The particle-in-cell simulation method: Concept and limitations

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Why (and when) particle-in-cell (PIC) simulations?

- Particle-in-cell / Vlasov codes can address all collisionless plasma processes
- Such codes can be used to verify linearized plasma dispersion relations
- The plasma dynamics can be followed through its non-linear phase
- PIC simulations have an 'unlimited' dynamical range for the particle velocities and no boundary conditions along $v$
- PIC codes have a limited signal-to-noise ratio and phase space density resolution
- PIC schemes parallelize well
What do PIC / Vlasov codes solve?

\[ \nabla \times E = -\frac{\partial B}{\partial t} \]  

(1)

\[ \nabla \times B = \mu_0 \epsilon_0 \frac{\partial E}{\partial t} + \mu_0 J \]  

(2)

\[ \nabla \cdot B = 0 \]  

(3)

\[ \nabla \cdot E = \rho / \epsilon_0 \]  

(4)

Vlasov equation for phase space distribution \( f(x, v, t) \)

\[ \frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{q}{m} (E + v \times B) \cdot \nabla_v f = 0 \]  

(5)

\[ \rho(x, t) = q \int_{-\infty}^{\infty} f(x, v, t) \, dv, \quad J(x, v, t) = q \int_{-\infty}^{\infty} v f(x, v, t) \, dv \]  

(6)
Numerics / Principle

Field equations

Replace continuous fields $B(x, t)$, $E(x, t)$ and Maxwell’s equations by their discretized counterparts.

(1) Introduce finite spatial resolution $x \rightarrow j \Delta x$ and finite time resolution $t \rightarrow j \Delta t$, with integer values $j$.

(2) Replace differential operators by difference operators. Example: $\frac{d}{dx} f(x) \rightarrow \frac{f[(j + 1) \Delta x] - f[j \Delta x]}{\Delta x}$.

⇒ Replaces differential equations by algebraic equations.

Particle equations (PIC codes only)

Replace continuous probability distribution by phase space elements

$$f(x, v, t) \Rightarrow \sum_{i=1}^{N} S(x - x_i) \delta(v - v_i), \quad (7)$$

where $S(x)$ is a shape function, e.g. a triangle.

⇒ Replaces phase space probability function by 'computational particles'.
**Phase space distribution:** Maxwellian distributions are often used.

Quantitatively different results are sometimes obtained with Vlasov codes (upper phase space distribution) and PIC codes (lower phase space distribution)!

- If particle weights are equal, the statistical representation of the plasma close to the mean speed of the species is good.

- The statistical representation is poor, if $|v - \bar{v}| \geq 2v_t$ for a Maxwellian $\exp\left(-\frac{(v - \bar{v})^2}{2v_t^2}\right)$. 
Particle-grid interaction

- The fields are defined on a grid (Field nodes).
- The particles move on ’continuous’ paths.
- Particles interact with the grid through \( \rho \) and \( \mathbf{J} \).
- The grid interacts with the particles through \( \mathbf{E} \) and \( \mathbf{B} \).

⇒ Interpolation schemes must be specified
• A computational electron is located between the cells $i, i + 1$ with the positions $X_i$ and $X_{i+1}$.
• It has the distance $D1$ from $X_i$ and $D2$ from $X_{i+1}$.
• Electron charge $Q$ is assigned to the grid nodes $i, i + 1$:
  \[ C_i = f_1(D1, D2) \] and \[ C_{i+1} = f_2(D1, D2). \]
• Example: $C_i = Q D2$ and $C_{i+1} = Q D1$ if $(X_{i+1} - X_i) = 1$.

Electric field $\vec{E}$

- Calculate potential $\Phi$ with $\nabla^2 \Phi = -\rho/\epsilon_0$ with $\rho_i \sim C_i$ and $\rho_{i+1} \sim C_{i+1}$.
- $\mathbf{E} = -\nabla \Phi$.
- Interpolate $\mathbf{E}$ to particle position: $\mathbf{E}(x) = D2 \cdot \mathbf{E}(x_i) + D1 \cdot \mathbf{E}(x_{i+1})$
1. Initialize plasma phase space distribution:
   - Place particles in space according to density
   - Initialize velocities with random numbers
2. Initialize E and B fields
3. From E,B fields calculate acceleration
4. Multiply acceleration with time step
   -> Velocity increment
5. Multiply velocity with time step
   -> Position increment
6. From new positions and velocities:
   Calculate new E,B
Limitations:

Known limitations with known consequence: Field discretization

- Spatial step $\Delta x \approx$ Debye length $\lambda_d = v_t/\omega_p$.
- Numerical stability $\rightarrow$ small time step $\Delta t$.
  For my code: $\Delta t = N_c \Delta x / \sqrt{2} c$ with $0 < N_c < 1$.
- We have $\Delta x = v_t/\omega_p$ and for $N_c = 1$ we get $\sqrt{2} \Delta t \omega_p = v_t/c$.
  $\Rightarrow$ Low $v_t$ requires high sampling rate. Critical speed $v_t \approx 10^6 m/s$.

Known limitations with unknown consequence:

Particle per cell count rates follow Poisson statistics $\rightarrow$ For $N_e$ particles per cell, the relative fluctuations are $1/\sqrt{N_e}$.

- Fluctuations result in particle-wave collisions.
- Parametric instabilities speed up.
- Dispersive properties change. Bernstein modes are damped 'close' to $n\omega_c$.
- Signal-to-noise ratio is low.
Spatial grid effects

In ‘continuous infinite plasmas’: Fourier integral

Infinitely extended and continuous position $x$ and wavenumber $k$ domains.

\[ f(x) \leftrightarrow g(k) \quad (8) \]
\[ f(x) = \int_{-\infty}^{\infty} g(k) \exp(ikx) \, dk \quad (9) \]
\[ g(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) \exp(-ikx) \, dx \quad (10) \]
In 'continuous confined plasmas': Fourier series

Limited position $0 < x < L$, $f(x)$ continuous. Unlimited, discrete $k$ spectrum.

$$f(x) \leftrightarrow g_k = g(k_k)$$  \hspace{1cm} (11)

$$f(x) = \sum_{k=-\infty}^{\infty} g_k \exp(\imath k_k x)$$  \hspace{1cm} (12)

$$g_k = \frac{1}{L} \int_{x=0}^{x=L} f(x) \exp(-\imath k k x) \, dx$$  \hspace{1cm} (13)

Periodicity of $\exp(\imath k x) \rightarrow$ The $f(x)$ is periodic, but not $g_i$. 

![Graph showing Amplitude vs Position and Power vs Wavenumber](image-url)
In ’PIC plasmas’: Discrete Fourier transform

The PIC code cannot represent a Fourier series → The \( k \)-spectrum is truncated.

\[
f_n = f(x_n) \Leftrightarrow g_k = g(k_k)
\]  \hspace{1cm} (14)

\[
f_n = \sum_{k=0}^{N-1} g_k \exp\left(\frac{2\pi i k n}{N}\right), \ n = 0, \ldots, N - 1
\]  \hspace{1cm} (15)

\[
g_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n \exp\left(-\frac{2\pi i k n}{N}\right), \ k = 0, \ldots, N - 1
\]  \hspace{1cm} (16)
Finite grid instability

- Phase space distribution has rapid oscillations: \( F(k_s, x) = \sin(k_s x) \).
- Grid imposes a maximum \( k_{Ny} = \pi / \Delta x \).
- A box with length \( L \) has the minimum \( k_M = 2\pi / L \).

(a) \( k_1 = k_{Ny}/25 \) and \( k_2 = k_{Ny}/100 \). Integer values for \( k_1/k_M \) and \( k_2/k_M \).
Wave oscillation is well-resolved.

Finite-box effects 'fill up' the $k$-spectrum: power leaks to other $k$ (aliasing).
(c) \( k_1 = \frac{k_{Ny}}{2} \) and \( k_2 = \frac{3k_{Ny}}{2} \). Integer values for \( k_1/k_M \) and \( k_2/k_M \).

Peaks are identical in power but have different phases.
Some consequences:

- The aliasing is introduced by mapping oscillations with an 'unlimited' \( k \)–spectrum onto a grid with \( |k| < k_{Ny} \).

- Case (3) showed that \( k_1, k_2 \) with \( k_1 - k_2 = k_{Ny} \) differ only in phase.

- Truncated Fourier series \( \rightarrow \) forced periodicity in \( x \) and \( k \).
  Signals with \( k_1 \) and \( k_2 \) differing by \( 2k_{Ny} \) can’t be distinguished!

- Relation to crystals / metals: Brillouin zones

- First Brillouin zone \( |k\Delta_x| < \pi \). Other zones differ by \( 2k_{Ny} = k_g = 2\pi/\Delta_x \).

- In PIC simulations, elementary sine waves are actually not (!) eigenfunctions of the system.
Finite grid instability

Counterstreaming two-stream instability

\[ 1 - \frac{\omega_p^2}{\omega^2} = \frac{\Omega_b^2}{(\omega - kv_b)^2} + \frac{\Omega_b^2}{(\omega + kv_b)^2} \quad (17) \]

- Physical resonance term: \( \omega - kv_b = 0 \)
- Aliasing: \( \omega - (k + pk_g)v_b = 0 \), with integer \( p \).
- The term \( k_gv_b \) has the dimension of a frequency. It is the grid crossing frequency \( \omega_g \) of the particle beam.
- The beam drives many resonances \( \frac{(\omega - p\omega_g)}{k} = v_b \). Only \( p = 0 \) is physical.
- Consequence: In non-relativistic 1D simulations with \( k \parallel v_b \) the nonphysical instabilities are electrostatic and only heat the beam \( \rightarrow \) Harmless.
Finite grid instability of relativistic beams in 2D

- The phase speeds of the waves are \( \frac{\omega}{k} = v_b + p \frac{\omega\phi}{k} \).

- For speeds \( 1 - \epsilon < v_b/c < 1 \) and \( \epsilon \ll 1 \), a \( p \neq 0 \) introduces superluminal waves that couple directly to the beam. The resonance is sharp.

- Particle oscillations due to a wave with \( k \parallel v_b \) couple through \( \gamma \) to other velocity components.
  Quiver motion acts as antenna!

- In 2D/3D simulations, obliquely propagating electromagnetic waves couple to the fast moving charge density modulation
  \( \Rightarrow \) Electromagnetic radiation similar to free electron laser.
PIC simulation

- Spatially homogeneous system in x-y plane, periodic boundary conditions.
- Initially, $E = 0$ and $B = (0, 0, B_0)$ with $eB_0/m_e = \Omega_p/10$ ($\Omega_p =$ plasma frequency).
- Bulk electrons and protons at rest, number densities $n_e$ and $n_p$.
- Counter-streaming proton beams with velocity vector $\pm(v_b, 0, 0)$ and $v_b = 0.8c$. Beam density: $n_b$ each. Both beams differ in their temperature.
- $n_e = n_p + 2n_b$.
- Rectangular simulation box, sidelength $= 6\pi v_b / \Omega_p$. Resolved by a $1200 \times 1200$ mesh.
- The system is advanced in time for $t\Omega_p = 194$. 

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Numerics / Principle
Phase space distribution
Particle-grid interaction
Assignment scheme:
Particles ↔ Grid
PIC algorithm
Limitations
Spatial grid effects
Finite grid instability
PIC simulation
Discussion
Results 1:

- Left plot, upper row: 10-logarithmic wavenumber (power) spectrum of physical wave. \( v_b \) is parallel to the x-axis.

- Right plot, upper row: 10-logarithmic wavenumber (power) spectrum of grid instability waves.

- Left plot, lower row: Low-pass filtered \( |E_x + \nu E_y| \) in a rectangular sub-interval with the side length \( 2 \pi v_b / \Omega_p \).

- Right plot, lower row: \( |E_x + \nu E_y| \) in a rectangular sub-interval with the side length \( \pi v_b / 2 \Omega_p \).
Results 2:

- Two straight lines going through $k = 0, \Omega = 0$: Beam dispersion relation.
- Two curved lines going through $k = 0, \Omega = 0$ (on this scale): Light modes.
- Straight line at large $\Omega$ parallel to the lower beam dispersion relation: Sideband separated from beam mode by grid crossing frequency.
Discussion

- The particle-in-cell simulation method is currently the tool of choice for the investigation of non-linear processes in kinetic, collision-less plasma.

- In contrast to fluid / magnetohydrodynamic codes, its resolution is set by the plasma Debye length → it can not be scaled to fit best a problem.

- Its signal-to-noise ratio is limited by noise. Noise can introduce 'unknown' modifications.

- The statistically poor representation of plasma by PIC simulations can give different results compared to Vlasov simulations.  

- The finite grid instability turns out to be a severe simulation constraint for the investigation of relativistic plasma flows. It can be reduced only moderately by finer grids.  