x$, the dispersion relation has a complex solution at $k\,\Delta x \simeq 1$; the imaginary part leads to a (numerical) instability
- For $c\,\Delta t < \Delta x$, the numerical phase velocity of EM waves depends on k and is less than the speed of light at high k numbers
- As a consequence of the latter condition there can be PIC particles moving faster than the numerical speed of light (numerical Cherenkov radiation)

Use of upwind scheme leads to a severe constraint on the choice of the time step respect to the spatial resolution

Summarising

In 1D the scheme is stable for $c\,\Delta t \leq \Delta x$

This is called the **Courant Friedrichs Lewy (CFL) condition**

Generalising to more than one dimension, the CFL reads:

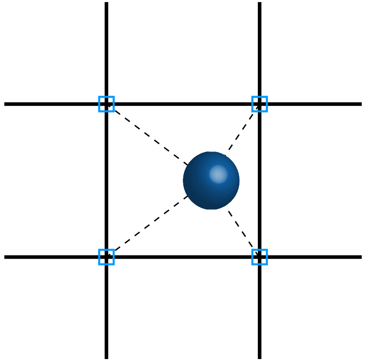
$$c\Delta t \leq \left(\sum_l \frac{1}{\Delta x_l^2} \right)^{-\frac{1}{2}}$$

At high k numbers, EM waves in vacuum can propagate slower than the speed of light

The scheme is affected by a numerical dispersion

Numerical dispersion can be mitigated or eliminated using instead a spectral solver.

Once E and B are computed on the grid, they have to be interpolated to the particle position



$$(\mathbf{E},\mathbf{B}) = \sum_g W(\mathbf{x}-\mathbf{x}_g)(\mathbf{E}_g,\mathbf{B}_g)$$

Interpolation function

The interpolation function is connected to the macroparticle shape function S(x):

$$W(x-x_g) = W_g(x) = \int_{x_g-\frac{\Delta x}{2}}^{x_g+\frac{\Delta x}{2}} S(x'-x)\,dx' = \int_{-\infty}^{\infty} \Pi\left(\frac{x'}{\Delta x}\right) S(x'-x)\,dx' = \Pi\left(\frac{x}{\Delta x}\right) \star S(x)$$

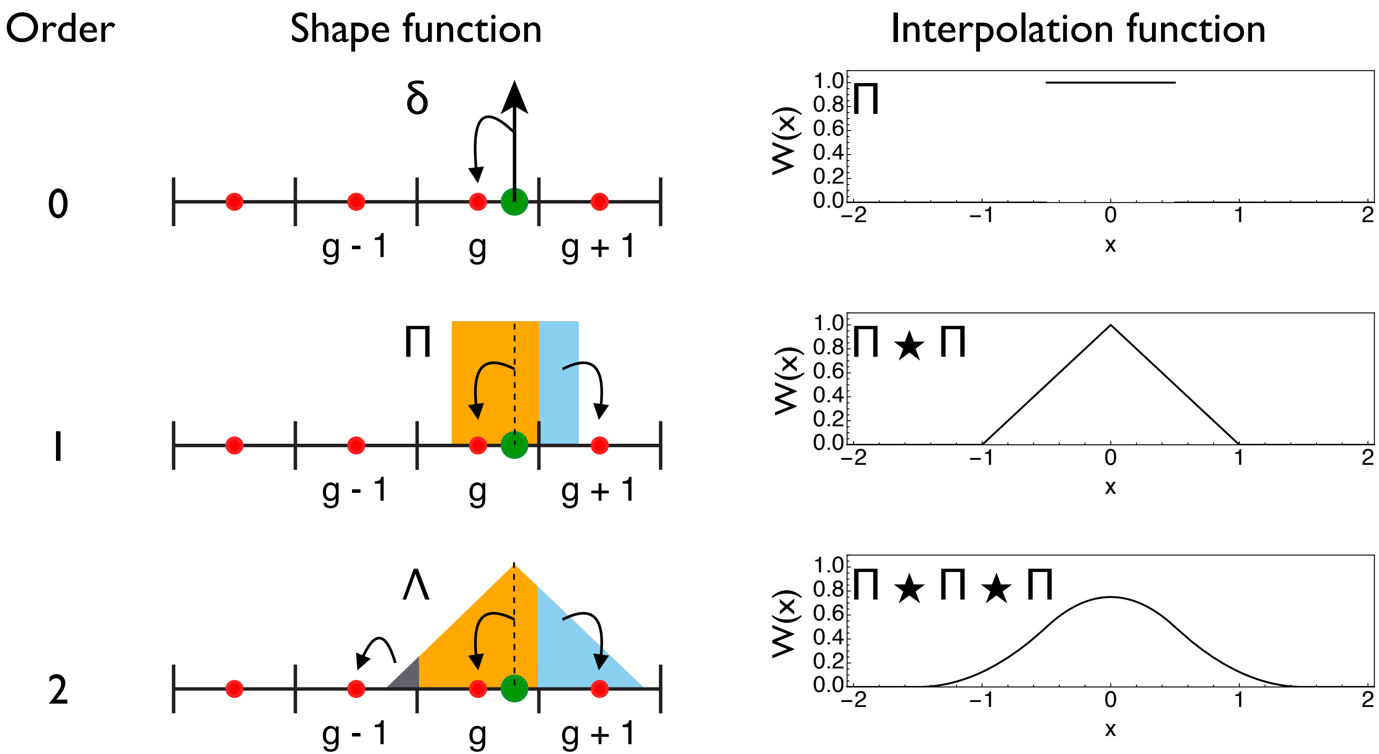
Hat function

$$\Pi\left(\frac{x}{\Delta x}\right) = \begin{cases} 1 & \text{if } x \leq \left|\frac{\Delta x}{2}\right| \\ 0 & \text{otherwise} \end{cases}$$

General properties of shape functions:

- compact support (e.g. shape function is 0 outside a small range)
- integral over the whole domain is unitary
- symmetric

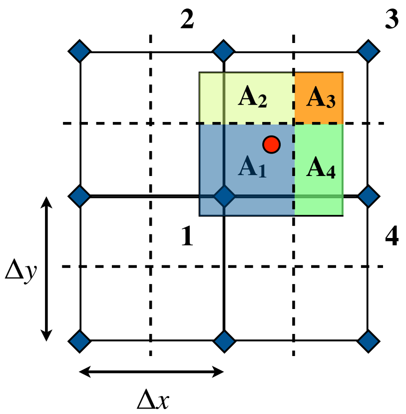
Once E and B are computed on the grid, they have to be interpolated to the particle position



Once E and B are computed on the grid, they have to be interpolated to the particle position

Modern PIC codes implement at least the first order shape function (linear interpolation).
This is referred to as cloud-in-cell (CIC)

First order shape function 2D



$$A = \Delta x \Delta y$$

$$E_p = \frac{A_1 E_1 + A_2 E_2 + A_3 E_3 + A_4 E_4}{A}$$

In order to ensure momentum conservation of the scheme and avoid numerical instability
the shape function used to interpolate fields to particles
must be consistent with current/charge deposition scheme

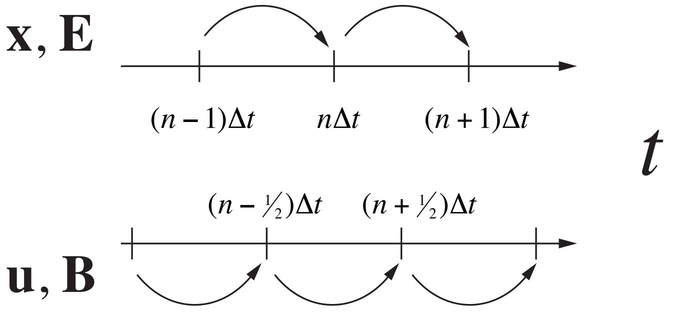
Fields at particle positions are used to advance the particles

Particles are advanced integrating numerically their respective equation of motion employing a leapfrog scheme (e.g. velocity and position are staggered in time)

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

$$\frac{\mathbf{x}^{n+1}-\mathbf{x}^n}{\Delta t}=\frac{\mathbf{u}^{n+1/2}}{\gamma^{n+1/2}}$$

with $\gamma^{n+1/2}=\sqrt{1+\left(\frac{\mathbf{u}^{n+1/2}}{c}\right)^2}$



The accuracy in time of the scheme is second order

Fields at particle positions are used to advance the particles

Particle velocity is updated using a relativistic Boris pusher

The first step is to notice that electric and magnetic contribution in Newton equation can be separated:

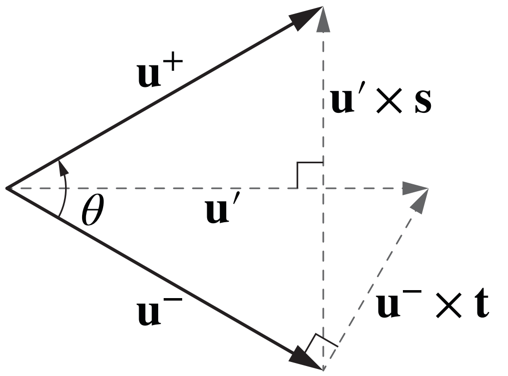
Introducing these definitions into Newton equation $\mathbf{u^{n-1/2}} = \mathbf{u}^- - \frac{q}{m}\frac{\Delta t}{2}\mathbf{E}^n \quad \mathbf{u^{n+1/2}} = \mathbf{u}^+ + \frac{q}{m}\frac{\Delta t}{2}\mathbf{E}^n$

the following is obtained $\frac{\mathbf{u}^+ - \mathbf{u}^-}{\Delta t} = \frac{q}{2\gamma^n mc}\left(\mathbf{u}^+ + \mathbf{u}^-\right) \times \mathbf{B}^n$

This is a rotation of $\theta = 2\arctan\left(\frac{qB\Delta t}{2\gamma^n m}\right)$

Fields at particle positions are used to advance the particles

The Boris pusher can be implemented following 4 steps:



Step 1: add half electric impulse $\mathbf{u}^- = \mathbf{u}^{n-1/2} + \frac{q\mathbf{E}^n}{m}\frac{\Delta t}{2}$

Step 2: rotate the result with half magnetic impulse $\mathbf{u}' = \mathbf{u}^- + \mathbf{u}^- \times \mathbf{t}$

$$\mathbf{t} = -\frac{q\mathbf{B}^n}{\gamma^n mc}\frac{\Delta t}{2}$$

Step 3: rotate the result with full magnetic impulse $\mathbf{u}^+ = \mathbf{u}^- + \mathbf{u}' \times \mathbf{s}$

$$\mathbf{s} = \frac{2\mathbf{t}}{1+\mathbf{t}^2}$$

Step 4: add remaining electric impulse $\mathbf{u}^{n+1/2} = \mathbf{u}^+ + \frac{q\mathbf{E}^n}{m}\frac{\Delta t}{2}$

$$\gamma^n = \sqrt{1+\left(\frac{\mathbf{u}'}{c}\right)^2}$$

Particles must be deposited on the grid to compute source term in Ampère equation

Particle current must be deposited following a scheme that ensures charge conservation

Simply depositing particles violates charge continuity equation

If charge continuity equation is violated,
a divergence cleaning must be implemented to ensure charge conservation

This means solving the elliptic Poisson equation on top of Faraday and Ampère equations

The current deposition technique proposed by Villasenor & Buneman in 1992 is the simplest scheme that allows for charge conservation; it is valid for linear interpolation

Later, current deposition schemes for higher order interpolation were conceived by Esirkepov

Villasenor & Buneman: Comp. Phys. Comm. 69, 306 (1992)
Esirkepov, Comp. Phys. Comm. 135, 144 (2001)

Particles must be deposited on the grid to compute source term in Ampère equation

The Villasenor & Buneman's scheme

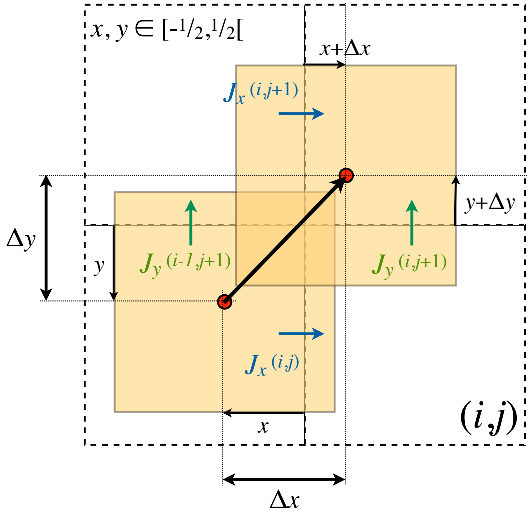
Charge moves $(\Delta x, \Delta y)$ in Δt

For $J_x(i,j)$ depth of charge moved is Δx:

- Initial height: $1/2 - y$
- Final height: $1/2 - (y+\Delta y)$
- Average: $1/2 - y - 1/2\,\Delta y$
- $J_x(i,j) = \Delta x(1/2 - y - 1/2\,\Delta y)\,q/\Delta t$

For all the J components, we get:

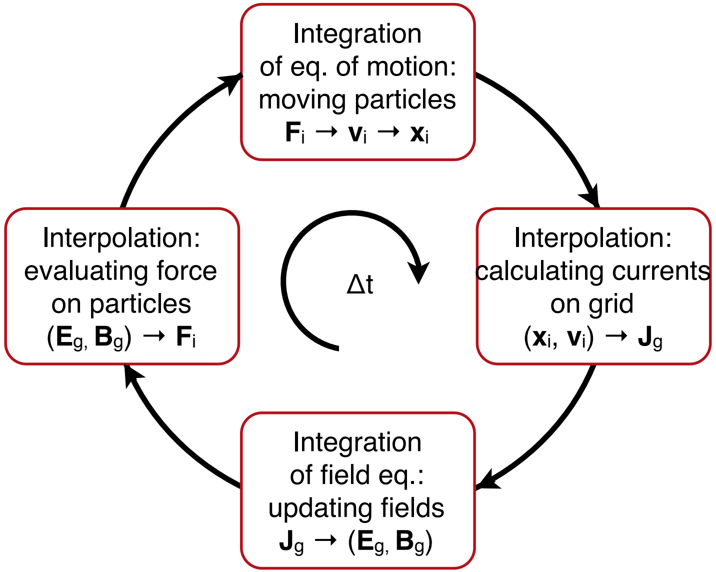
$$
\begin{aligned}
J_{x(i,j)} &= \Delta x\left(\frac{1}{2} - y - \frac{1}{2}\Delta y\right)\frac{q}{\Delta t}\\
J_{x(i,j+1)} &= \Delta x\left(\frac{1}{2} + y + \frac{1}{2}\Delta y\right)\frac{q}{\Delta t}\\
J_{y(i-1,j+1)} &= \Delta y\left(\frac{1}{2} - x - \frac{1}{2}\Delta x\right)\frac{q}{\Delta t}\\
J_{y(i,j+1)} &= \Delta y\left(\frac{1}{2} + x + \frac{1}{2}\Delta x\right)\frac{q}{\Delta t}
\end{aligned}
$$



Particles can cross more than 4 boundaries; in this case motion is split into series of motions that cross only one boundary (x and/or y)

Villasenor & Buneman: Comp. Phys. Comm. 69, 306 (1992)
Esirkepov, Comp. Phys. Comm. 135, 144 (2001)

Combining everything together: the PIC loop



Usually normalised units are employed

Careful choice of units and normalisation is critical

- Avoids multiplication by several constants (e.g. m_e, e and c) improving performance and numerical accuracy.
- By expressing the simulation quantities in terms of fundamental plasma quantities the results are general and not bound to some specific units we may choose

Common choice of units and normalisation in PIC codes

- The frequencies are normalised to a normalisation frequency, ω_n. Time is normalised to ω_n^{-1}
- Proper velocities are normalised to the speed of light, c. Space is normalised to c/ω_n.
- Charge and mass are normalised to the absolute electron charge, e, and the electron mass, m_e. The fields are then normalised appropriately.
- The density is normalised to ω_n^2 (the normalisation frequency squared). So if the density is 1 at a given location then the normalisation frequency is the plasma frequency at that location.
- If the laser frequency is 1, then the normalisation frequency is the laser frequency and the density is normalised to the critical density (for that laser frequency).

$$\mathbf{x}' = \frac{\omega_n}{c}\mathbf{x} \quad \mathbf{p}' = \frac{\mathbf{p}}{m_{sp}c} = \frac{\gamma\mathbf{v}}{c} = \frac{\mathbf{u}}{c} \quad \mathbf{E}' = e\frac{c/\omega_n}{m_e c^2}\mathbf{E} \quad \mathbf{B}' = e\frac{c/\omega_n}{m_e c^2}\mathbf{B}$$

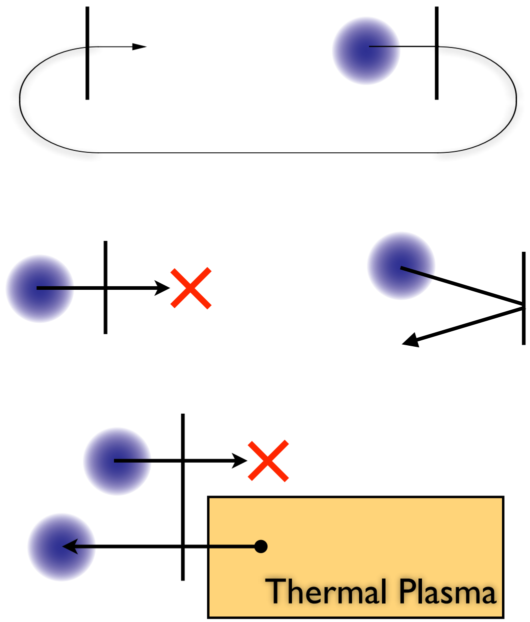
Different boundary conditions can be implemented

Particles

- Periodic
- Open
- Specular Reflection
- Thermal Bath

Fields

- Periodic
- Conducting
- Open



E. Lindmann, J. Comp. Phys. 18, 66 (1975)
J.Vay, J. Comp. Phys. 165, 511 (2000)

Hands-on: electrostatic PIC

Exercises and scripts on a GitHub repo

git clone https://github.com/eboella/Python-ePIC.git

or download from https://github.com/eboella/Python-ePIC

The scripts implement a 1D electrostatic PIC scheme

They solve Poisson equation to advance the fields

Normalisation done respect to λ_D and ω_p

Beware of the finite grid instability (more details during next class)

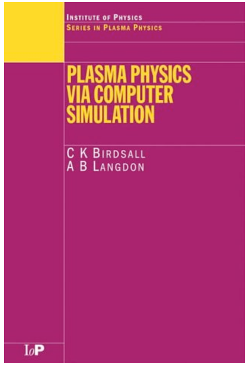
Numerical instability that causes unphysical electron heating

Requires adopting $\Delta x/\lambda_D \ll \pi$ for linear interpolation

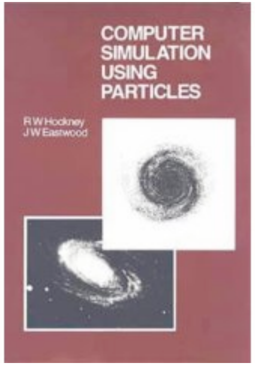
In general, it is recommended resolving λ_D to avoid numerical heating

To switch from Python 3 to 2: https://docs.anaconda.com/anaconda/user-guide/tasks/switch-environment/

References



C. K. Birdsall, A. B. Langdon
Plasma Physics via Computer Simulation
IoP Publishing, Bristol, UK (1991)



R. W. Hockney, J. W. Eastwood,
Computer Simulation Using Particles
McGraw-Hill, New York (1981)

Particle simulation of plasmas

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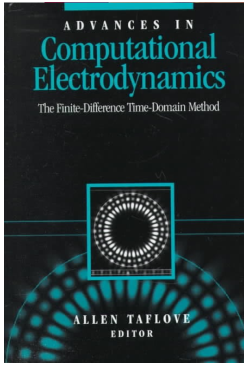
For plasma with a large number of degrees of freedom, particle simulation using high-speed computers can offer insights and information that supplement those gained by traditional experimental and theoretical approaches. The technique follows the motion of a large assembly of charged particles in their self-consistent electric and magnetic fields. With proper diagnostics, these numerical experiments reveal such details as distribution functions, linear and nonlinear behavior, stochastic and transport phenomena, and approach to steady state. Such information can both guide and verify theoretical modeling of the physical processes underlying complex phenomena. It can also be used in the interpretation of experiments.

J. M. Dawson,
Particle simulation of plasmas
Rev. Mod. Phys. 55, 403 (1983)



Taflove, S. C. Hagness,
Computational Electrodynamics: The Finite- Difference Time-Domain Method.
Artech House Publishers (2005).