Self-consistent intrabeam scattering methods

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Introduction

Direct Simulation
P3M model

$$\frac{d^2}{dt^2}\mathbf{x}_1 = F^{\text{far}} + F^{\text{near}}$$

$$\frac{d^2}{dt^2}\mathbf{x}_1 = F(\mathbf{x}_1, \mathbf{v}_1, \ldots)$$

Exact Description

Kinetic Description
Langevin model

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{\text{diff}} + \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$$

- F denotes a force, f is the phase space distribution function
- The direct simulation approach has two terms representing the far field F^{far} and the near field F^{near} forces
- In the kinetic description, $\left(\frac{\partial f}{\partial t}\right)_{\text{diff}}$ refers to the diffusion term, which contains the mean field, while $\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$ represents the collision operator

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Ultracold Sources

Data from [XHM+, KAS+20]

- Applications in electron diffraction (imaging) and free electron lasers profit greatly from high brightness beams.
- A promising candidate for such beams are photoinjectors with ultracold photocathodes.

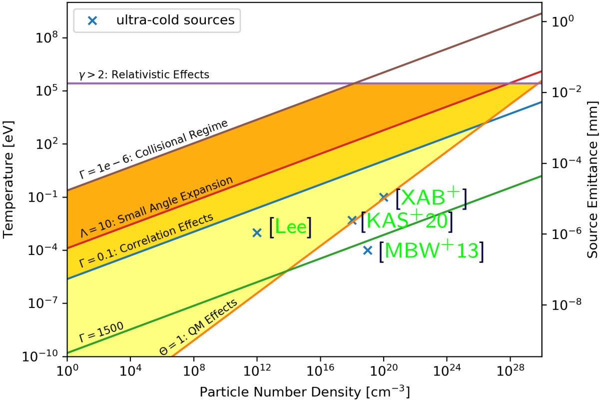
Observable	Magneto Optical Traps	Ultra Cold Photo Injector	Regular Photo injector
e^- Temperature [K]	< 10	$50 <$	1e3 - 1e4
Beam Charge [pC]	1000	-	100-3000
Emittance [mm.mrad]	0.04	$\propto$ 0.05	1
Brightness [A/m^2·sr]	1e16	$\propto$ 1e16	1e12 - 1e13
Bunch Length [ps]	0.1-1	-	$<$ hundreds

Direct Computation
Boltzmann
Landau

is valid for

& &

&



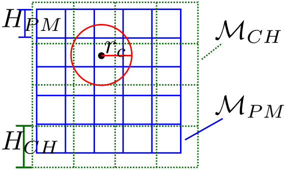
Γ: Coupling
Θ: Degeneracy
Λ: Coulomb Log.
γ: Relativ. Factor

The P^3M Algorithm

Implementation following [HE]

P^3M = **P**article-**P**article + **P**article-**M**esh

- high resolution from PP part
- good performance from PM part
- adjustable influence of Coulomb collisions



Particle-Particle (PM):

1. interpolate charges to mesh (CIC, NGP,...)
2. solve for potential Φ using an FFT solver (fast Possion solver)
3. compute forces by $F = -\nabla\Phi$
4. interpolate forces to particles $\Rightarrow$ Electric field

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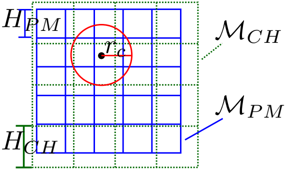

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Particle-Particle (PP):

1. compute linked lists for particles in interaction radius r_e
2. compute short range forces
3. update electric field

The Poisson Equation

The electrostatic potential $\Phi(\boldsymbol{r})$ of a system of interacting point charges $q_i(\boldsymbol{r})$ with charge distribution $\rho(\boldsymbol{r})$ is described by the Poisson Equation.

$$\boldsymbol{\nabla}^2\Phi(\boldsymbol{r}) = -\rho(\boldsymbol{r})$$

With the appropriate Green's function

$$G(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

interpreted as the potential that arises due to a point charge at $\boldsymbol{r}'$, the solution for an arbitrary charge distribution is given by the convolution

$$\boldsymbol{\Phi}(\boldsymbol{r}) = \int G(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}')d^3\boldsymbol{r}'$$

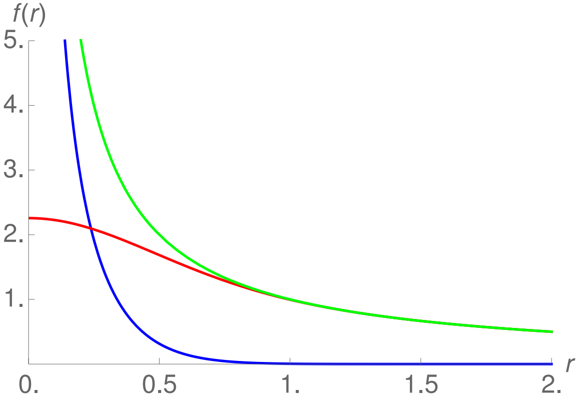
Interaction Splitting I

The main concept behind the P3M algorithm is a splitting of the interaction function $G(r)$ into a **short-range** contribution $G_{pp}(r)$ and a **long-range** contribution $G_{pm}(r)$. This splitting can be done using a Gaussian screening charge distribution

$$G(r) = \frac{1}{r} = \underbrace{\frac{1 - erf(\alpha r)}{r}}_{G_{PP}} + \underbrace{\frac{erf(\alpha r)}{r}}_{G_{PM}}$$

Interaction Splitting II

Gaussian shaped (S3) screening charge, $\alpha = 2$



Disorder Induced Heating (DIH) Process

- in a cold beam (near-zero temperature) with high density, stochastic Coulomb interactions (collisions) encounter
- Γ and known from (cold) plasma theory to be between 0.2 and 2 [MBW+13]
- in order to achieve this ratio, the local disorder is transformed into disorder associated with the particle momenta during the simulation
- the phase space volume increases $\Rightarrow$ the beam is heated
- equilibrium solution $\Rightarrow$ solving the hypernetted-chain equation

DIH Setup for Validation

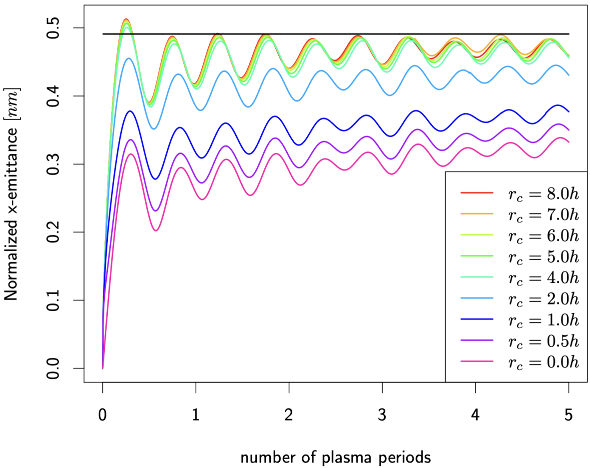
The experimental setup and simulation parameters from [MQ15].

- spherical, cold beam of radius $R = 17.74\,\mu\text{m}$ and charge $Q = 25\,\text{fC}$ with uniform spatial distribution
- constant focusing applied
- cubical domain with edge length $L = 100\,\mu\text{m}$
- $\mathrm{P^3M}$ simulation over 5 plasma periods
- $\mathcal{M}_{PM} = 256^3$; r_c varying from $0\,\mu\text{m}$ to $3.125\,\mu\text{m}$
- simulation over 1000 time-steps
- the normalized $x-$emittance for the thermal equilibrium is

$$\varepsilon_{x,n}^{eq} = 0.491\,\text{nm}$$

obtained by solving the hypernetted-chain equation

P3M Results - DIH



Vlasov-Poisson Equation

Vlasov-Poisson Equation

$$\begin{cases} \dfrac{\partial f}{\partial t} + \boldsymbol{v} \cdot \dfrac{\partial f}{\partial \boldsymbol{r}} + \dfrac{\boldsymbol{F}}{m} \dfrac{\partial f}{\partial \boldsymbol{v}} = \left(\dfrac{\partial f}{\partial t} \right)_{\text{coll}}, \\ \nabla^2_{\boldsymbol{r}} \phi(\boldsymbol{r}) = -\dfrac{\rho(\boldsymbol{r})}{\varepsilon_0}. \end{cases} \tag{1}$$

$\longrightarrow$ How do we determine the r.h.s. $\left(\dfrac{\partial f}{\partial t} \right)_{\text{coll}}$?

Fokker-Planck Equation I

Story ...

- The collision term $(\partial f/\partial t)_{\text{coll}}$ should capture changes to the density function $f(\boldsymbol{r}, \boldsymbol{v})$ due to interactions between particles $\Rightarrow$ relaxation towards equilibrium.
- Picture: a test particle traveling through a background of equally charged particles ("scatterers"). On its path it gets influenced by the electric force of these nearby particles.
- However, the interactions are limited to a Debye radius λ_D, "shielding" the test particle off from particles farther away.

These collisions exhibit two important properties:

1. an individual collision (i.e. its potential energy) is weak compared to the thermal energy of the system [BS03], causing only small angle deflections. It can be shown that the accumulated effect of these far outweigh more rare strong interactions.

Fokker-Planck Equation II

2. Second, the considered time-scale is usually much larger than the collision time τ_c but still smaller than the dissipation time ν [Nic83]:

$$\tau_c \ll \Delta t \ll \nu, \tag{2}$$

where the dissipation time ν is of the scale after which a small perturbation to the phase space density is observed to be below a fixed threshold [FW03].

$\Rightarrow$ spatial position not affected, $(\partial f / \partial t)_{\mathrm{coll}}$ in velocity space

$\Rightarrow$ strong similarity to properties known from Brownian motion

$\Rightarrow$ Fokker-Planck formulation of the collision operator is applicable

Fokker-Planck Equation III

In the Fokker-Planck approach we advance our phase space density f in time by Δt via an integral over a probability function $\psi(\boldsymbol{v}, \Delta\boldsymbol{v})$ that defines how likely it is that a particle with velocity $\boldsymbol{v}$ experiences a change in velocity $\Delta\boldsymbol{v}$. Taylor expansion up to order 2 of this integral results in the FP operator:

$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}} = -\frac{\partial}{\partial \boldsymbol{v}} \cdot \left(f \frac{\langle \Delta\boldsymbol{v} \rangle}{\Delta t}\right) + \frac{1}{2} \frac{\partial^2}{\partial \boldsymbol{v} \partial \boldsymbol{v}} : \left(f \frac{\langle \Delta\boldsymbol{v}\Delta\boldsymbol{v} \rangle}{\Delta t}\right)$$

The Rosenbluth's approach to FP I

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{\partial}{\partial \boldsymbol{v}} \cdot \left(f \frac{\langle \Delta \boldsymbol{v} \rangle}{\Delta t}\right) + \frac{1}{2} \frac{\partial^2}{\partial \boldsymbol{v} \partial \boldsymbol{v}} : \left(f \frac{\langle \Delta \boldsymbol{v} \Delta \boldsymbol{v} \rangle}{\Delta t}\right)$$

Collision Coefficients

$$\boldsymbol{F}_d(\boldsymbol{v}) = \frac{\langle \Delta \boldsymbol{v} \rangle}{\Delta t} = \Gamma \frac{\partial h(\boldsymbol{v})}{\partial \boldsymbol{v}},$$

$$D(\boldsymbol{v}) = \frac{\langle \Delta \boldsymbol{v} \Delta \boldsymbol{v} \rangle}{\Delta t} = \Gamma \frac{\partial^2 g(\boldsymbol{v})}{\partial \boldsymbol{v} \partial \boldsymbol{v}}.$$

Poisson Problems [RMJ].

$$\nabla^2_{\boldsymbol{v}} h(\boldsymbol{v}) = -8\pi f(\boldsymbol{r}, \boldsymbol{v}),$$

$$\nabla^2_{\boldsymbol{v}} \nabla^2_{\boldsymbol{v}} g(\boldsymbol{v}) = -8\pi f(\boldsymbol{r}, \boldsymbol{v}).$$

$\boldsymbol{F}_d(\boldsymbol{v})$: Dynamic friction coefficient
$D(\boldsymbol{v})$: Diffusion coefficient

The Rosenbluth's approach to FP II

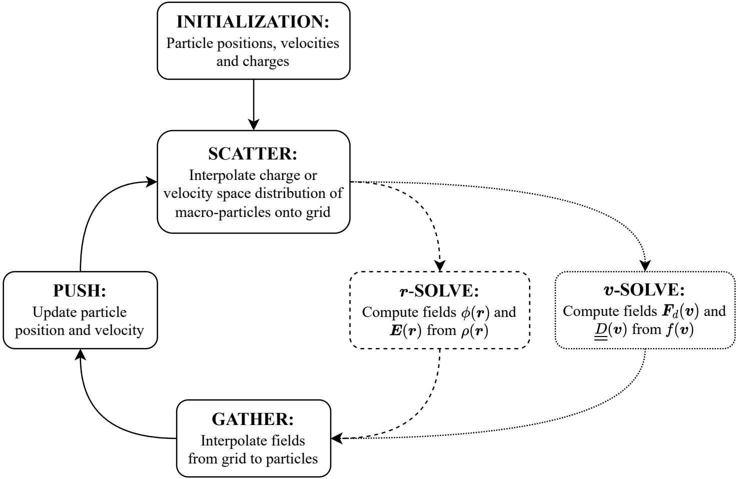
- We've talked about the randomness in how these collisions happen, how do we reflect this in the timestepping procedure?
- Langevin Eq. arises naturaly when a variable experience a slow time variation in velocity due to many small random forces.
- Idea based on Markov processes

Langevin Equation [Tab19]

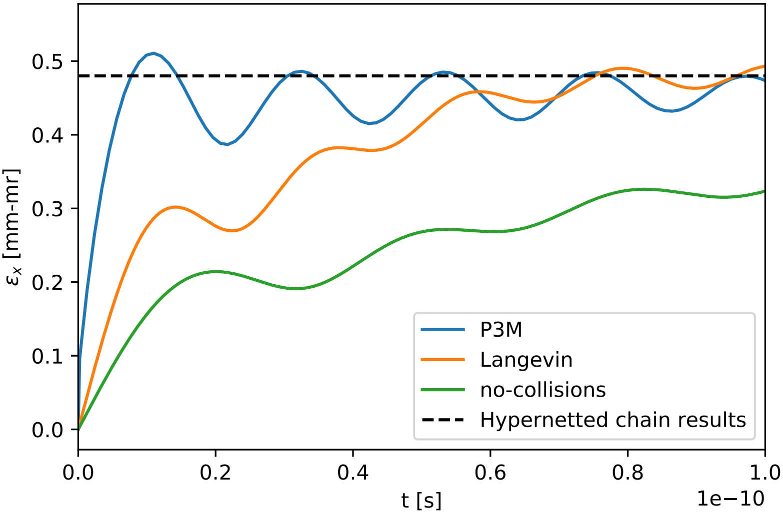
$$d\boldsymbol{v}(t) = \underbrace{\boldsymbol{a}(\boldsymbol{v}, t)}_{\boldsymbol{F}_d(\boldsymbol{v})} dt + \underbrace{\boldsymbol{b}(\boldsymbol{v}, t)}_{Q(\boldsymbol{v})} d\boldsymbol{W}(t), \tag{3}$$

$$d\boldsymbol{W}(t) = \boldsymbol{\xi}_t dt, \quad \boldsymbol{\xi}_t \sim \mathcal{N}(0, 1). \tag{4}$$

Particle-in-Cell + FP I



DIH again



0.5
0.4
0.3
0.2
0.1
0.0
ε_x [mm-mr]
0.0
0.2
0.4
0.6
0.8
1.0
1e−10
t [s]
P3M
Langevin
no-collisions
Hypernetted chain results

Preliminary P3M Results for SwissFEL @13m

in collaboration with Sven Reiche and Thomas Lucas Geoffrey

Can switch on/off collisions in OPAL:

```
FS_PM: Fieldsolver, FSTYPE = FFT, MX = 64, MY = 64, MT = 64, PARFFTX = decx, PARFFTY = decy,
       PARFFTT = decz, BCFFTX = open, BCFFTY = open, BCFFTT = open , GREENSF = INTEGRATED;

FS_P3M: Fieldsolver, FSTYPE = "P3M", MX = 64, MY = 64, MT = 64, PARFFTX = decx, PARFFTY = decy,
       PARFFTT = decz, BCFFTX = open, BCFFTY = open, BCFFTT = open, RC=6.25e-5,
       ALPHA=32000, EPSILON=0, P3MTEST=false;

//-----------------------------------------------------------------------------------
BEAM1:  BEAM, PARTICLE = ELECTRON, pc = P0, NPART = n_particles, BFREQ = rf_freq,
        BCURRENT = beam_current, CHARGE = -1;
//-----------------------------------------------------------------------------------


//TRACK, LINE = SWISSFEL, BEAM = BEAM1, MAXSTEPS = 1900000, DT = {1.0e-13, 2.0e-12}, ZSTOP={0.20, 0.50};
TRACK, LINE = SWISSFEL, BEAM = BEAM1, MAXSTEPS = 1900000, DT = {2.0e-12}, ZSTOP={7.0};
RUN, METHOD = "PARALLEL-T", BEAM = BEAM1, FIELDSOLVER = FS_PM, DISTRIBUTION = Dist;
ENDTRACK;
TRACK, LINE = SWISSFEL, BEAM = BEAM1, MAXSTEPS = 1900000, DT = {2.0e-12}, ZSTOP={13.1};
RUN, METHOD = "PARALLEL-T", BEAM = BEAM1, FIELDSOLVER = FS_P3M, DISTRIBUTION = Dist;
ENDTRACK;

STOP;
```

Preliminary P3M Results for SwissFEL @13m

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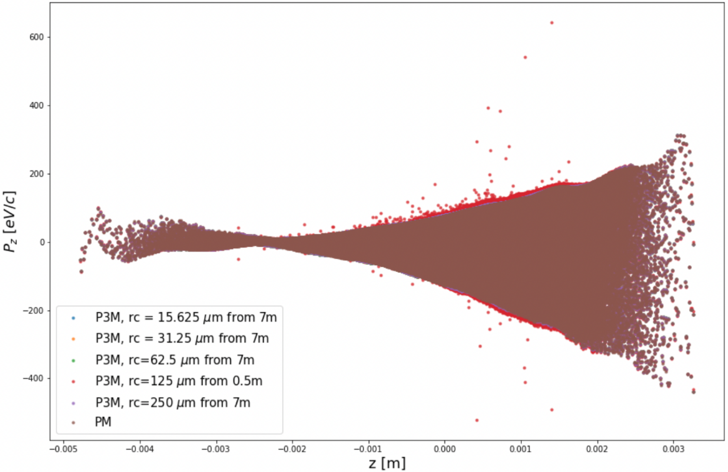
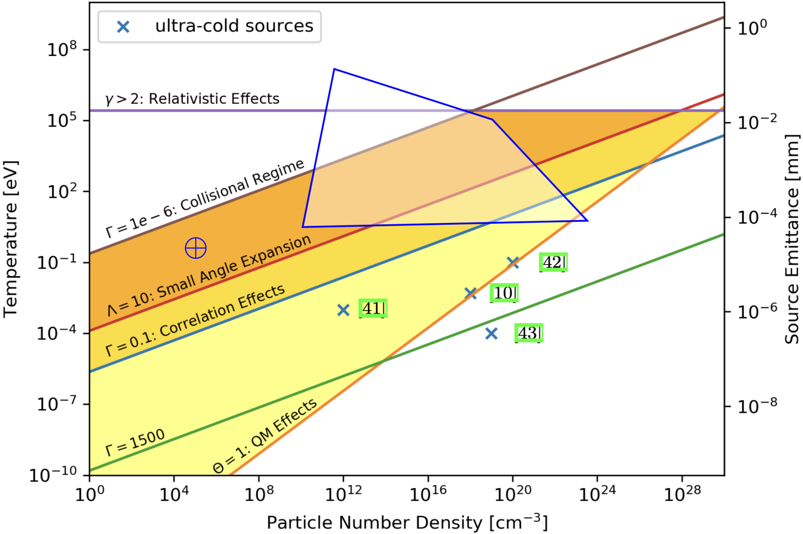


Conclusions and Outlook



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