Modeling cooling in HPRF cavities including atomic physics processes

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HPRF cavity experiments

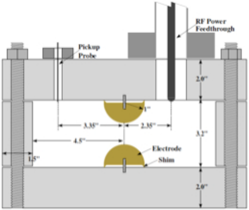


Figure: Schematic of HPRF cavity

- Dense hydrogen gas filled RF cavity has been proposed for muon beam phase space cooling and acceleration
- Proton beam: 400 MeV, H_2 gas: $P = 200$ bar, $\rho = 10^{21}\ cm^{-3}$
- External electric field: 20 MV/m, $f = 900$ MHz; 10 T external magnetic field

Critical Issues in HPRF cavity experiments

- RF power loading due to beam-induced gas effects
  - Incident particles produce many electron-ion pairs
  - Electrons transfer RF energy into hydrogen gas via interactions (10^{13} Hz collision frequency, ps-time scale for equilibrium)
  - Deviation of predictions from experimentally measures values
- Electronegative gas effect
  - Dry air containing 20% of O_2 was used
  - O_2 molecules captured ionized electrons and formed heavy negative ions
  - Residual electrons also remained in test cell
  - Experiments suggested that the electron capture by O_2 takes place via three-body reaction

$$O_2 + e + M \rightarrow O_2^- + M$$

Plasma Processes in HPRF cavity

- Energy loss of incident particle by ionization can be described by the Bethe-Bloch formula

$$\frac{dE}{ds} = 4\pi N_A r_e^2 m_e c^2 \rho \frac{Z}{A} \left(\frac{1}{\beta^2} \ln \frac{2 m_e c^2 \gamma^2 \beta^2}{I} - 1 - \frac{\delta(\beta)}{2\beta^2} \right), \tag{1}$$

- Atomic processes

$$p + H_2 \to p + H_2^+ + e^-,$$
$$H_2^+ + 2H_2 \to H_3^+ + H_2 + H,$$
$$H_3^+ + e^- \to 3H.$$

- In the case of O_2 presence,

$$O_2 + e + M \to O_2^- + M$$

- Intrinsically multiscale problem: relevant time scales change from ps to several μs.

Algorithms for EM-PIC with Atomic Physics

- Finite Difference Time Domain
- PIC approximation for charges
- Rigorous charge conservative method
- Symplectic explicit solvers (Boris scheme), 2nd order accurate
- Physically relevant boundary conditions
- Probabilistic algorithm for atomic physics
- Parallelization for traditional and multicore supercomputers

FDTD with Particles: Cloud-in-Cell method

- Uniform charge density cloud.

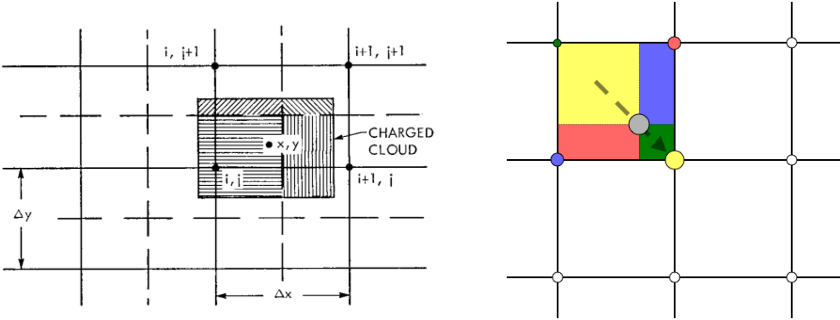


Figure: Cloud-in-Cell method concept and computation

Rigorous charge conservative method

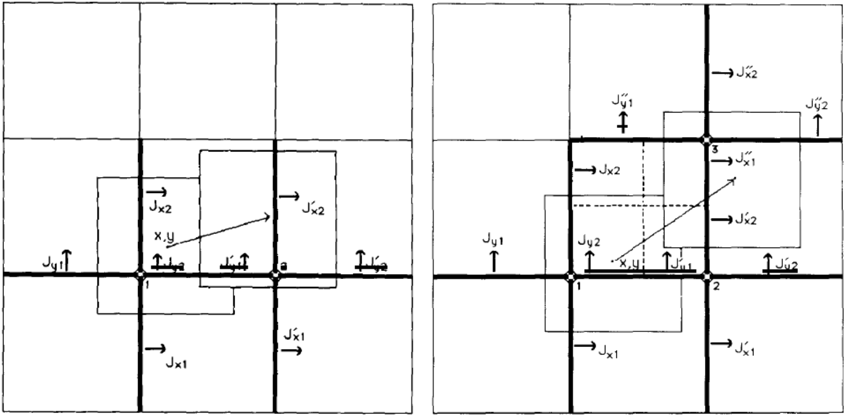


Figure: Computation in two cells and three cells

PIC Method for Electromagnetic Problems

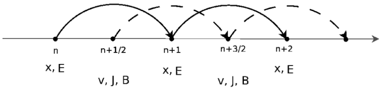
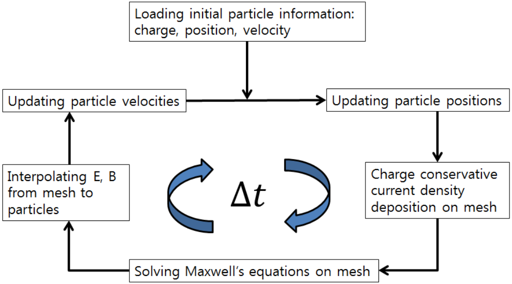


Figure: Computation sequence along time step


Loading initial particle information: charge, position, velocity

Updating particle velocities

Updating particle positions

Interpolating E, B from mesh to particles

Δt

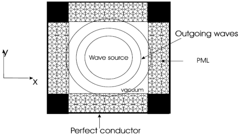
Charge conservative current density deposition on mesh

Solving Maxwell's equations on mesh

Figure: Processing flow in a time step of electrostatic problems

Boundary conditions

- Regular Boundary
    - Open Boundary: Absolving Boundary Condition by using Perfectly Matched Layer (PML) (In progress).



    - Superconducting Boundary (Implemented in the current code)
- Irregular Boundary (implemented in a serial FDTD code)

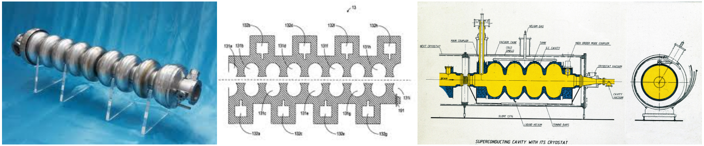


Figure: RF cavity

Code Structure

- C++, Object-Oriented Design
- Main components
    - FieldSolver: solves Maxwell's equations using FDTD
    - ParticleMover: propagate particles and implements rigorous charge conservation method
    - Visualization: FieldViewer, ParticleViewer (parallel data rendering using VisIt)
    - TimeController: control above objects
    - All components have passed careful verification tests

Parallelization Methods: Field Solver

- 3D parallel domain decomposition for solving Maxwell's equation
- Well balanced computation dominated problem
- Good weak scaling to thousands of processors on BG/P
- Hybrid parallelization method for multicore supercomputers (BG/P) using MPI and OpenMP
  - Gives only several percent of the performance increase for moderate-size problems
  - Is beneficial only if the MPI communication time is bigger than the computation time

Parallelization Methods: Particle solver

- Parallel particle decomposition is independent on their geometric location
- Particles in a parallel computing node can exist anywhere in the computational domain
- Very good load balance of computation
- Communication cost becomes high if the computational mesh is 128^3 or larger
- We have reduced communications by using ideas from parallel sparse matrix storage algorithms

Code Validation

- Step 1: Validation of FDTD solver without charges
  - Comparison with exact analytical solutions for rectangular cavities
  - Second order convergence
  - Good weak scalability to thousands of processors on BG/P
- Step 2: Validation of EM-PIC code was performed using electrostatic interaction and space charge problems

Validation of Embedded Boundary Method

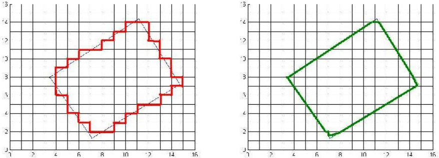


Figure: "Irregular boundary" can be obtained by simply rotating rectangular cavity with respect to the grid. Advantage: exact solution exists. Stair-case approximation (left) and EBM (right) for rectangular cavity.

grid size	EBM convergence order, $\frac{\log e_1/e_2}{\log h_1/h_2}$
16*16*16	NA
32*32*32	1.25
64*64*64	1.47
128*128*128	1.42

Previous simulation of muon beams in absorbers

- Muon bunch propagates in plasma cloud
- Constant particle number: ionization and recombination is neglected
- Muon bunch: 10^{12} particles, $\sigma_x = \sigma_y = 0.05$, $\sigma_z = 0.67$
- Ion / electron cloud: 10^{12} pairs, $\sigma_x = \sigma_y = 0.1$, $\sigma_z = 1.3$
- Muon beam has initially zero emittance. We study the muon scattering as the bunch propagates throgh plasma

Preliminary simulation of positive muon beam in absorbers

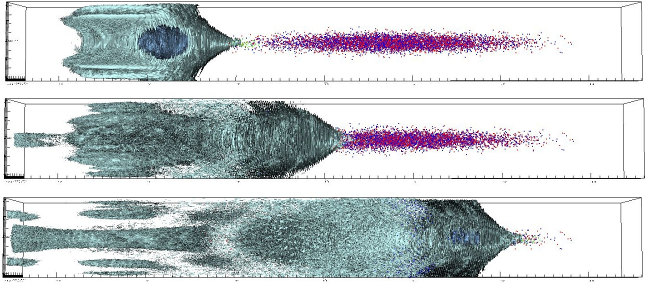


Figure: Muon bunch in absorber

Preliminary simulation of negative muon beam in absorbers

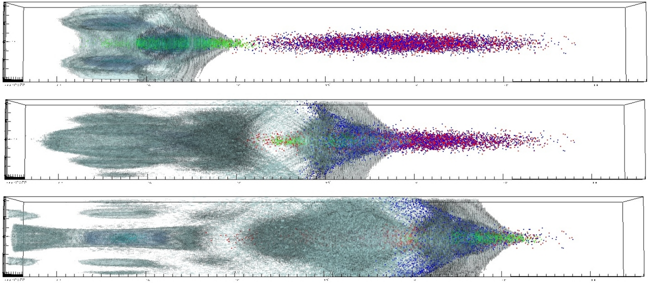


Figure: Muon bunch in absorber

Muon Scattering on Plasma

Muon bunch location	Transverse vel.	Longitudinal vel.
-6	2.678E+04	2.6376E+08
-3.2	2.692E+05	2.6356E+08
0.3	5.373E+05	2.6334E+08
2.5	8.415E+05	2.6307E+08
5	1.140E+06	2.6268E+08

Implementation of atomic physics processes in bean induced plasma

- Each macroparticle has extra degree of freedom: the life time (depending on state)
- Multiple species of particles are supported
- The energy loss of each incident macroparticle is calculated by integration the Bethe-Bloch formula along the particle trajectory $\Delta E = N_p \int f(v) ds$
- At each time step, ion - electron pairs are created along the proton macroparticle path by assigning them random direction velocities corresponding to their initial energy

Implementation of atomic physics processes in bean induced plasma (cont.)

- H_2^+ is transformed into H_3^+ ion on picosecond time scale. This simply requires changing the mass of the ion macroparticle and re-setting its internal time in the data structure
- In pure hydrogen, lifetime of electrons before recombination is very long, μs
- Electron capture by O_2 represents intermediate time scale
- Problem of electron mobility in high pressure gas

Current simulations (in progress)

- Plasma loading in pure hydrogen HPRF cavity
  - Run 1: simulate detailed atomic physics and plasma formation as proton beam passes through RF cavity (ns time scale)
  - Run 2: use input from step 1 and simulate long term dynamics (μs) of plasma in external fields using statistical models for electron dynamics
- Electronegative gas in HPRF cavity
  - Add atomic transformation involving O_2 and resolve fast capture of electrons by O_2 and dynamics of residual electrons