Accelerator Physics & Modelling

Zuoz Summer School Lecture 4: Collective Effects

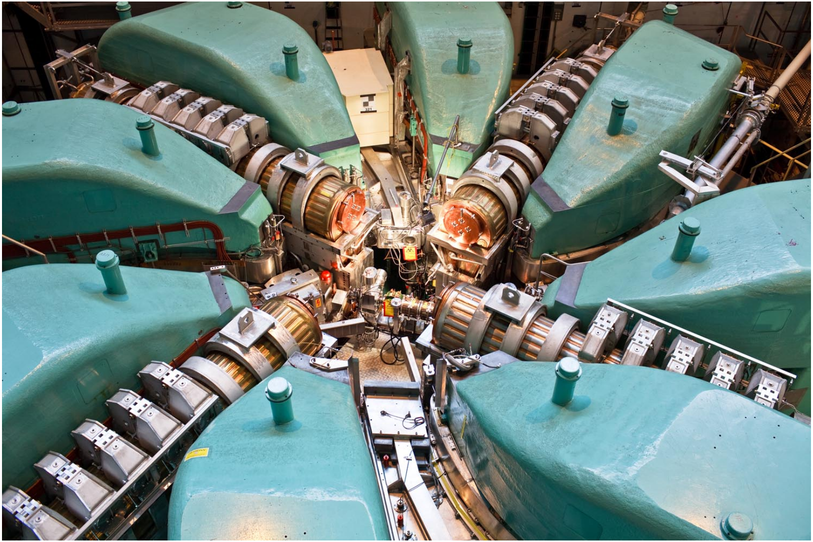
Andreas Adelmann

Paul Scherrer Institut, Villigen
E-mail: andreaad@ethz.ch

August 4-10, 2024

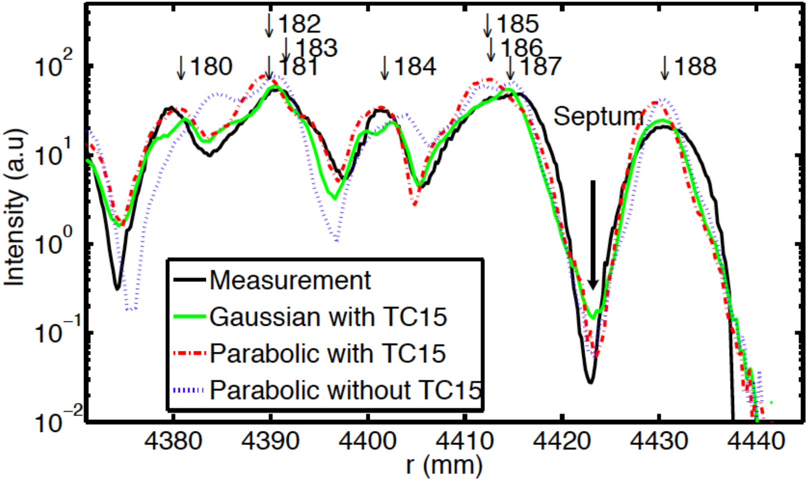
Precise Beam Dynamic Simulations I

PSI Ring Cyclotron



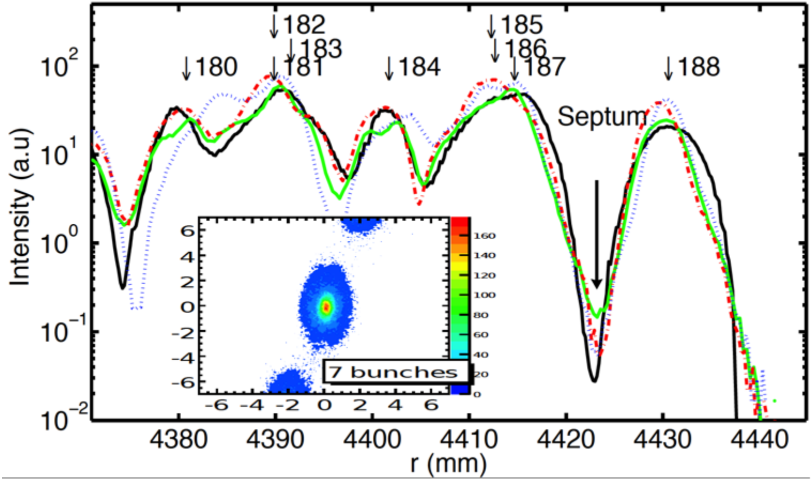
Precise Beam Dynamic Simulations II

PSI Ring Cyclotron



Precise Beam Dynamic Simulations III

PSI Ring Cyclotron



Collision-less (non relativistic) Vlasov-Maxwell equation

$f \subset (\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R} :\to \mathbb{R}.$

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

$$\left.\begin{aligned} \cancel{\partial_t \mathbf{E}} - c^2 \,\mathbf{curl}\, \mathbf{B} &= \frac{\mathbf{J}}{\varepsilon_0}, \qquad & \nabla \cdot \mathbf{E} &= \frac{\rho}{\varepsilon_0}, \\ \cancel{\partial_t \mathbf{B}} + \mathbf{curl}\, \mathbf{E} &= 0, \qquad & \nabla \cdot \mathbf{B} &= 0, \end{aligned}\right\} \qquad \text{Maxwell's equations}$$

where the source terms are computed by

$$\rho = \sum q \int f \, d\mathbf{v}, \qquad \mathbf{J} = \sum q \int f \mathbf{v} \, d\mathbf{v}.$$

- no transient behaviour $\cancel{\partial_t}$
- $\mathbf{J} \sim 0$

Collision-less (non relativistic) Vlasov-Poisson equation

$$\nabla \cdot \mathbf{E} = -\frac{\rho}{\varepsilon_0}$$

- $\mathbf{E} = \nabla\phi$
- $\nabla \cdot \nabla\phi = \Delta\phi = -\frac{\rho}{\varepsilon_0}$

with appropriate boundary conditions.

Field Maps &
Analytic Models

$$\nabla \cdot \mathbf{E}_{sc} = -\rho/\varepsilon_0 = \nabla \cdot \nabla \phi_{sc}$$
$$\Delta \phi_{sc} \;=\; -\frac{\rho}{\varepsilon_0}$$
& BC's

Electro
Magneto
Optics

$$\mathbf{H} = \mathbf{H}_{\mathrm{ext}} + \mathbf{H}_{\mathrm{sc}}$$

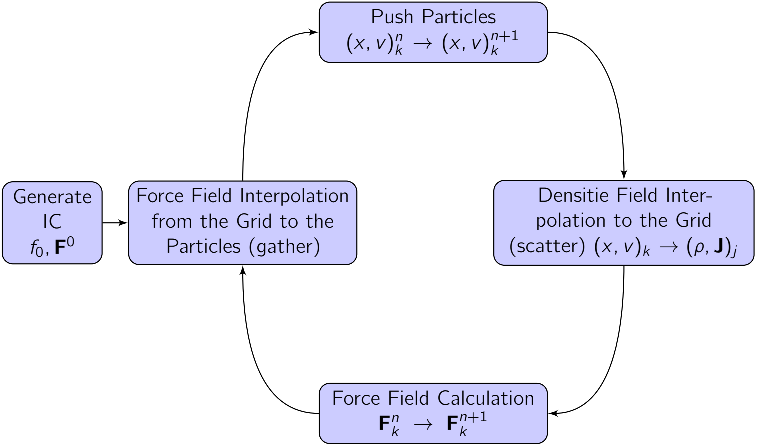
N-Body
Dynamics

Split Operator techniques: (Yoshida splitting)

$$\mathcal{M}(s) = \mathcal{M}_{\mathrm{ext}}(s/2)\mathcal{M}_{\mathrm{sc}}(s)\mathcal{M}_{\mathrm{ext}}(s/2) + \mathcal{O}(s^3)$$

Problem: s vs. t

Coupling Particle Dynamics with Electromagnetic Fields



In case of <u>precise</u> particle accelerator modelling, resolving losses at very low level, large N-body problems have to be solved.

A Direct FFT-Based Poisson Solver I

Assume you know G the Green's function

The solution of the Poisson's equation

$$\nabla^2\phi = -\rho/\varepsilon_0,$$

for the scalar potential, ϕ can be expressed as:

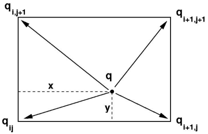
$$\phi(x,y,z) = \int\int\int dx'dy'dz'\rho(x',y',z')G(x-x',y-y',z-z'), \tag{1}$$

where G is the Green function and ρ is the charge density.

A Direct FFT-Based Poisson Solver II

Assume you know G the Green's function

Discretisation of Eq. (1) on a grid with cell sizes h_x, h_y and h_z

leads to: 

$$\phi_{i,j,k} = h_x h_y h_z \sum_{i'=1}^{M_x} \sum_{j'=1}^{M_y} \sum_{k'=1}^{M_z} \rho_{i',j',k'} G_{i-i',j-j',k-k'}, \qquad (2)$$

The solution of Eq. (2) can be obtained using FFT based convolution:

$$\phi_{i,j,k} = h_x h_y h_z \ \mathrm{FFT}^{-1}\{(\mathrm{FFT}\{\rho_{i,j,k}\}) \otimes (\mathrm{FFT}\{G_{i,j,k}\})\}$$

A Direct FFT-Based Poisson Solver III

Assume you know G the Green's function

Algorithm Electrostatic Field Calculation:

- ▷ Scatter all q_i to nearby mesh points to obtain ρ
- ▷ $\mathcal{L}$-transform to obtain ρ in beam rest frame.
- ▷ Use FFT on ρ and G to obtain $\widehat{\rho}$ and $\widehat{G}$
- ▷ Determine $\widehat{\phi}$ on the grid: $\widehat{\phi} = \widehat{\rho} \cdot \widehat{G}$
- ▷ FFT^{-1} on $\widehat{\phi}$ to obtain ϕ
- ▷ Finite Difference computation for $\mathbf{E} = -\nabla\phi$
- ▷ $\mathcal{L}^{-1}$-transform to obtain $\mathbf{E}_{sc}$ and $\mathbf{B}_{sc}$
- ▷ Interpolate (gather) $\mathbf{E}$, $\mathbf{B}$ at particle positions $\mathbf{x}$ from $\mathbf{E}_{sc}$ and $\mathbf{B}_{sc}$

1. Go to Fourier space $\rho_h \rightarrow \widehat{\rho}_h$, $G_h \rightarrow \widehat{G}_h$ and convert the convolution into a multiplication $\widehat{\phi}_h = \widehat{\rho}_h * \widehat{G}_h$ in $\mathcal{O}(N \log N)$
2. Use a parallel FFT, particle and field load balancing

Object Oriented Parallel Particle Library (OPAL)

https://gitlab.psi.ch/OPAL/src/wikis/home

OPAL is a versatile open-source tool for charged-particle optics in large accelerator structures and beam lines including 3D EM field calculation, collisions, radiation, particle-matter interaction, and multi-objective optimisation

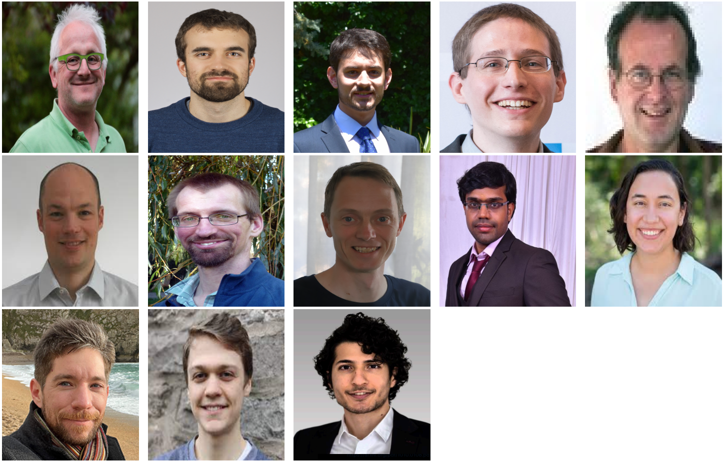
- OPAL is built from the ground up as an HPC application
- OPAL runs on your laptop as well as on the largest HPC clusters
- OPAL uses the MAD language with extensions
- OPAL is written in C++, uses design patterns,
- The OPAL Discussion Forum:
  https://psilists.ethz.ch/sympa/info/opal

Object Oriented Parallel Particle Library (OPAL)

https://gitlab.psi.ch/OPAL/src/wikis/home

- International team of 13 active developers and a user base of $\mathcal{O}(100)$
- The OPAL **sampler** command can generate labeled data sets using the largest computing resources and allocations available

The Active OPAL Developer Team



Two OPAL flavours, OPAL-t & OPAL-cycl

- Common features
  - 3D space charge: in unbounded, and bounded domains
  - particle Matter Interaction (protons)
  - parallel hdf5 & SDDS output
  - sampler & multi-objective optimisation
  - from e, p to Uranium (q/m is a parameter)
- OPAL-cycl (+ FFAs + Synchrotrons)
  - neighbouring turns
  - time integration, 4th-order RK, LF, adaptive schemes
  - find matched distributions with linear space charge
  - spiral inflector modelling with space charge
- OPAL-t
  - rf-guns, injectors, beamlines [1]
  - auto-phasing (with veto)
  - full EM in `undulator` element since OPAL 2021.1
  - Particle-Particle-Particle-Mesh solver since OPAL 2022.1

[1] Proton therapy gantries & degrader

Software Architecture

MPI based

OPAL

classic	MAD-Parser	Flavors: t,Cycl	Distributions
classic	Solvers: ES/EM	Integrators	PMI, WFC
H5hut	FFT	D-Operators	NGP,CIC,TSI
H5hut	Fields	Mesh	Particles
BOOST	Load Balancing	Domain Decomp.	Communication
BOOST	Particle-Cache	PETE	Trillions Interface
	GSL	MITHRA	Trilinos

Collisions

Introduction

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

Exact Description

Direct Simulation
P3M model

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

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

Ultracold Sources

- 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

The $\mathrm{P}^3\mathrm{M}$ Algorithm

Implementation following [?]

$\mathrm{P}^3\mathrm{M}$ = **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

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

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

With the appropriate Green's function

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

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

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

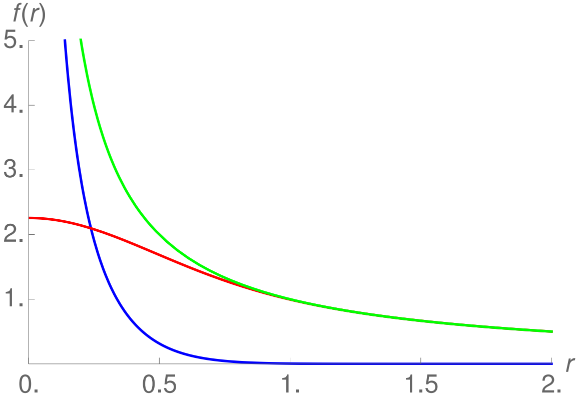
Interaction Splitting I

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

- case relevant for electron diffraction
- after the electron gun in an accelerator particle positions are disordered and the beam is rather cold
- in a cold beam (near-zero temperature) with high density, stochastic Coulomb interactions (collisions) encounter
- 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

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

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

obtained by solving the hypernetted-chain equation

P3M Results - DIH