Kinetic Plasma Simulations

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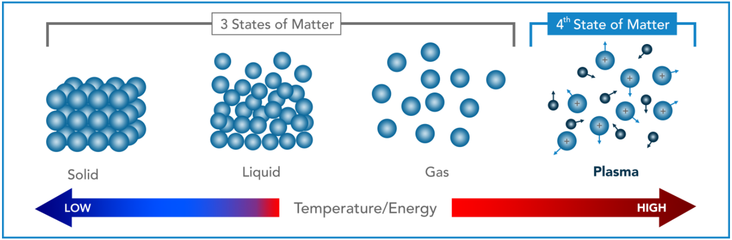
Outline

Plasma state of matter

Plasma

- Plasma: ionized gas ($T > 10^4 K$) and its electromagnetic field.
- Plasma physics: studies plasma behavior through experiment, theory and simulation!
- Simulation needed to study collective and kinetic effects, especially in the nonlinear development.
- Applications: reconnection, anomalous resistivity, instabilities, transport, heating, etc.



Time and length scale of plasma physics

Strongly interacting systems

- Plasma frequency: $\omega_p = \left(\frac{4\pi \mathrm{ne}^2}{\mathrm{m}}\right)^{1/2}$.
- Larmor frequency: $\omega_L = \frac{eB}{mc}$
- Debie length: $\lambda_\mathrm{D} = \frac{\mathrm{v_{th}}}{\omega_\mathrm{p}} \propto \left(\frac{\mathrm{T}}{\mathrm{n}}\right)^{1/2}$.
- Skin depth: $\lambda_{\mathsf{skin}} = c/\omega_\mathrm{p}$

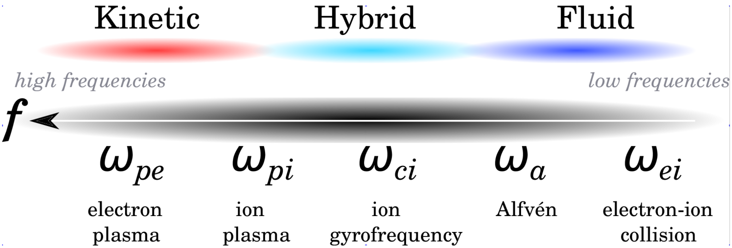


Figure 2: Time scale.

Thought experiment

The first step to decide how to model a system of interacting particles is to distinguish between weakly and strongly interacting systems.

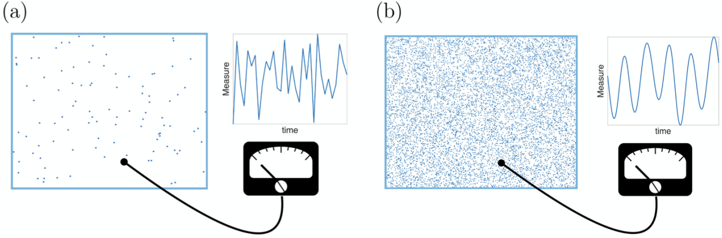


Figure 3: Thought experiment for strongly (a) versus weakly (b) coupled systems.

Types of interacting systems

Strongly interacting systems

- Presence of few particles in the Debye box.
- Evolution is determined by the close encounters and by the relative configuration of any two pairs of particles $\rightarrow$ Collisions.
- Spiky behaviour of the electric field.

Weakly interacting systems

- Extremely large number of particles in the Debye box.
- The mean field is produced by the superposition of contributions from a large number of particles.
- Smooth behaviour of the electric field.

Are important collision?

- We are interested in: $\mathrm{L} >> \lambda_{\mathrm{D}}, \quad \mathrm{t} >> \omega_{\mathrm{p}}^{-1}, \omega_{\mathrm{L}}^{-1}$.
- Number of particles in Debye cube: $N_{\mathrm{D}} = n\lambda_{\mathrm{D}}^{3}$.
- Plasma is collisionless if: $L >> \lambda_{\mathrm{D}}, \quad N_{\mathrm{D}} >> 1$.

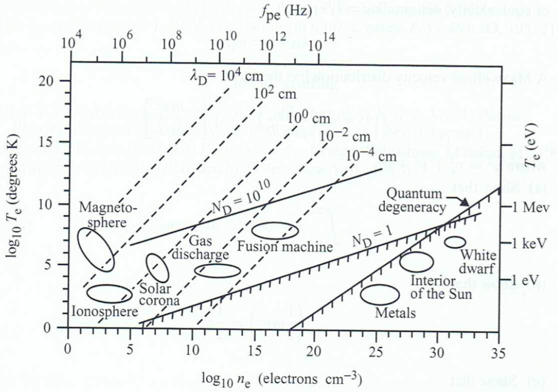


Figure 4: Plasma parameter from various sources.

Strength of interaction

Electrostatic potential energy:

$$E_{\mathrm{pot}} = \frac{q^2}{4\pi\epsilon_0 a}, \quad a \equiv n^{-1/3} \tag{1}$$

Thermal energy:

$$E_{\mathrm{th}} = k_B T \tag{2}$$

Plasma coupling parameter

$$\Gamma = \frac{E_{\mathrm{pot}}}{E_{\mathrm{th}}} = \frac{q^2}{4\pi N_D^{2/3}} = \begin{cases} \Gamma >> 1 & \text{Strongly coupled} \\ \Gamma << 1 & \text{Weakly coupled} \end{cases} \tag{3}$$

Outline

A bit of history

- 1950's John Dawson began 1D electrostatic "charge-sheet" experiments at Priceton, later at UCLA.
- 1965's Hockney and Buneman introduced grids and direct Poisson solve.
- 1970's Langdon developed the theory of electrostatic PIC $\Rightarrow$ first electromagnetic codes.
- 80's-90's 3D EM PIC takes off (always in step with Moore's law).

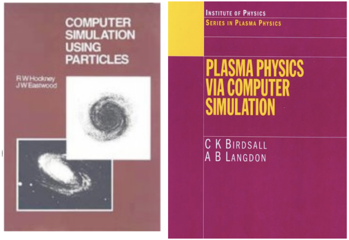


Figure 5: Holy bibles of PiC.

Computer simulation of interacting systems

Particle-particle (P-P) approach

- Evolving the equations of Newton for each of the N particles.
- Method used for strongly coupled systems (molecular dynamics, cosmological studies).

Particle-in-cell (PIC) method

- Finite-size particle approach $\rightarrow$ computational particles can be visualized as a small piece of phase space.
- Behave as point particles but when they overlap, the overlap zone is neutralized.
- Even though we have few computational particles in the Debye cube, the behavior resembles that of weakly coupled systems.
- Finite-size particles $\Rightarrow$ reduction of the potential energy for the same kinetic energy.

Phase space discretization: finite-size computational particles

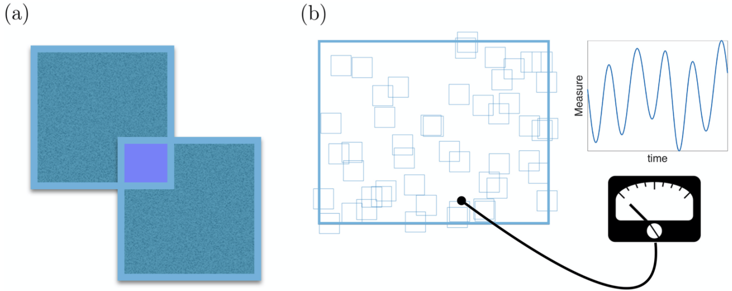


Figure 6: (a) Finite-size part behave as point particles until their respective surfaces start to overlap: the force starts to decrease to become zero for complete overlap. (b) Shows a Debye cube filled by a set of computational particles to illustrate the idea of the PIC method.

Coulomb force in comparison

To simulate of weakly coupled systems we use finite-size part: group of particles with similar phase space coordinate.

Point particles:

- Short range $\rightarrow$ collision effects.
- Long range $\rightarrow$ collective effects.

Finite-size particles:

- Long range $\rightarrow$ the force is identical to the Coulomb force.
- Short range $\rightarrow$ reduction.

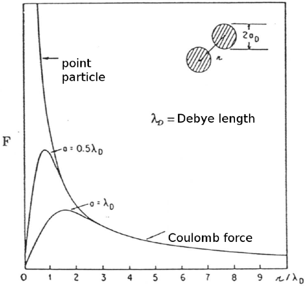


Figure 7: Coulomb force between two spherical charged particles as a function of their distance.

Set of equations

The kinetic description of a plasma aims to describe the system via electromagnetic fields and distribution functions.

Boltzmann equation

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \frac{\partial f_s}{\partial \mathbf{x}} + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_s}{\partial \mathbf{v}} = St\left(f_s\right) \tag{4}$$

Maxwell's equations

$$\partial_\nu F^{\mu\nu} = \frac{1}{c} j^\mu \tag{5}$$

Charge and current density

$$\begin{cases} \rho(\mathbf{x}, t) = \sum_s q_s \int_{\mathbb{V}} f_s(\mathbf{x}, \mathbf{v}, t) \mathrm{d}\mathbf{v} \\ \mathbf{j}(\mathbf{x}, t) = \sum_s q_s \int_{\mathbb{V}} \mathbf{v} f_s(\mathbf{x}, \mathbf{v}, t) \mathrm{d}\mathbf{v} \end{cases} \tag{6}$$

Mathematical formulation of PiC

The distribution function of each species is given by the superposition of several elements (called computational particles) represents by a large number of physical particle

$$f_s(\mathbf{x}, \mathbf{v}, t) = \sum_p f_p(\mathbf{x}, \mathbf{v}, t) \tag{7}$$

The functional dependence is assumed to be a tensor product of the shape functions in each direction of phase space

$$f_p(\mathbf{x}, \mathbf{v}, t) = N_p S_{\mathbf{x}}\left(\mathbf{x} - \mathbf{x}_p(t)\right) S_{\mathbf{v}}\left(\mathbf{v} - \mathbf{v}_p(t)\right) \tag{8}$$

Prop. of shape functions

- Compact in order to describe a small portion of phase space.
- Unitary integral over the domain: $\int_{V_\xi} S_\xi\left(\xi - \xi_p\right) \mathrm{d}\xi = 1$.
- Simmetric shape: $S_\xi\left(\xi - \xi_p\right) = S_\xi\left(\xi_p - \xi\right)$.

Definition of shapes function

For velocity Dirac's delta

$$S_{\mathrm{v}}\left(\mathbf{v}-\mathbf{v}_p\right)=\delta\left(v_x-v_{xp}\right)\delta\left(v_y-v_{yp}\right)\delta\left(v_z-v_{zp}\right) \tag{9}$$

$\Rightarrow$ particles within the element of phase space remain closer in phase space during the subsequent evolution.

For space b-splines

$$S_{\mathbf{x}}\left(\mathbf{x}-\mathbf{x}_p\right)=\frac{1}{\Delta x_p \Delta y_p \Delta z_p} b_\ell\left(\frac{x-x_p}{\Delta x_p}\right) b_\ell\left(\frac{y-y_p}{\Delta y_p}\right) b_\ell\left(\frac{z-z_p}{\Delta z_p}\right) \tag{10}$$

- Def.: $b_\ell(\xi)=\int_{-\infty}^{\infty}\mathrm{d}\xi' b_0\left(\xi-\xi'\right) b_{\ell-1}\left(\xi'\right)$
- Sum over all points of evaluation is unitary: $\sum_i b_\ell(\xi+i)=1$.
- The integral of b-splines of any order is unitary: $\int_{-\infty}^{\infty} b_\ell(\xi)\mathrm{d}\xi=1$.
- $\delta(\xi)\equiv b_{-1}(\xi)$

PiC choiche is 0 order b-splines

A choice referred to as cloud-in-cell (CiC) because the particle is a uniform square cloud in space with an infinitesimal span in the velocity directions.

$$b_0(\xi) = \begin{cases} 1 & \text{if } |\xi| < 1/2 \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

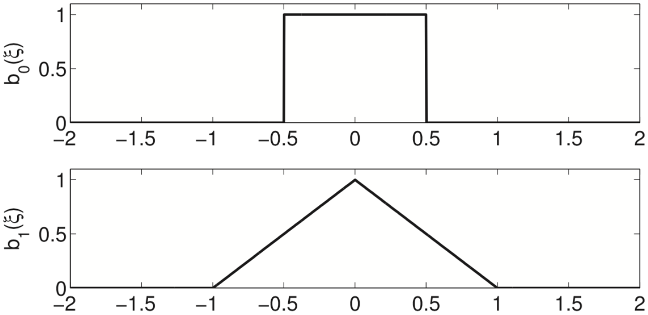


Figure 8: The first two b-spline functions.

Derivation of the equations of motion (physical part.)

Phase space

$$\frac{\partial f_p}{\partial t} + \mathbf{v} \cdot \frac{\partial f_p}{\partial \mathbf{x}} + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_p}{\partial \mathbf{v}} = 0 \tag{12}$$

- The Vlasov eq. is not linear in f_p because f_s is involved inside total fields.
- The function (8) cannot satisfied locally the Vlasov eq. (12) but only in average.

Time evolution

$$\frac{\mathrm{d}\mathbf{v}_p}{\mathrm{d}t} = \frac{q_s}{m_s}\left(\mathbf{E}_p + \mathbf{v}_p \times \mathbf{B}_p\right) \tag{13}$$

- Fields as average over the shape function: $\mathbf{E}_p = \int S_{\mathbf{x}}\left(\mathbf{x} - \mathbf{x}_p\right)\mathbf{E}(\mathbf{x})\mathrm{d}\mathbf{x}$.

Derivation of the equations of motion (PiC)

Computational part.

- Vlasov eq. is formally linear in f_s.
- The continuum distribution function is replaced by a discrete mathematical representation provided by the superposition of moving fixed-shape computational particles of finite size.
- Element of phase space described by the shape functions (9) (10) chosen for the discretization would be distorted by non-uniform electric and magnetic fields. Instead thr Liouville teorem requires the conservation of the phase-space volume of each element.

Coupling with the field equations: spatial discretization on a grid (I)

Discretized Maxwell eq.

- Continuum operator and sources are replaced by discrete ones: $\nabla, \rho, J \rightarrow \nabla_g, \rho_g, J_g$.
- Hp $\rightarrow$ fields are known at grid points, not necessarily the same for both fields (Yee lattice). Are defined as point values or averages over control volumes: E_g, B_g

Sources

$$\begin{cases} \rho_g = \frac{1}{V_g} \sum_p q_p W\left(\mathbf{x}_g - \mathbf{x}_p\right) \\ \mathbf{j}_g = \frac{1}{V_g} \sum_p q_p \mathbf{v}_p W\left(\mathbf{x}_g - \mathbf{x}_p\right) \end{cases} \tag{14}$$

Interpolation function:

$$W\left(\mathbf{x}_g - \mathbf{x}_p\right) = b_{l+1}\left(\frac{x_g - x_p}{\Delta x}\right) b_{l+1}\left(\frac{y_g - y_p}{\Delta y}\right) b_{l+1}\left(\frac{z_g - z_p}{\Delta z}\right) \tag{15}$$

Coupling with the field equations: spatial discretization on a grid (II)

Interpolation func. for the electric and magnetic fields

$$S_{\mathrm{E,B}}\left(\mathrm{x}-\mathrm{x}_g\right) = b_0\left(\frac{x_g - x_p}{\Delta_x}\right) b_0\left(\frac{y_g - y_p}{\Delta_y}\right) b_0\left(\frac{z_g - z_p}{\Delta_z}\right) \tag{16}$$

Total fields

$$\begin{aligned} \mathbf{E}(\mathbf{x}) &= \sum_g \mathbf{E}_g S_{\mathbf{E}}\left(\mathbf{x}-\mathbf{x}_g\right) \\ \mathbf{B}(\mathbf{x}) &= \sum_g \mathbf{B}_g S_{\mathbf{B}}\left(\mathbf{x}-\mathbf{x}_g\right) \end{aligned} \tag{17}$$

Particles field

$$\begin{aligned} \mathbf{E}_p &= \sum_g \int S_{\mathbf{x}}\left(\mathbf{x}-\mathbf{x}_p\right) \mathbf{E}_g S_{\mathbf{E}}\left(\mathbf{x}-\mathbf{x}_g\right) \mathrm{d}\mathbf{x} \\ \mathbf{B}_p &= \sum_g \int S_{\mathbf{x}}\left(\mathbf{x}-\mathbf{x}_p\right) \mathbf{B}_g S_{\mathbf{B}}\left(\mathbf{x}-\mathbf{x}_g\right) \mathrm{d}\mathbf{x} \end{aligned} \tag{18}$$

Temporal discretization

Maxwell's and Newton's equations are coupled. Newton's equations need the electric and magnetic fields and Maxwell's equations need the particle positions to compute the sources: current and density.

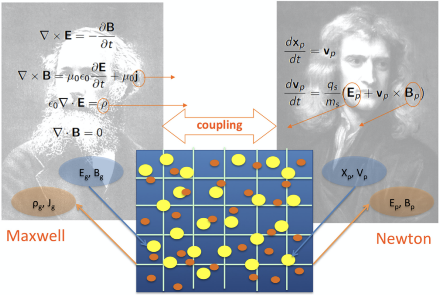


Figure 9: The computational part.are indicated as coloured dots, the larger yellow ones are ions, and the smaller orange ones electrons. The dot size is indicative of the mass of the particles, not their sizes. All computational particles have the same size (equal to the size of the cells).

Outline

Explicit temporal discretization of the particle equations (I)

The leap-frog algorithm is based on staggering the time levels of the velocity and position by a half time step; it's used to discretizing in time Newton's equations for the particles.

$$
\begin{aligned}
&\frac{\mathbf{x}_p^{n+1}-\mathbf{x}_p^n}{\Delta t} = \mathbf{v}_p^{n+1/2} \\
&\frac{\mathbf{v}_p^{n+1/2}-\mathbf{v}_p^{n-1/2}}{\Delta t} = \frac{q_s}{m_s}\mathbf{E}^n\left(x_p^n\right) + \frac{q_s}{m_s}\left(\frac{\mathbf{v}_p^{n+1/2}+\mathbf{v}_p^{n-1/2}}{2}\right)\times\mathbf{B}^n\left(x_p^n\right)
\end{aligned}
\tag{19}
$$

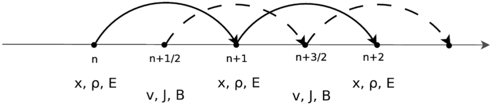


Figure 10: The time discretization is staggered, with the electric field, charge density, and particle positions at integer times, and the magnetic field, current, and particle velocity at half time steps.

Explicit temporal discretization of the particle equations (II)

The first equation (19) is clearly explicit, the second can be formulated explicitly as a roto-translation of the vector $v_p^{n-1/2}$:

$$\mathbf{v}_p^{n+1/2} = 2\left(\hat{\mathbf{v}}_p + \beta_s \hat{\mathbf{E}}_p\right) - \mathbf{v}_p^{n-1/2} \tag{20}$$

where hatted quantities have been rotated by the magnetic field:

$$\begin{aligned} \hat{\mathbf{v}}_p &= \alpha_p^n \mathbf{v}_p^{n-1/2} \\ \hat{\mathbf{E}}_p &= \alpha_p^n \mathbf{E}_p^n \end{aligned} \tag{21}$$

via a rotation matrix α_p^n defined as:

$$\alpha_p^n = \frac{1}{1 + \left(\beta_s B_p^n\right)^2} \left(1 - \beta_s \mathbf{I} \times \mathbf{B}_p^n + \beta_s^2 \mathbf{B}_p^n \mathbf{B}_p^n\right) \tag{22}$$

Where $\mathbf{I}$ is the dyadic tensor (matrix with diagonal of 1) and $\beta_s = q_p \Delta t / 2 m_p$ (independent of the particle weight and unique to a given species).

Explicit PIC cycle: curl eq.

We discretize Maxwell's eq. in time using use the leap-frog algorithm for the fields:

$$\begin{aligned} \nabla_g \times \mathbf{E}^n &= \tfrac{\mathbf{B}^{n+1/2} - \mathbf{B}^{n-1/2}}{\Delta t} \\ \nabla_g \times \mathbf{B}^{n+1/2} &= \mu_0 \mathbf{J}_g^{n+1/2} + \mu_0 \epsilon_0 \tfrac{\mathbf{E}^{n+1} - \mathbf{E}^n}{\Delta t} \end{aligned} \tag{23}$$

When quantities are not at the same time level we do average. The current needs to be accumulated from the particle information:

$$\mathbf{j}_g^{n+1/2} = \frac{1}{V_g} \sum_p q_p \mathbf{v}_p^{n+1/2} \frac{W\left(\mathbf{x}_g - \mathbf{x}_p^n\right) + W\left(\mathbf{x}_g - \mathbf{x}_p^n\right)}{2} \tag{24}$$

In a similar manner the magnetic field:

$$\mathbf{B}^n = \frac{1}{2}\left(\mathbf{B}^{n+1/2} + \mathbf{B}^{n-1/2}\right) \tag{25}$$

Explicit PIC cycle: divergence eq.

The divergence conditions are valid at all times if they are valid at the initial time and if the charge continuity eq. is satisfied. The divergence of the magnetic field is always zero, for the electric field there are some issues.

Solutions:

- Charge conserving: ρ, $\mathbf{J}$ interpolation from particles to grid can be modified to ensure continuity equation.
- Divergence cleaning: every step $\mathbf{E}$ field can be cleaned for any component not satisfying Gauss law (numericalal expensive).

This sol. can be combined to avoid numerical error to get the PiC cycle.

Pros and Cons

- Pro: no iteration needed $\rightarrow$ each step requires only info from the privious one.
- Con: small t. step $\leftrightarrow$ in a fixed step fields are frozen while particles evolve and vice versa.

Four step PiC cycle

$$\mathbf{E}_p^n = \sum_g \mathbf{E}_g^n W(\mathbf{x}_g - \mathbf{x}_p^n) d\mathbf{x}$$

$$\mathbf{B}_p^n = \sum_g \mathbf{B}_g^n W(\mathbf{x}_g - \mathbf{x}_p^n) d\mathbf{x}$$

$$\mathbf{v}_p^{n+1/2} = 2\left(\widehat{\mathbf{v}}_p + \beta_s \widehat{\mathbf{E}}_p\right) - \mathbf{v}_p^{n-1/2}$$

$$\widehat{\mathbf{v}}_p = \alpha_p^n \mathbf{v}_p^n$$

$$\widehat{\mathbf{E}}_p = \alpha_p^n \mathbf{E}_p^n$$

$$\alpha_p^n = \frac{1}{1+(\beta_s B_p^n)^2}\left(\mathbb{I} - \beta_s \mathbb{I} \times \mathbf{B}_p^n + \beta_s^2 \mathbf{B}_p^n \mathbf{B}_p^n\right)$$

$$\mathbf{j}_g^{n+1/2} = \frac{1}{V_g} \sum_p q_p \mathbf{v}_p^{n+1/2} \frac{W(\mathbf{x}_g - \mathbf{x}_p^n) + W(\mathbf{x}_g - \mathbf{x}_p^n)}{2}$$

$$\mathbf{E}^{n+1} = \mathbf{E}^n + \frac{\Delta t}{\mu_0 \epsilon_0}\left(\nabla_g \times \mathbf{B}^{n+1/2} - \mu_0 \mathbf{J}_g^{n+1/2}\right)$$

$$\mathbf{B}^{n+3/2} = \mathbf{B}^{n+1/2} - \Delta t \nabla_g \times \mathbf{E}^{n+1}$$

$$\mathbf{B}^{n+1} = \frac{1}{2}\left(\mathbf{B}^{n+3/2} + \mathbf{B}^{n+1/2}\right)$$

Figure 11: Starting from the top: (1) electric and magnetic fields from the previous time step are interpolated to the particles; (2) particles are advanced over Δt to find the new position and velocity; (3) particle information is then interpolated to the grid to obtain the current density in each cell; (4) fields are then advanced for the same Δt on the grid.

Electostatic PiC $\Rightarrow$ J is small

Gauss law that can be rewritten in terms of the electrostatic potential:

$$\begin{aligned} \Delta_g \phi &= -\frac{\rho_g}{\epsilon_0} \\ E_g &= -\nabla_g \phi \end{aligned} \tag{26}$$

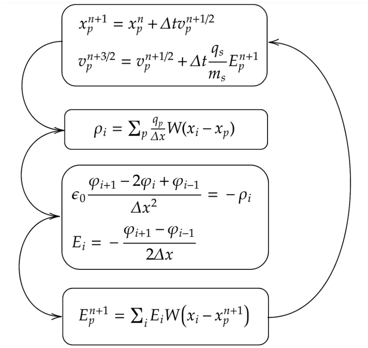


Figure 12: Electrostatic PiC cycle.

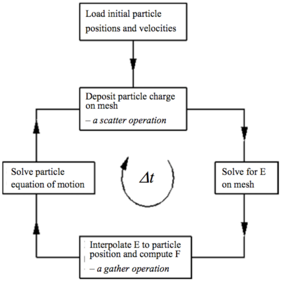


Figure 13: Electrostatic PiC cycle.

Stability of the explicit PiC

Explicit PIC have limitations to avoid numerical heating(energy explode):

Particle mover

$$\Delta t < 2/\omega_{pe}, \quad (\omega_{pe}\Delta t = 0.1) \tag{27}$$

Von Neuman Analisys applied to Langmiur wave.

Explicit time differencing of the field equations

$$\Delta x > c\Delta t \tag{28}$$

Courant–Friedrich–Levy cond. to discretize hyperbolic func. explicitly.

Finite grid instability

$$\Delta x > \lambda_D \zeta \tag{29}$$

Collapsing the continuum particle shapes to discrete contributions in a set of points.

Solution to prohibitive stability condition

Some solution to avoid small time steps and grid spacing required by explicit methods:

- Darwin approx.: for slow-varying magnetic fields $\rightarrow$ from Maxwell's equations the terms allowing the propagation of light.
- Hybrid approx.: eliminate some of the electron physics needed to resolve Debye length $\rightarrow$ treating electron like fluids.
- Gyrokinetic approx.: averaging over the gyration of particles in large magnetic fields (widely used in fusion research).
- Modern solution: introduce a new numerical method more sofisticated.

Outline

Implicit particle methods (ECPiC)

Particle and field equations are solved simultaneously (coupled), additionally particles eq. are non-linear.

- Replace the leap-frog algorithm with a new mover (remuve stability constraints).
- Exactly energy conserving ($\epsilon_r < 10^{-9}$).
- Inconditionally stable.

θ-scheme

$$\begin{aligned} \mathbf{x}_p^{n+1} &= \mathbf{x}_p^n + \Delta t \mathbf{v}_p^{n+\theta} \\ \mathbf{v}_p^{n+1} &= \mathbf{v}_p^n + \frac{q_p \Delta t}{m_p}\left(\mathbf{E}_p^{n+\theta}(\bar{\mathbf{x}}_p) + \bar{\mathbf{v}}_p \times \mathbf{B}_p^{n+\theta}(\mathbf{x}_p)\right) \end{aligned} \tag{30}$$

Where barred variables are average between time level n and n+1 $\bar{\mathbf{x}} = \frac{\mathbf{x}^{n+1} + \mathbf{x}^{n+1}}{2}$, and variables of time index $n+\theta$ are defined as $\mathbf{x}^{n+\theta} = \theta \mathbf{x}^{n+1} + (1-\theta)\mathbf{x}^n$.

Implicit vs Explicit

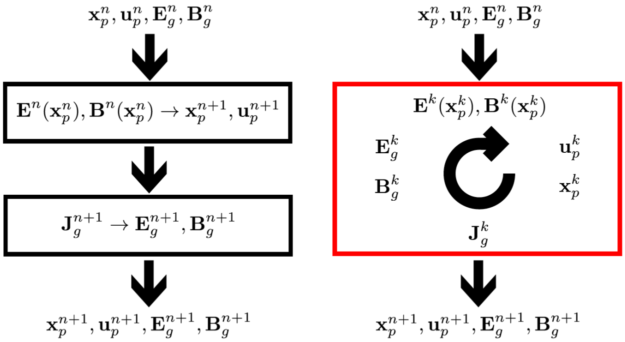


Figure 14: Schematic comparison between the typical computational cycle of an explicit PiC method (left) and an implicit method (right). Black boxes indicate explicit (non-iterative) operations, while red boxes indicate the use of an iterative solution process.

References

@incollectionch4, author = "Lapenta Giovanni", title = "Particle-based simulation of plasmas", booktitle = "Plasma Modeling", publisher = "IOP Publishing", year = "2016"