OPAL-CYCL : A Parallel PIC Code Including Neighboring Bunches Effects in Cyclotron

Work in Progress

Jianjun Yang[1], Andreas Adelmann[2]

1. Ph.D Candidate, CIAE & Tsinghua Univ.
2. AMAS Group, PSI

22th April, 2008

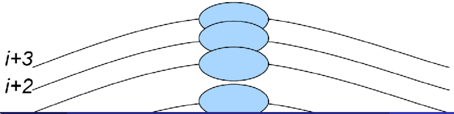
Outline

Background

Brief Review

Space charge effects play an important role in high intensity cyclotrons (space charge dominated PSI Injector2). Two different types can be distinguished.

- Space charge effects of single bunch.
  M.M.Gordon, M.Joho, S.Adam, A.Adelmann and P. Bertrand have done very nice work on this.
- Space charge effects of radially neighboring bunches .
  As a pioneer, E.Pozdeyev developed a model in his code CYCO (Ph.D thesis, MSU, 2003)
  $\Rightarrow$ Not self-consistent model & serial code & θ as independent variable.



Background

Turn Separation

In an ideal machine, the "radial gain per turn" $\Delta R_{n,n+1}$ produced by the increment of energy can be expressed as:

$$\Delta R_{n,n+1} = \left[\sqrt{1 + \frac{2\Delta E_{n,n+1}(E_k+E_0) + \left(\Delta E_{n,n+1}\right)^2}{2E_k E_0 + {E_k}^2}} \Bigg/ \left(1 + \frac{\Delta E_{n,n+1}}{E_k+E_0}\right) - 1 \right] R_n .$$

E_0: rest energy,
E_k: kinetic energy,
$\Delta E_{n,n+1}$: energy gain in one turn,
R_n: average radius of nth turn.

If $\Delta E_{n,n+1}$ keeps constant, $E_k \nearrow \Rightarrow \Delta R_{n,n+1} \searrow$

Motivation: Upgrade Project of PSI Cyclotron Facility

590MeV Ring

- Beam Current/Power:
  2mA/1.2MW ⇒ 3mA/1.8MW
  The highest current cyclotron in the world.
- Turns number
  200 ⇒ less than 160.
- After upgrade, turn seperation better.

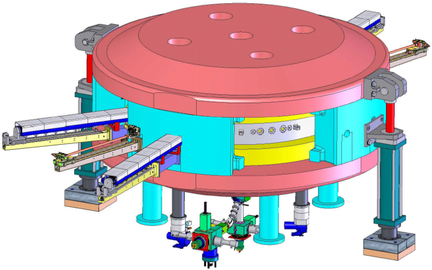
After upgrade, without deliberately added field for extraction purpose, at extraction point,

$$\Delta R_{n,n+1} = 5.7\text{mm}.$$

Motivation: Compact Cyclotron under Building in CIAE

100MeV H^- CYCIAE-100

- Designed beam current 0.2mA, future 0.5mA .
- Turns number is about 500.
- Energy gain per turn is 0.2MeV.
- Multi-turn extraction by striper at radius of 1.9m.
- Turn separation far smaller than beam size at outer Radius, multi-bunches will overlap together.



At extraction point,

$$\Delta R_{n,n+1} = 1.5\text{mm}.$$

Outline

Basic Formula

Particle Motion Equation

Common equations of motion of single charged particle in electromagnetic field.

$$\dot{\mathbf{p}} = \mathbf{F}(\mathbf{v}, \mathbf{x}, t) = q\,(\mathbf{v} \times \mathbf{B} + \mathbf{E})$$

$$\mathbf{E} = \mathbf{E}_{ext} + \mathbf{E}_{sc}$$

$$\mathbf{B} = \mathbf{B}_{ext} + \mathbf{B}_{sc}$$

the evolution of beam's distribution function $f(\mathbf{x}, \mathbf{v}, t)$ can be expressed by collisonless Vlasov-Maxwell Equations:

$$\frac{df}{dt} = \partial_t f + \mathbf{v} \cdot \nabla_x f + \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f = 0.$$

3D Parallel Poisson equation Solver using PIC/FFT

The external fields are given, space charge field can be obtain by solving Poisson equation using PIC (Particle-In-Cell) methods.

Solve Poisson equation on discrete domain

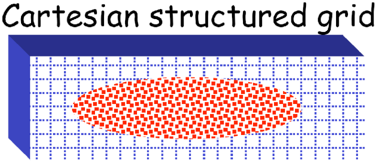
In PIC/FFT, a 3D rectangle grid which contains all particles is built(following quantities with superscript of D means on grid). The solution of the discretized Poisson equation with $\vec{k} = (l, n, m,)$

$$\nabla^2 \phi^D(\vec{k}) = -\frac{\rho^D(\vec{k})}{\epsilon_0}, \vec{k} \in \Omega^D.$$

ϕ^D is given by convolution with the appropriate discretized Green's function G_D:

$$\phi^D = \rho^D * G^D.$$

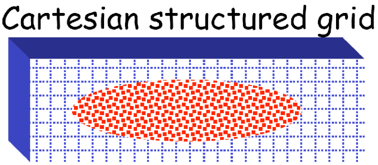
3D Parallel Poisson Solver using PIC/FFT



Basic Process of the Poisson Solver

▷ Assign all particles charges q_i to nearby mesh points to obtain ρ^D

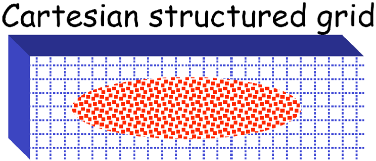
3D Parallel Poisson Solver using PIC/FFT



Basic Process of the Poisson Solver

- ▷ Assign all particles charges q_i to nearby mesh points to obtain ρ^D
- ▷ Lorentz transform to obtain ρ^D in beam rest frame $\mathbf{S}_{beam}$.

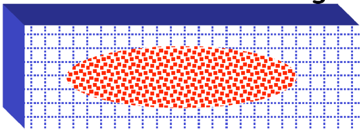
3D Parallel Poisson Solver using PIC/FFT



Basic Process of the Poisson Solver

- ▷ Assign all particles charges q_i to nearby mesh points to obtain ρ^D
- ▷ Lorentz transform to obtain ρ^D in beam rest frame $\mathbf{S}_{beam}$.
- ▷ Use FFT on ρ^D and G^D to obtain $\widehat{\rho}^D$ and $\widehat{G}^D$

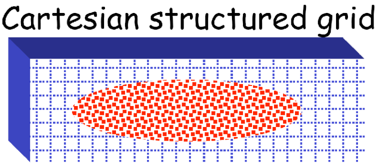
3D Parallel Poisson Solver using PIC/FFT



Basic Process of the Poisson Solver

- ▷ Assign all particles charges q_i to nearby mesh points to obtain ρ^D
- ▷ Lorentz transform to obtain ρ^D in beam rest frame $\mathbf{S}_{beam}$.
- ▷ Use FFT on ρ^D and G^D to obtain $\widehat{\rho}^D$ and $\widehat{G}^D$
- ▷ Determine $\widehat{\phi}^D$ on the grid using $\widehat{\phi}^D = \widehat{\rho}^D \cdot \widehat{G}^D$

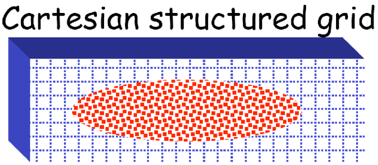
3D Parallel Poisson Solver using PIC/FFT



Basic Process of the Poisson Solver

- ▷ Assign all particles charges q_i to nearby mesh points to obtain ρ^D
- ▷ Lorentz transform to obtain ρ^D in beam rest frame $\mathbf{S}_{beam}$.
- ▷ Use FFT on ρ^D and G^D to obtain $\widehat{\rho}^D$ and $\widehat{G}^D$
- ▷ Determine $\widehat{\phi}^D$ on the grid using $\widehat{\phi}^D = \widehat{\rho}^D \cdot \widehat{G}^D$
- ▷ Use inverse FFT on $\widehat{\phi}^D$ to obtain ϕ^D

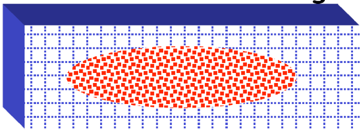
3D Parallel Poisson Solver using PIC/FFT



Basic Process of the Poisson Solver

- ▷ Assign all particles charges q_i to nearby mesh points to obtain ρ^D
- ▷ Lorentz transform to obtain ρ^D in beam rest frame $\mathbf{S}_{beam}$.
- ▷ Use FFT on ρ^D and G^D to obtain $\widehat{\rho}^D$ and $\widehat{G}^D$
- ▷ Determine $\widehat{\phi}^D$ on the grid using $\widehat{\phi}^D = \widehat{\rho}^D \cdot \widehat{G}^D$
- ▷ Use inverse FFT on $\widehat{\phi}^D$ to obtain ϕ^D
- ▷ Compute $\mathbf{E}^D = -\nabla\phi^D$

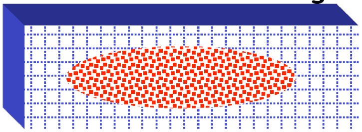
3D Parallel Poisson Solver using PIC/FFT



Basic Process of the Poisson Solver

- Assign all particles charges q_i to nearby mesh points to obtain ρ^D
- Lorentz transform to obtain ρ^D in beam rest frame $\mathbf{S}_{beam}$.
- Use FFT on ρ^D and G^D to obtain $\widehat{\rho}^D$ and $\widehat{G}^D$
- Determine $\widehat{\phi}^D$ on the grid using $\widehat{\phi}^D = \widehat{\rho}^D \cdot \widehat{G}^D$
- Use inverse FFT on $\widehat{\phi}^D$ to obtain ϕ^D
- Compute $\mathbf{E}^D = -\nabla\phi^D$
- Interpolate $\mathbf{E}$ at particle positions $\mathbf{x}$ from $\mathbf{E}^D$

3D Parallel Poisson Solver using PIC/FFT



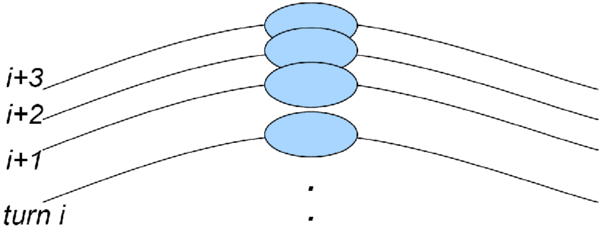
Basic Process of the Poisson Solver

- ▷ Assign all particles charges q_i to nearby mesh points to obtain ρ^D
- ▷ Lorentz transform to obtain ρ^D in beam rest frame $\mathbf{S}_{beam}$.
- ▷ Use FFT on ρ^D and G^D to obtain $\widehat{\rho}^D$ and $\widehat{G}^D$
- ▷ Determine $\widehat{\phi}^D$ on the grid using $\widehat{\phi}^D = \widehat{\rho}^D \cdot \widehat{G}^D$
- ▷ Use inverse FFT on $\widehat{\phi}^D$ to obtain ϕ^D
- ▷ Compute $\mathbf{E}^D = -\nabla\phi^D$
- ▷ Interpolate $\mathbf{E}$ at particle positions $\mathbf{x}$ from $\mathbf{E}^D$
- ▷ Lorentz back transform to obtain $\mathbf{E}_{sc}$ and $\mathbf{B}_{sc}$ in laboratory frame $\mathbf{S}_{lab}$.

3D Parallel Poisson Solver using PIC/FFT

Specialization in Cyclotron

- The orientation of laboratory frame $\mathbf{S}_{lab}$ changes from time to time.
- For multi-bunch simulation, the energy span is huge, so particles are divided into different energy bins. For each bin, apply Lorentz transformation and calculate field.



Outline

Implementation of OPAL-CYCL

Characteristics of OPAL-CYCL

- Based on OPAL framework (IPPL, CLASSIC, H5Part, HDF5)
- Store intermediate phase space data in hdf5 format
- Read in measured field map of median plane
- Treat electric field of cavity as a δ function with correction of transit effects
- Use 4th-order RK as integrator
- Use time as independent variable
- Track in global cartesian coordinates
- Has three working modes:
    - Single particle tracking mode.
    - Tune calculation mode.
    - Multi-bunches tracking mode (single bunch & multi-bunches)

Implementation of OPAL-CYCL

Implement neighboring bunches effects in electrostatic approximation

- When $\Delta R \leq M\sigma_{x,y}$, the execution will transfers from single bunch mode to multi-bunch mode automatically, namely, inject new bunches consecutively after each revolution period.
- Integrate particles in all the bunches simutaniously.
- For each time step, calculate space charge field for each energy bin using PIC/FFT, then add contribution of all bins together.
- Reset energy bin when the bunches' energy span overlap together.

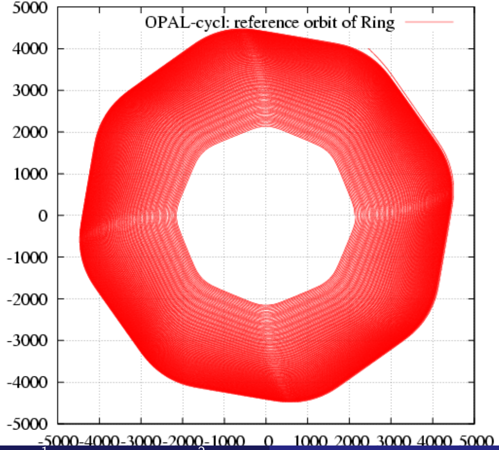
Fully self-consistent model of dealing with radially neighboring bunches effects in time domain!

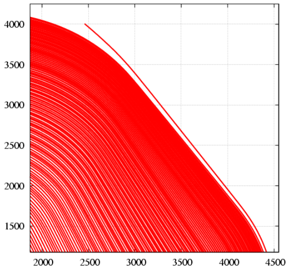
Outline

Single particle track result

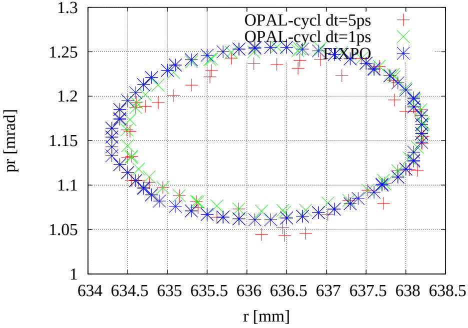
Reference Orbit of Ring

Before upgrade, set $V_{main} = 0.735MV$, $V_{flattop} = 11.2\% V_{main}$, 206 turns
After upgrade, set $V_{main} = 0.900MV$, $V_{flattop} = 11.2\% V_{main}$, 168 turns





Single particle track result

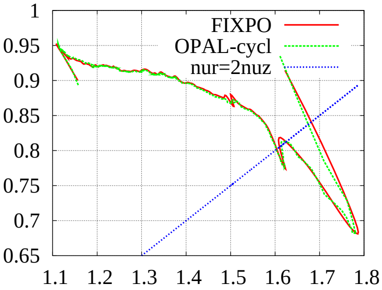


Eigen ellipse of Inj.2 @ 2MeV

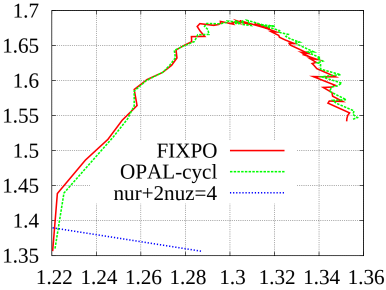
Radial eigen ellipse agree with FIXPO code very well !

Tune calculation result

PSI Ring



PSI Injector2



Tune diagram

The calculation results agree with FIXPO code very well !

Test for parallel Scalability

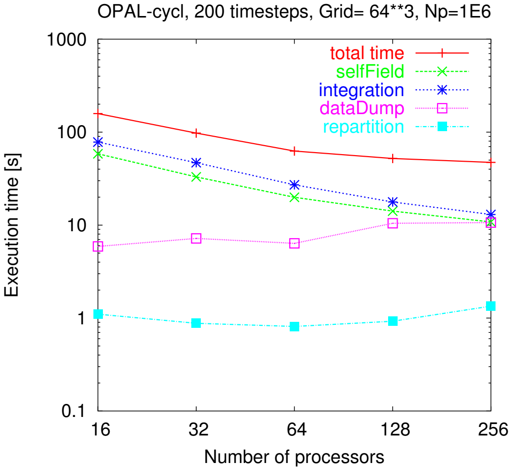
OPAL-CYCL Scaling on Cray XT3 Cluster at CSCS

Production Run Setup

- 10^6 particles
- 3D FFT on a 64^3 grid
- 2D domain decomposition
- track 200 time steps
- Gaussian distribution
- Dump data into single HDF5 file

Observations

- The code scales well
- Good load-balancing
- 128 processors is best choice for this job.



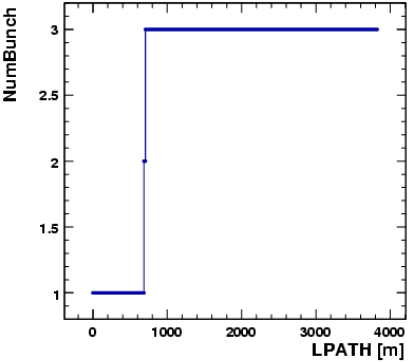
Animation of Single Bunches and Multi-Bunches

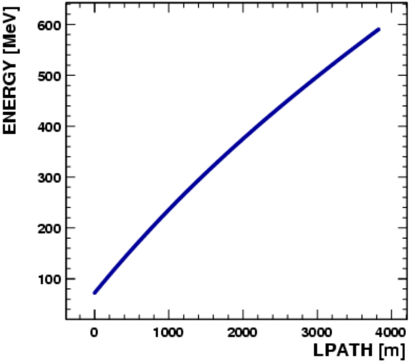
Movies show

Single Bunch Run

3 Bunches Run

Multi-Bunches Test in Ring

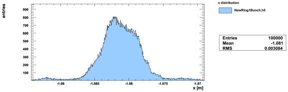




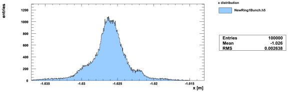
Multi-Bunches Test in Ring

Single Bunch Run

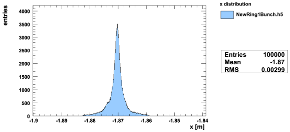
40th turn



41th turn

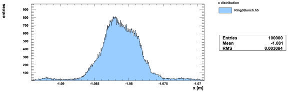


42th turn

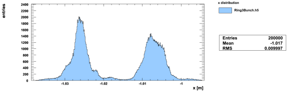


3 Bunches Run

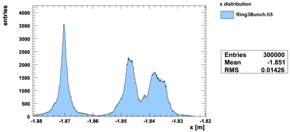
40th turn



41th turn



42th turn



Outlook

Future plan

- Study in detail on beam dynamics issues of PSI Ring and CYCIAE-100 machine to do some substantial contribution.
- Add Radial and vertical collimator.
- Include high order expansion of magnetic field, RF magnetic field.

Outline

Acknowledgments

Many Thanks To :

T.J. Zhang
M. Humbel
Ch. Kraus
W. Joho
AMAS Group Members