Particle-in-Cell (PIC) Simulations of Plasmas

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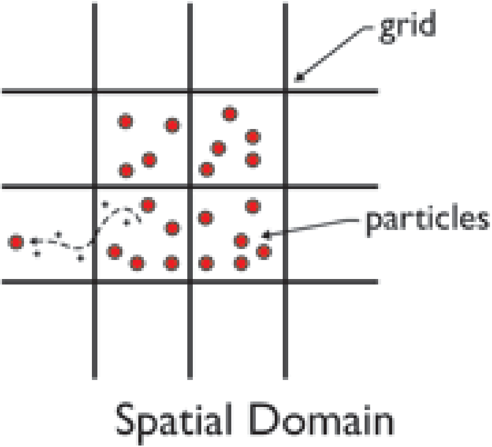
Cartoon PIC

Adapted from
https://www.lanl.gov/science/NSS/issue2_2010/story4.shtml



E and **B** are known on the grid. Particles move freely.

Why Doing Plasma Physics via Computer Simulations Using Particles Makes Good Physical Sense

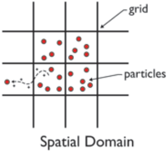
Inspired by Birdsall & Langdon, *Plasma Physics via Computer Simulation*

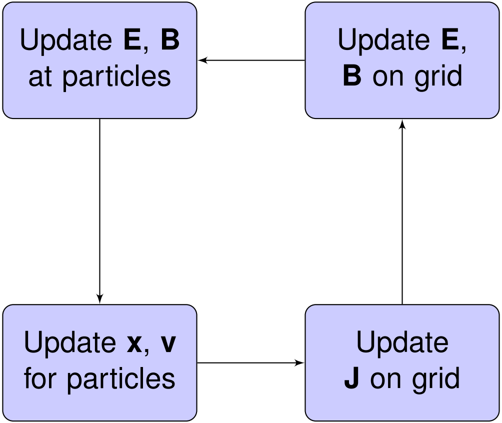
- Debye length $\lambda_D = v_{th}/\omega_{pe} \ll L$; we care about $\lambda \gtrsim \lambda_D$.
- For a meaningful plasma $N_D = n\lambda_D^3 \ggg 1$
- But that means

$$\frac{\text{KE (thermal kinetic energy)}}{\text{PE (electrostatic potential energy)}} = N_D^{2/3} \gg 1$$

- $\therefore$ *Particles interact collectively, not discretely*.
- Grids with $\Delta x \lesssim \lambda_D$ capture the important physics without the unimportant inter-particle effects.

Cartoon Timestep





Updating $\mathbf{x}$, $\mathbf{v}$, $\mathbf{J}$, $\mathbf{B}$, and $\mathbf{E}$

- Field advancement:

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

- Particle advancement:

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

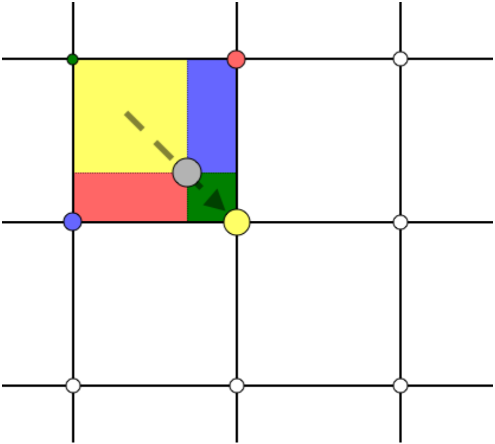
- Current density update:

$$\mathbf{J} = \sum_i q_i \mathbf{v}_i S(\mathbf{X} - \mathbf{x}_i)$$

where $S(\mathbf{X} - \mathbf{x})$ is a shape function.

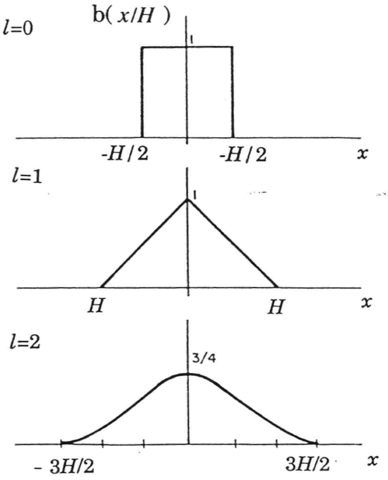
Translating Between Particles and the Grid

Adapted from `https://www.particleincell.com/2010/es-pic-method/`



Effective Particle Shapes (1D)

Adapted from `https://perswww.kuleuven.be/~u0052182/weather/pic.pdf`



- Nearest gridpoint
- First-order (cloud-in-cell)
- Quadratic spline

Does PIC Satisfy $\nabla \cdot \mathbf{B} = 0$ and $\nabla \cdot \mathbf{E} = 4\pi\rho$?

Numerically, $\nabla \cdot (\nabla \times) = 0$

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

If $\nabla \cdot \mathbf{B} = 0$ at $t = 0$, it remains so (ignoring round-off)

In contrast,

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

To satisfy Gauss's Law requires

$$\frac{\partial\rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

Unfortunately $\cdots$

Continuity is not, in general, satisfied

Corrections fall into two broad categories

- “Fix” **E**
- “Fix” **J**

An approach of the first type: Suppose a Φ exists such that

$$\mathbf{E}' = \mathbf{E} - \boldsymbol{\nabla}\Phi \qquad \text{where} \qquad \boldsymbol{\nabla}\cdot\mathbf{E}' = 4\pi\rho$$

Find Φ by solving

$$\nabla^2\Phi = \boldsymbol{\nabla}\cdot\mathbf{E} - 4\pi\rho \equiv b$$

This ($\nabla^2\Phi = b$) is Poisson’s equation and can be solved many different ways: FFTs, matrix methods, multigrid methods, $\cdots$

An Alternative: Fluid vs. PIC Simulations

Fluid (MHD)

Advantages:

- Correct on large scales
- Computationally fast

Disadvantages:

- Wrong at small scales

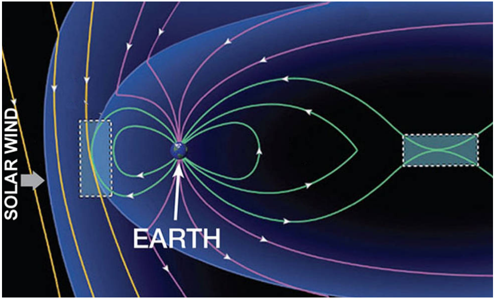
Kinetic (PIC)

Advantages:

- $\approx$ All of the physics

Disadvantages:

- Must resolve important scales
- Computationally painful



Resolution for Explicit PIC

For timestep Δt, grid spacing Δx, and velocity u a general constraint is

- CFL (Courant-Friedrichs-Lewy):

$$\frac{u\Delta t}{\Delta x} \leq 1$$

For plasmas also need to resolve important physical scales

- $\Delta x < (\lambda_D, \omega_{pe}, \rho_{Le})$
- $\Delta t < (\omega_{pe}, \omega_{ce})$

Not resolving generally leads to numerical instability.

Kinetic Scales

How painful?

- Solar corona: $B = 50$ G, $n = 10^9$ cm^{-3}, $L \approx 10^9$ m, $\tau \approx 10^3$ s
  - $d_p \approx 10$ m
  - $\Omega_{pc}^{-1} \approx 2 \times 10^{-6}$ s
  - $\omega_{pi}^{-1} \approx 2 \times 10^{-8}$ s
- Magnetosphere: $B = 2 \times 10^{-4}$ G, $n = 20$ cm^{-3}, $L \approx 10^4$ km, $\tau \approx 10^3$ s
  - $d_p \approx 50$ km
  - $\Omega_{pc}^{-1} \approx 0.5$ s
  - $\omega_{pi}^{-1} \approx 2 \times 10^{-4}$ s
- Tokamak: $B = 3 \times 10^4$ G, $n = 2 \times 10^{13}$ cm^{-3}, $L \approx 10^2$ cm, $\tau \approx 10^{-2}$ s
  - $d_p \approx 5$ cm
  - $\Omega_{pc}^{-1} \approx 3 \times 10^{-9}$ s
  - $\omega_{pi}^{-1} \approx 2 \times 10^{-10}$ s

The Annoyances of Reality

And How to Get Around Them

Besides real systems being much larger than kinetic scales, nature insists on making the situation worse.

- $m_p/m_e \approx 1836$
- $c/v_A \gg 1$

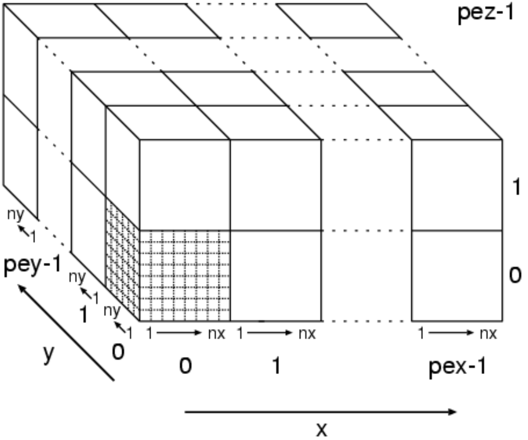
The resulting separation of scales is computationally challenging. To combat it, artificial values are often used

- $m_p/m_e = 400, 100, 25$
- $c/v_A = 20 - 50$

Potential unwanted side-effects (e.g., $v_{th,e} \to c$) must be kept in mind.

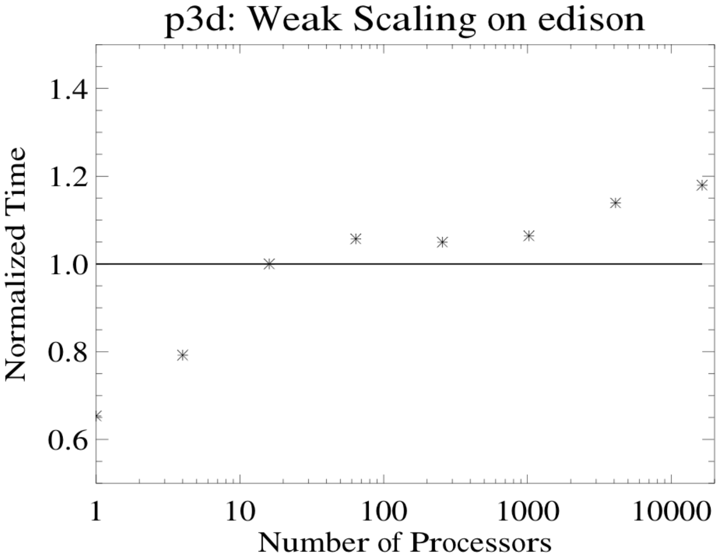
PIC on Supercomputers

Domain Decomposition



A useful simulation ($\gtrsim 10^{10}$ particles) needs many cores working in parallel. Communication should be minimized.

Supercomputer Performance



Brief Notes on PIC-Related Topics

Accurate Numerical Differentiation

Not PIC-Specific

From the Taylor series

$$f(x_0 + \Delta x) = f(x) + \Delta x \left.\frac{df}{dx}\right|_{x_0} + \frac{(\Delta x)^2}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_0} + \mathcal{O}(\Delta x^3)$$

comes the approximation

$$\frac{df}{dx} = \frac{f(x + \Delta x) - f(x)}{\Delta x} + \mathcal{O}(\boldsymbol{\Delta x})$$

Incorporating a variation

$$f(x_0 - \Delta x) = f(x) - \Delta x \left.\frac{df}{dx}\right|_{x_0} + \frac{(\Delta x)^2}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_0} + \mathcal{O}(\Delta x^3)$$

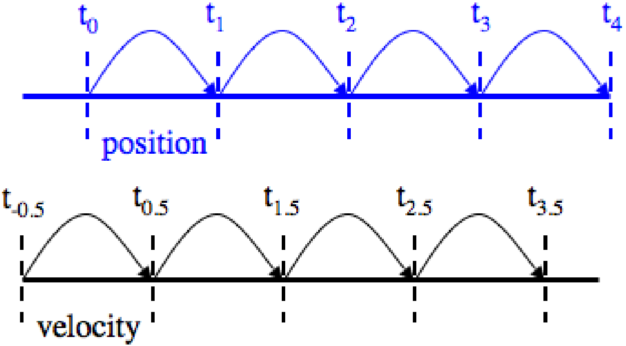
gives something more accurate

$$\frac{df}{dx} = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} + \mathcal{O}(\boldsymbol{\Delta x^2})$$

Symmetry Reduces Errors and Helps Stability

From https://www.particleincell.com/2011/velocity-integration/

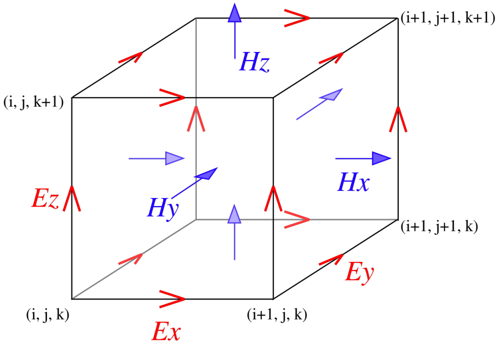
Basic leapfrog algorithm



Gridding Systems

Adapted from `https://commons.wikimedia.org/wiki/File:Yee-cube.svg`

The Yee lattice is a popular – but not the only – choice.
E is known on edges, **B**/**H** on faces.



The finite-difference versions of Maxwell's equations are nice, but bookkeeping is an annoyance.

Explicit Versus Implicit Algorithms

Consider

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

Explicit discretization:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D\left[\frac{u_{j+1}^{\mathbf{n}} - 2u_j^{\mathbf{n}} + u_{j-1}^{\mathbf{n}}}{(\Delta x)^2}\right]$$

Implicit discretization:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D\left[\frac{u_{j+1}^{\mathbf{n+1}} - 2u_j^{\mathbf{n+1}} + u_{j-1}^{\mathbf{n+1}}}{(\Delta x)^2}\right]$$

Implicit is typically much more stable but requires much more work to solve.