Conservative Particle-Mesh Algorithms and Parallel Software for Electromagnetism and Applications

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Introduction: Motivation

- High priority BNL projects
  - Physics of high-gradient hadron laser-plasma accelerator.
  - Advanced cooling and polarizing techniques for high energy hadron and lepton collider.
  - Simulation of short electron bunches in accelerators in support of the e-RHIC project.
- Muon Cooling

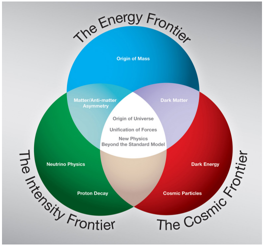


Figure: Muon collider's important role in three research fields

Notation and Terminology

- Notations
  - $\mathbf{E}$ Electric field intensity (V/m)
  - $\mathbf{D}$ Electric flux density (Electric displacement) (C/m^2)
  - $\mathbf{H}$ Magnetic field intensity density (T)
  - $\mathbf{B}$ Magnetic flux density (A/m)
  - μ_0 Permeability in free space (H/m) $(4\pi \times 10^{-7})$
  - ϵ_0 Permittivity in free space (F/m) $(\frac{1}{36\pi} \times 10^{-9})$
  - c speed of light in free space (m/s)
- Relations
  - $\mathbf{D} = \epsilon_0 \mathbf{E}$
  - $\mathbf{H} = \frac{1}{\mu_0}\mathbf{B}$
  - $c = \frac{1}{\sqrt{\epsilon_0 \mu_0}}$

Finite-Difference Time-Domain (FDTD)

Maxwell's Equations

Differential Form	Integral Form
$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$ $\Rightarrow (\nabla \cdot \mathbf{B})_t = 0$	$\oint_C \mathbf{E} \cdot dl = -\frac{d}{dt} \int_S \mu \mathbf{H} \cdot d\mathbf{s}$
$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}$	$\oint_C \mathbf{H} \cdot dl = I + \frac{d}{dt} \int_S \mathbf{D} \cdot d\mathbf{s}$
$\nabla \cdot \mathbf{D} = \rho$ $(\rho_t = -\nabla \cdot \mathbf{J})$	$\oint_C \mathbf{D} \cdot d\mathbf{s} = Q$
$\nabla \cdot \mathbf{B} = 0$	$\oint_C \mathbf{B} \cdot d\mathbf{s} = 0$

Yee Mesh

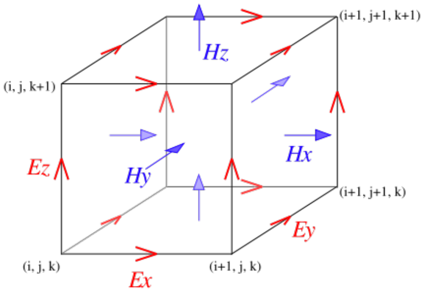


Figure: Yee Cell: Locations of grid indexes in three dimensions

Space-Time Chart of FDTD

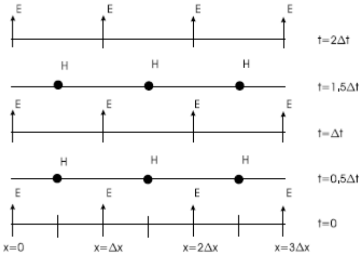


Figure: The one dimensional space-time chart of FDTD

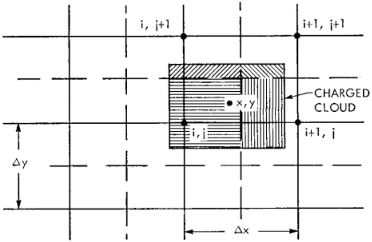
Divergence equations

- By using centered space scheme of $\nabla \cdot \mathbf{B} = 0$
  $\nabla \cdot \mathbf{B} = 0$ initially $\Rightarrow \nabla \cdot \mathbf{B} = 0$ at later time step.
- This is true for $\nabla \cdot \mathbf{E}$ by assuming no charge.
- In the case of having charges,
  $\nabla \cdot \mathbf{E} = \nabla \cdot (-\nabla \phi) = \nabla^2 \mathbf{E} = -\frac{\rho}{\epsilon}$.
- However, solving the Poisson's equation can be circumvented by using the rigorous charge conservative method.

FDTD with Particles

Cloud-in-Cell method

- Uniform charge density cloud.



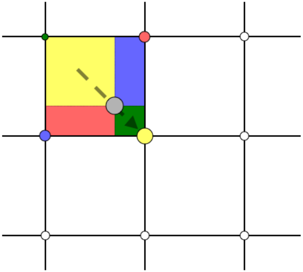


Figure: Cloud-in-Cell method concept and computation

Dynamics of Particles in EM Fields & its Discretization

- Newton - Lorentz force equation

$$m\frac{d\mathbf{u}_p}{dt} = \mathbf{F}_p = q_p\left(\mathbf{E}(\mathbf{x}_p) + \mathbf{u}_p \times \mathbf{B}(\mathbf{x}_p)\right)$$

- Leapfrog scheme for Newton - Lorentz force equation

$$\begin{cases} \dfrac{\mathbf{x}^{n+1} - \mathbf{x}^{n}}{\Delta t} = \mathbf{u}^{n+1/2} \\ \dfrac{\mathbf{u}^{n+\frac{3}{2}} - \mathbf{u}^{n+\frac{1}{2}}}{\Delta t} = \\ \dfrac{q}{m}\left(\mathbf{E}^{n+1}(\mathbf{x}^{n+1}) + \left(\dfrac{\mathbf{u}^{n+\frac{3}{2}} + \mathbf{u}^{n+\frac{1}{2}}}{2} \times \mathbf{B}^{n+1}(\mathbf{x}^{n+1})\right)\right) \end{cases}$$

Relativistic Corrections

- Particles moves at nearly the speed of light. $\Rightarrow$ Relativistic correction.
- $\frac{\Delta \mathbf{u}}{\mathbf{u}} \simeq 0 \Rightarrow$ Constant Lorentz factor $\gamma = \frac{1}{\sqrt{1-\mathbf{u}^2/c^2}}$.
- Relativistic equation of motion

$$(\gamma m)\frac{d\mathbf{u}_p}{dt} = \mathbf{F}_p = q_p\left(\mathbf{E}(\mathbf{x}_p) + \mathbf{u}_p \times \mathbf{B}(\mathbf{x}_p)\right).$$

Symplectic Integrator

PIC Method for Electromagnetic Problems

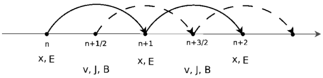


Figure: Computation sequence along time step

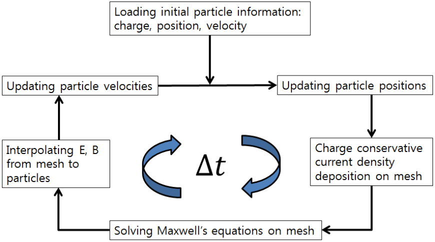


Figure: Processing flow in a time step of electrostatic problems

Explicit Symplectic Time Integration (Boris Scheme)

- The main drawback of the Leap-Frog scheme is that

$$\frac{\mathbf{u}^{n+\frac{1}{2}} - \mathbf{u}^{n-\frac{1}{2}}}{\Delta t} = \frac{q}{m}\left(\mathbf{E}^n(\mathbf{x}^n) + \left(\frac{\mathbf{u}^{n+\frac{1}{2}} + \mathbf{u}^{n-\frac{1}{2}}}{2} \times \mathbf{B}^n(\mathbf{x}^n)\right)\right)$$

  is implicit.
- Boris scheme is an explicit transformation of the implicit scheme.
- Boris scheme is explicit and symplectic.

Rigorous charge conservative method

- By assuming charge density conservation, that is, assuming $\rho_t = -\nabla \cdot \mathbf{J}$ equation holds, Ampère's circuital law implies Gauss's law because we have $(\nabla \cdot \mathbf{D})_t = \nabla \cdot \mathbf{D}_t = \nabla \cdot (\nabla \times \mathbf{H}) - \nabla \cdot \mathbf{J} = -\nabla \cdot \mathbf{J} = \rho_t$.
- We want this property also holds in FDTD and CIC discretization.
- First, consider the dual grid of Yee mesh grid.

Rigorous charge conservative method (cont.)

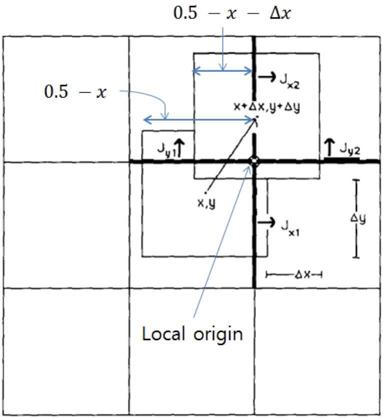


Figure: Current computation in one cell

Rigorous charge conservative method (cont.)

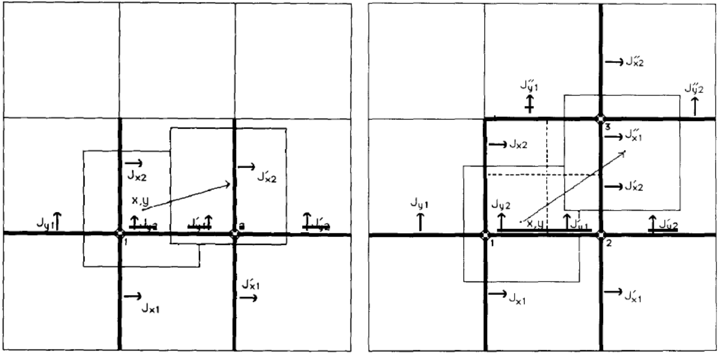
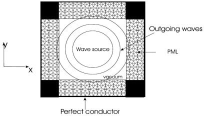


Figure: Current computation in two cells and three cells

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)

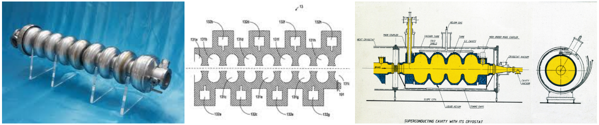
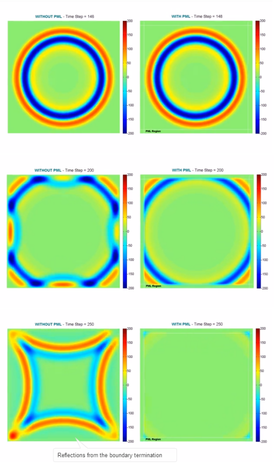


Figure: RF cavity

Boundary conditions: Comparison between non-PML and PML boundaries



Code Structure

- We use C++ and applied Object-Oriented Design.
- The software mainly operated by three objects.
  - FieldSolver: solve Maxwell's equations using FDTD.
  - ParticleMover: solve Maxwell's equations using FDTD.
  - TimeController: control above two objects and any other miscellaneous objects such as FieldViwer and ParticleViewer which deal with visualization of electromagnetic field and particle respectively.

Parallelization Methods

- The parallel code is using domain decomposition in solving of Maxwell's equation.
- Parallel particle decomposition is independent on their geometric location
- Particles in a parallel computing node can exist in whole computational domain whereas Maxwell's equation is solved in a local domain of a parallel computing node.
- Although the particle decomposition has a drawback, it has very good load balance.
- Ill-balanced load to computing nodes in solving particle motion is affecting the performance. We are working on resolving it

Code Validation

Figure: Coulomb's Law

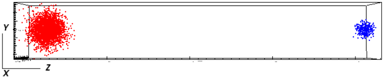


Figure: Simulation result for code validation

Code Validation (cont.)

- Simulation setting

	Left bunch	Right Bunch
Charge per particle	-1.602e-9 (C)	-1.602e-12 (C)
Mass per particle	9.109e-10 (Kg)	9.109e-24 (Kg)
# of particles	3000	300

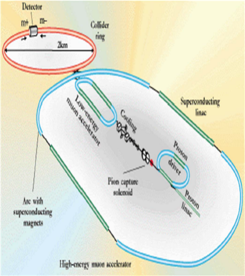
- Analytic result: $(0.0, 0.0, 2.0604e + 6)$ (m/s)
- Simulation results

# of particles	Relative error of velocity (m/s)
300	(-3.34e-03, 6.55e-03, 1.5e-3)
3000	(3.37e-4, 6.75e-4, 1.e-5)

Applications

Muon Collider and Neutrino Factory

- The purpose of a muon collider is to create and accelerate in opposite directions two muon beams in a circular machine, and to bring them into collision.
- A neutrino factory stores dense muon beams in a ring.



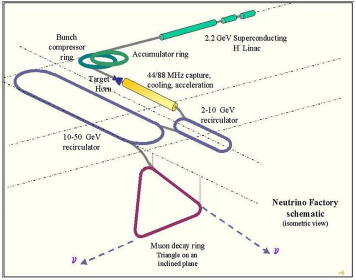


Figure: Schematic of Muon collider and Neutrino Factory

Muon Cooling: Theory

- In both the muon collider and neutrino factory, generated muons are sufficiently "hot": they have large spreading energy or a large volume in the 6-dimensional phase space.
- Before accelerating or storing such muon beans in a circular rings, the phase space of muon beams must be reduced (so-called beam cooling).
- As the magnetic field does not change the total energy of particle, according to Liouville's theorem, it will not change the phase space.
- The transverse phase space coordinates of a beam can be reduced by passing the beam through an absorber (called the ionization cooling proposed in 1981).

Muon Cooling: Theory (cont.)

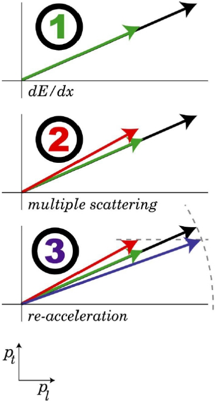


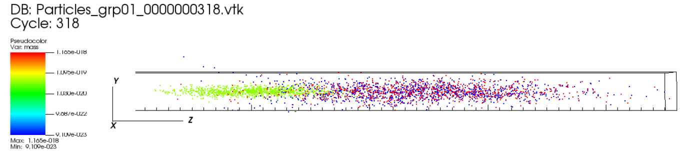
Figure: Schematic of muon ionization cooling (courtesy S. Holmes).

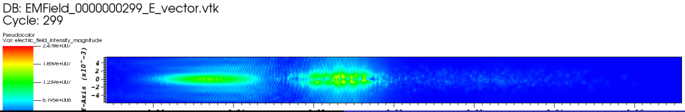
Previous work and its limitations

- The ICOOL code (1996) has been designed to track muons in magnetic focusing lattices, together with interactions in shaped absorbers.
- Being a single-particle serial code, ICOOL is missing collective effects such as space charge that have important implication on the beam dynamics and the cooling process.
- The limitations of ICOOL are partially resolved in the code Geant.
- However, in the both codes, ionization processes produce sufficiently ionized plasma in the absorber that may strongly influence the incoming muon bunch.
- The production of plasma in the absorber and the muon bunch - plasma interaction, unresolved in previous simulations, will be among most important applications of our code.

Preliminary simulation of muon beams in absorbers

- Muon bunch goes through a lithium plasma cluod
- 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 muon beams in absorbers

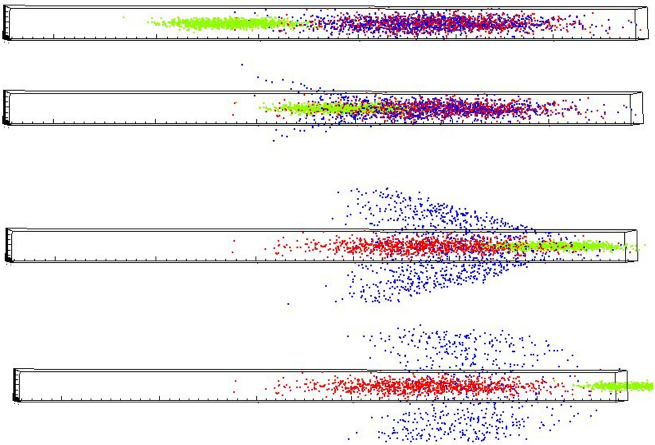


Figure: Muon bunch in lithium absorber

Muon Scattering on Lithium 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