PIC solvers for Intense Beams in Synchrotrons

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Space Charge Simulations in Synchrotrons

\[ \varepsilon_0 \nabla \cdot \vec{E} = \rho \]

(in the rest system of the beam)

\[ v_0 = \beta_0 c \]

\[ \beta_0 = 0.1 - 0.99 \quad \text{Bunch (rms length: 0.1 m–dc)} \]

\[ \text{Bunch length} \gg \text{pipe diameter} \]

Space charge tune shift: \[ \Delta Q_y^{sc} \propto -\frac{q^2 N}{m B_f} \frac{4}{\epsilon \beta_0^2 \gamma_0^3} \]

The transverse space charge force is the main intensity limiting effect in the FAIR synchrotrons at GSI and in other high current synchrotrons.

**Time scales:** 1000-10^6 turns (1 ms - 1 s)

\[ \rightarrow \text{Emittance growth, Beam loss (< 1%)} \]

**Challenge:** Control of numerical emittance growth!

**‘Space charge’ collaboration**
(CERN, GSI, FNAL, SNS, KEK, ...)

- Codes for long-term simulations
  \[ \rightarrow \text{Effect of stochastic noise!} \]
- (PIC) codes used for FAIR at GSI:
  pyORB11T, Micromap, PATRIC
PIC simulation scheme (for 2D beams)

- **\( q \)**: beam particle charge
- **\( Q = q \frac{N}{M} \)**: macro particle charge
- **\( N \)**: number of beam particles
- **\( M \times N \)**: number of macro-particles

\[
x''_i - \kappa(s)x_i - \frac{qE_x(x_i, y_i, s)}{\gamma_0mv_0^2} = 0
\]
\[
y''_i + \kappa(s)y_i - \frac{qE_y(x_i, y_i, s)}{\gamma_0mv_0^2} = 0
\]

‘Error’ sources:
1) ‘artificial’ collisions of macro-particles \( Q \) and test particles \( q \).

(Coulomb’s law)

\[
\vec{F}_i = \sum_{j=0}^{M} \frac{qQ'S(\vec{x}_i - \vec{x}_j)(\vec{x}_i - \vec{x}_j)}{2\pi\epsilon_0\gamma_0mv_0^2|\vec{x}_i - \vec{x}_j|}
\]

\( \rightarrow \) energy conserving.

2) Grid/stochastic heating

Depending on particle shape \( S \) the macro-particles have a finite width: \( \Delta \approx \Delta x \)

2.5D electric fields: bunches are long (m)

Compared to their transverse width (cm).

\[
\rho(x, y, s) = Q \sum_{i=0}^{M} S(\vec{x} - \vec{x}_i)
\]

Integrate Poisson's equation on the grid: \( \rho_p \rightarrow E_p \)

\[
\epsilon_0 \nabla \cdot \vec{E} = \rho(x, y, s)
\]

\( \Delta s \rightarrow \Delta x \)

Integrate equation of motion, assign new coordinates:

- Weighting: \( E_p \rightarrow F_i \)
- Weighting: \( x_i \rightarrow \rho_p \)
What physics system does a PIC code represent?

The system we would like to solve: **Collision-free Vlasov-Poisson (V-P) system**

\[
\frac{df}{dt} + x' \frac{df}{dx} + F_\perp \frac{df}{dx} = 0
\]

(Vlasov equation)

\[
\dot{\phi} \nabla \phi = \rho(x, y)
\]

(Poisson equation)

\[
\rho(x, y) = q \int f(x, x')d^2x
\]

(charge density)

\[
F_\perp = \kappa_{x,y}(s)x - \frac{q}{\gamma_0mv_0^2} \nabla \phi(x, y, s)
\]

(AG focusing) (space charge)

\[
\Rightarrow \quad S = -k \int f \ln fdx dx' = \text{const.} \quad \text{(Entropy)}
\]

What in fact we solve is (forget about the grid for a moment):

\[
\frac{dF}{dt} + x' \frac{dF}{dx} + F_\perp \frac{dF}{dx} = 0
\]

(Klimontovich equation)

\[
F(x, x') = \sum_{j=0}^{M} S(x - x_j) \delta(x' - x'_j)
\]

\[
\Rightarrow \quad S_{4M} = -k \int F \ln F dx dx' = \text{const.} \quad \text{(Entropy)}
\]

Artificial collisions in a 2D computer beam

In a 2D beam the beam macro-particles are rods: **Collision angle independent on b**!

All particles with relative velocities less than

\[ v_{1}^2 = \frac{qQ'}{2\pi \varepsilon_0 m} \]

are deflected by angles > 90°.

Friction force on a test particle:

\[ F_p(\vec{v}) = m\vec{v} = m \int d^2vdbu^2 f(\vec{v}) \sin^2 (\theta / 2) \]

\[ v \propto \frac{N^2}{M} \left( 1 - \frac{\Delta}{\lambda_D} \right) \]  

(2D collision rate for finite-sized macro particles)

\[ v \propto \frac{N^2}{M} \ln \left( \frac{\lambda_D}{\Delta} \right) \]  

(3D collision rate)

\[ \Delta \approx \Delta x \]  

(grid spacing)

Debye length:

\[ \lambda_D \propto \frac{1}{\sqrt{N}} \]

Collision angle:

\[ \theta(b) = \frac{qQ'}{\pi \varepsilon_0 m u^2} \arccos \frac{b}{\lambda_D} \]

Impact parameter b:

Test beam ion: q

Friction force on a test particle:

\[ F = \frac{qQ'}{2\pi \varepsilon_0 r} \]  

(2D ‘Coulomb’ force)

Relation between friction and diffusion in a system with energy conservation:

\[ D = v \frac{k_B T}{m} \]  

(Einstein relation)

\[ T(s) = \left( T_x + T_y \right) / 2 \]

\[ k_B T_x \propto mc^2 \frac{\varepsilon_x}{\beta_x} \]

Entropy and emittance growth due to artificial collisions in computer beams


Entropy/Emittance growth for anisotropic beams: \( T_x \neq T_y \)

\[
D = \nu \frac{k_B T}{m} \Rightarrow \frac{1}{\nu} \frac{d\varepsilon}{dt} = \frac{1}{2} k_B \nu \frac{(T_x - T_y)^2}{T_x T_y} \quad \varepsilon = \varepsilon_x \varepsilon_y
\]

(4D emittance)

**Emittance growth due to AG focusing in a FODO channel!**

**No growth for constant focusing (CF) and for FODOXX channels.**

\( FODOXX: \ k_x(s) = k_y(s) \Rightarrow \hat{\beta}_x = \hat{\beta}_y \)

\( \text{CF: } k_x = k_y = \text{const.} \)

**PATRIC (2D PIC):**

Emittance growth after 100-500 FODO cells


\[\varepsilon_0, x = \varepsilon_0, y\]

\[\nu \propto \frac{N^2}{M}\]

\[\mu_0 = 60^\circ\]

\[\Delta \mu^c_x = -10^\circ\]

Emittance growth in CF/FODOXX channels.

\( \nu \propto \frac{N^2}{M} \)

\( \varepsilon / \varepsilon_0 \)

\[1 / \text{macro-particle number}\]

Short comment on the effect of the grid spacing on emittance growth

**PATRIC (2D PIC):**
Emittance growth after 100-500 FODO cells

<table>
<thead>
<tr>
<th>Grid Size</th>
<th>Emittance Growth</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N_x=64)</td>
<td>(M = 1000)</td>
</tr>
</tbody>
</table>

**Artificial collisions**

**PATRIC (2D PIC):**
FODO vs. CF

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<td>FODO</td>
</tr>
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Artificial collisions
Stochastic or grid heating ('inelastic collisions')

Random walk in grid induced error fields:

\[
kT \approx n \frac{1}{2} \frac{q^2}{m} (\delta E)^2 (\Delta s)^2
\]

Numerical heating due to grid!

\[
D > \nu k_B T \frac{m}{\nu}
\]

\(\delta E\) Random grid induced electrical error field: rounding, time step, finite differences,…

A non-conservative force (\(\rightarrow\) heating) is introduced by grid undersampling.

\(\rightarrow\) Standard PIC integrators are non-symplectic

'Noise is not bad, the grid (undersampling) is'

Stochastic heating in computer plasmas:

Application to computer beams:
Digital filters for PIC

+ Reduce noise at short wavelengths (smoothing of the charge density).
+ Relatively fast.
- Can lead to non-physical results and numerical instabilities
- (Non-) Energy conservation (e.g. damping of modes)

$$\rho_{i,k} = \frac{M \rho_{i,k} + S(\text{side terms}) + K(\text{corner terms})}{M + 4(S + K)}$$

$$(M, S, K) = \text{Middle, side and corner weights}$$

Examples:
Hollow 8-point filter (0,1,1): Studied in [2]. Has negative spectral representation.
Binomial 9-point filter (4,2,1): Proposed for PIC codes in [1].

Digital filters:

Wavelet denoising:
Example results for FODO channel with filters

**PATRIC 2D:** Numerical emittance growth in a FODO channel after 100-500 cells with 9-point filter

\[ \mu_0 = 60^\circ, \quad \Delta \mu_x^{sc} = -10^\circ \]

- With digital filters:
  - Emittance growth rate is slower (approx. factor 10).
  - However, emittance growth is not the only benchmark -> resonances,...
‘Symplectic Particle-In-Cell’

Conventional PIC: Total momentum is conserved, but not energy (grid heating).

‘Energy conserving’ PIC [3]: Momentum is not conserved (self-force on the grid).

-> PIC codes are usually not symplectic

An ideal beam particle integrator with space charge would conserve:

Phase space (Symplectic), Emittance, Entropy, Energy (only for constant focusing)

‘Multi-symplectic’ integrators offer bounded variations of those constants.

Starting point is usually the Lagrangian (here for a 2D beam with space charge):

\[
L = \int dx_0 dy_0 dx'_0 dy'_0 f(x_0, y_0, x'_0, y'_0) \left( \frac{1}{2} (x'^2 + y'^2) - \frac{1}{2} \kappa (x^2 - y^2) - \frac{q}{E_0 \gamma_0^2 \beta_0^2} \phi(x) \right) - \frac{\dot{\phi}_0}{E_0 \gamma_0^2 \beta_0^2} \int dx dy \nabla \phi \cdot \nabla \phi
\]

Equations of motion (for particles and fields) from Euler-Lagrange equations:

\[
\frac{\partial L}{\partial \xi} - \frac{d}{ds} \frac{\partial L}{\partial \xi'} = 0 \quad \Rightarrow \quad x'' + \kappa(s)x = -\frac{q}{E_0 \gamma_0^2 \beta_0^2} \frac{\partial \phi}{\partial x} \quad y'' - \kappa(s)y = -\frac{q}{E_0 \gamma_0^2 \beta_0^2} \frac{\partial \phi}{\partial y} \quad \dot{\phi}_0 \Delta \phi = -\rho
\]

Spectral (grid-less) computer beam Lagrangian

Beam macro-particle distribution:

\[ f(x, x') = w \sum_{j=0}^{M} S(x - x_j) \delta(x' - x'_j) \]

Spectral space charge potential

\[ \phi(x) = \sum_{k} \phi_k \exp(ik \cdot x) \]

Resulting discrete Lagrangian:

\[ L_D = W_k - W_{AG} - W_{sc} - W_{field} \]

\[ W_k = w \sum_{j=0}^{M} \frac{1}{2}(x')^2 \quad W_{sc} = w \frac{q}{E_0 \gamma_0^2 \beta_0^2} \sum_{j=0}^{M} \sum_{k} S(k) \phi_k \exp(ik \cdot x_j) \quad W_{field} = \frac{1}{E_0 \gamma_0^2 \beta_0^2} \sum_{k} \sum_{k'} kk' \phi_k \phi_{k'} \]

(kinetic) (space charge potential) (space charge field energy)

Equations for macro-particles and spectra field) from Euler-Lagrange equations:

\[ \frac{\partial L_D}{\partial \xi_j} - \frac{d}{ds} \frac{\partial L_D}{\partial \dot{\xi}_j} = 0 \quad \Rightarrow \quad x''_j + \kappa(s)x_j = -\frac{iq}{E_0 \gamma_0^2 \beta_0^2} \sum_{k} k \phi_k S(k)e^{ik \cdot x_j} \quad \varepsilon_0 k^2 \phi_k = \rho_k \]

Spectral (grid-less) PIC for plasmas:

Spectral algorithm for 2D beams

Spectral charge density: \( \rho_k = wS(k)\sum_j e^{-ik\cdot x_j} \)

Space charge potential: \( \varepsilon_0 k^2 \phi_k = \rho_k \)

Space charge kick:

\[
\Delta x'_n = -\Delta s \frac{iq}{E_0} \frac{1}{\beta_0^2} \sum_k k_x \phi_k S^*(k) e^{ik\cdot x''_j} 
\]

Time step (\( \Delta s \)):

\[
\begin{pmatrix}
  x_j \\
x'_j \\
y_j \\
y'_j 
\end{pmatrix}_{n+1} = M(s_n, s_{n+1}) \begin{pmatrix}
  x_j \\
x'_j + \Delta x'_j \\
y_j \\
y'_j + \Delta y'_j 
\end{pmatrix}_n
\]

‘Tent’ particles shape:

\[
S(x) = \begin{cases}
  1 - |x / \Delta x|, & |x| \leq \Delta x \\
  0, & |x| > \Delta x
\end{cases}
\]

2D spectral particle shape:

\[
S(k) = \frac{1}{\sqrt{2\pi}} \int dx S(x) \exp(-ikx)
\]

Algorithm derived from a grid-less macro-particle Lagrangian.

We expect the system to follow: \( D \approx v \frac{k_B T}{m} \)
Tests: Spectral PIC vs. Conventional PIC

**PATRIC 2D:** Numerical emittance growth in a FODO channel after 500 cells.

- \[ \mu_0 = 60^\circ, \quad \Delta \mu_x^{sc} = -10^\circ \]
- \[ N_k = N_x = 64 \]

Noise still present (in k-space), but no emittance growth.

However, spectral PIC is (still) much slower:

\[ T \propto \alpha \cdot M \cdot \text{cells} \quad \frac{\alpha_{\text{spectral}}}{\alpha_{\text{grid}}} \approx 20 - 50 \]

Remark: For a python/numpy/cython implementation and on a Mac Pro. Process running on one core.
Spectral PIC: More results for FODO channel

Numerical emittance growth in a FODO channel after 100-500 cells.
Spectral PIC with M=1000.

\[ \mu_0 = 60^\circ, \quad \Delta \mu_x^{sc} = -10^\circ \]

Artificial collisions?

Because ‘symplectic’ PIC solves a macro-particle model, collisions should be present and the emittance should growth in AG focusing according to (still to be shown):

\[ D = v \frac{k_B T}{m} \Rightarrow \frac{1}{\varepsilon} \frac{d\varepsilon}{dt} = \frac{1}{2} k_B v \frac{(T_x - T_y)^2}{T_x T_y} \]
Conclusions and Outlook

Numerical emittance growth is a concern for long-term PIC particle tracking simulations with space charge in synchrotrons.
Two sources of numerical emittance growth:
1) Artificial collisions (or ‘numerical IBS’): Emittance growth in AG focusing
2) Stochastic or grid heating (‘inelastic collisions’) -> dominant in conventional PIC

Collision rate: \( \nu \propto \frac{N^2}{M} \quad D > \nu \frac{k_B T}{m} \) (diffusion, not balanced by friction -> heating)

Counter measures to decrease the growth rate: Larger M, particle shapes, filters, ….

’Symplectic’ PIC:
+ Still collisional (we don’t solve the Vlasov-Poisson equations)!
+ Noise/collisions do not cause emittance growth -> Bounded emittance \( D \approx \nu \frac{k_B T}{m} \) - Usually slower than conventional PIC.

To do:
-> optimized implementations, e.g. using a properly chosen S(x) one a grid.
-> check other benchmarks: Resonances, Landau damping and echoes,…..
-> compare with other approaches, like symplectic Vlasov-Poisson solvers