ALGORITHMS FOR SELF-CONSISTENT SIMULATIONS OF BEAM-INDUCED PLASMA IN MUON COOLING DEVICES

R. Samulyak*, Stony Brook University, Stony Brook, NY and BNL, Upton, NY, USA
K. Yu, Stony Brook University, Stony Brook, NY, M. Chung, A. Tollestrup,
K. Yonehara, FNAL, Batavia, IL, R. D. Ryne, LBNL, Berkeley, CA, USA

Abstract

A code called SPACE for the simulation of beam-induced plasma in gas-filled RF cavities has been developed. The core code uses the particle-in-cell (PIC) method for the Maxwell equations coupled to the dynamics of particles. In the SPACE code, the electromagnetic PIC methods are coupled with probabilistic treatment of atomic physics processes. The aim of the project is to demonstrate the feasibility of the RF cavity with muon collider beams. The most critical part is investigating how intense muon beams influence the plasma dynamics. Initial phase of simulations demonstrating the plasma generation and its short time dynamics in the high pressure hydrogen filled RF test cell has been performed.

INTRODUCTION

A dense hydrogen gas filled RF cavity has been proposed for muon beam phase space cooling and acceleration. The aim of the simulation program is the development of mathematical and numerical models and parallel software for the simulation of processes occurring in gas-filled RF cavities. An important issue in high-pressure gas filled cavity is a RF power loading due to beam-induced plasma [1]. Incident particle beam interacts with dense hydrogen gas and causes significant ionization level. Due to high frequency of collisions with neutrals, electrons reach equilibrium within picosecond time scale and move with a slow drift velocity. The recombination processes occur on the millisecond time scale. In order to induce the three-body electron capture, electronegtive gas has been tested in the test cell. This is the most critical process in the final cooling stage and should be modeled accurately in simulations. Other important processes include the interaction between positive and negative ions and the interaction of the beam with wakefields. A parallel electromagnetic PIC code with atomic physics, called SPACE, has been developed at Stony Brook University / BNL. It implements new mathematical models and numerical algorithms for the interaction of high-energy proton and muon beams with neutral gas and plasmas.

NUMERICAL METHODS

PIC method for Maxwell's equations

The system of Maxwells equations is discretized using the finite difference time domain (FDTD) method on a staggered mesh [2] that achieves second order accuracy in space and time. Electric charges are represented by discrete macroparticles coupled with electromagnetic fields by the action of Lorentz forces and electric currents. When one solves Maxwells equations analytically, solving two equations describing the Faraday and Ampere laws is sufficient as the equations expressing the Gauss law and the divergence-free constraint for the magnetic field are invariants of motion. The numerical method of Yee [2] for electromagnetic fields in vacuum also preserves the divergence-free properties of the electric and magnetic fields. To deal with the last two equations in the presence of charges and currents, the rigorous charge conservation method was developed within the PIC framework in [3]. The method calculates electric currents along computational grid edges by solving a geometrical problem of sweeping the computational mesh by finite volumes associated with each macroparticle. By using this method, we find first a set of initial conditions consistent with the Maxwell equations by either solving the Poisson problem for the electric potential or by a superposition of electric fields and changes created by each particle. Then only the first two Maxwell equations and the Newton-Lorentz equation are solved numerically thus avoiding solving the Poisson problem at each time step.

A schematic of processes computed at each time step is depicted in Figure 1. We would like to note that the conservative Leapfrog time discretization scheme for the Newton-Lorentz equations of particle motion becomes implicit. We use the Boris scheme for the time update [4], which is a modification of the Leapfrog scheme resulting in an explicit and conservative scheme. We also implement modifications of the Boris scheme proposed in [5] for dealing with rapidly accelerating particles for which the relativistic factor is not constant.

For accurate simulations of electromagnetic fields in geometrically complex structures, we have implemented the embedded boundary method [6] in a stand-alone Maxwell equation solver. The coupling of algorithms for complex boundaries with the main electromagnetic PIC code will be performed in the next phase.

Code Structure and Properties

The code is developed in C++ utilizing the advantages of Objected-Oriented Programming. The code is composed of three major parts. The first part, the FieldSolver class, contains FDTD solvers of the Maxwell equations. The second part, the ParticleMover class, contains solvers for the Newton-Lorentz equation. This class also includes various physics models describing particle interactions and trans-

* roman.samulyak@stonybrook.edu

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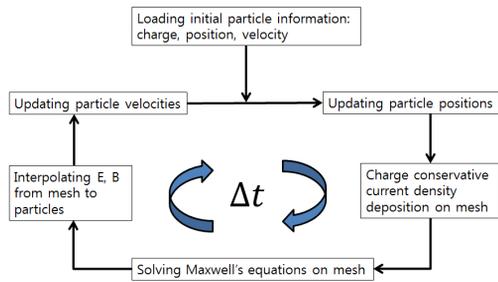D06 - Code Development and Simulation Techniques

Figure 1: Interaction of muons with plasma in cooling absorbers. Negative (top) and positive (bottom) muons (red dots) interacting with ions (green) and electron (blue dots). Semi-transparent iso-surfaces represent electric field intensity.

formations by atomic physics processes. The code is capable of tracking numerous particle species. Finally, the third, TimeController class, controls the above classes and any miscellaneous classes such as classes performing the visualization of electromagnetic fields and particle data. The visualization is done using the visualization software called VisIt developed at LLNL for the remote parallel visualization on distributed memory supercomputers. Since the main classes of the code are connected via the interface classes, the code can easily be extended by implementing additional functions and physics models. For convenience of a new problem setup, the initialization routines use XML (eXtensible Markup Language).

Parallelization Methods

The electromagnetic PIC code is parallelized using a hybrid MPI / tread programming for distributed memory multicore supercomputers. The FieldSolver uses a three-dimensional domain decomposition for solving Maxwell's equations. The ParticleMover uses a decomposition of particles that is independent of the FieldSolver domain decomposition. Namely, particles in a parallel computing node can be distributed in the whole computational domain whereas Maxwell's equations are solved in a local domain of a parallel computing node. As the distribution of particles is usually very non-uniform in the space, such a decomposition maximizes the load balance.

In the electromagnetic-PIC code, computations performed by the ParticleMover are more time consuming compared to computations by the FieldSolver. The described parallel decompositions minimizes the CPU computing time but requires a large amount of communications between the FieldSolver and ParticleMover. We have adopted ideas from the sparse matrix storage to minimize the amount of communications and send field data to ParticleMover from only those computational cells that contain macroparticles.

Verification and Validation

The electromagnetic PIC code has undergone a V&V program and its accuracy and parallel scalability has been
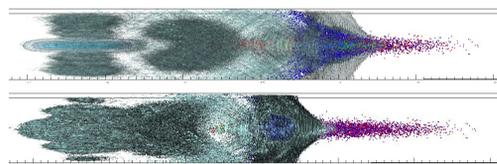
Figure 2: Example of simulation using SPACE code. Interaction of muons with preset plasma in cooling absorbers. Negative (top) and positive (bottom) muons (red dots) interacting with ions (green) and electron (blue dots). Semi-transparent iso-surfaces represent electric field intensity.

estimated. The FieldSolver has been verified using analytical solution for electromagnetic fields in a rectangular cavity. The FieldSolver achieves the second order accuracy and achieves close to linear weak scalability on thousands of processors. The embedded boundary solver has also been verified using analytical solutions for rectangular cavities initialized under some angle to the computational mesh. While the stair-case approximation of boundaries results in a zero-order accuracy, the use of the embedded boundary method restores the accuracy to the order of 1.4 1.5. The ParticleMover has been verified using space charge problems and problems with special distributions of particles.

ATOMIC PHYSICS EFFECTS

In this section, we describe the implementation of probabilistic models for atomic physics processes in gases under the influence of high energy particles and high gradient electromagnetic fields. As each macroparticle passes through the absorber, it ionizes the medium in real time by creating electron - ion pairs. The motion of ions and electrons is explicitly tracked, and their recombination and other atomic physics transformation are resolved as described below. The code supports the dynamics of multiple particle species.

Consider a high-energy particle entering an absorber medium. The energy loss of this particle by ionization can be described by the Bethe-Bloch formula [7]

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

where N_A is the Avogadro number, ρ, A, and Z are the density, atomic weight and number of the absorbing material, and m_e and r_e are the mass and the classical radius of the electron. Numerically,

$$4\pi N_A r_e^2 m_e c^2 = 0.3071 \, MeV \, cm^2/g.$$

The ionization constant I is approximately $16Z^{0.9}$eV, and δ is the density effect factor that arises from the screening of remote electrons by close electrons and results in a reduction of energy loss for higher energies.

Implementation of Atomic Physics Processes

While various atomic physics transformations are supported in the code, we currently resolve the following processes that are most essential for the problem of interest:

$$p + H_2 \rightarrow p + H_2^+ + e^-, \qquad (2)$$

$$H_2^+ + 2H_2 \rightarrow H_3^+ + H_2 + H, \qquad (3)$$

$$H_3^+ + e^- \rightarrow 3H. \qquad (4)$$
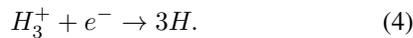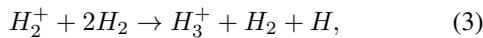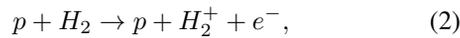
The implementation using macroparticles is as follows. The energy loss of each proton macroparticle is calculated by integration the Bethe-Bloch formula along the particle trajectory

$$\Delta E = N_p \int f(v) ds,$$

where $f(v)$ denotes the right hand side of the Bethe-Bloch formula and N_p is the number of real protons represented by one macroparticle. At each time step,

$$(int) \frac{\Delta E}{I N_H}$$

of ion – electron pairs are created along the proton macroparticle path by assigning them random direction velocities corresponding to their initial energy. Here N_H is the number of real H_2 molecules represented by one macroparticle. The initial time is recorded for each new ion and electron macroparticles and they are then tracked in the code. (int) stands for the rounding-off to integer as only integer number of ion-electron pairs can be created. The rounding-off error is saved and used in the next time step to satisfy the energy balance.

When the macroparticle of H_2^+ propagates the distance equal to the mean free path of the second atomic transformation (2.3), it is transformed into the H_3^+ ion. This simply requires changing the mass of the ion macroparticle and resetting its internal time in the data structure. As there is no need to track neutral particles, the molecule H_2 and atom H in (2.3) are ignored. The error due to the fact that the atomic weight of neutrals in the left and right sides of (2.3) differ by one atomic mass is negligible in terms of changing properties (density and pressure) inside of the RF cavity.

Finally, when the ion H_3^+ macroparticle propagates the distance equal to the mean free path of the transformation (2.4), it captures the closest electron and neutralizes into $3H$. In the code, the corresponding H_3^+ and e^- macroparticles are simply eliminated from data structures.

The interaction of electrons and ions with neutrals is modeled in the code using theory and available experimental data. For instance, electrons equilibrate on the picosecond time scale due to high frequency collisions with neutral molecules. The experimental measurements [8] suggest that the electron drift velocity in the conditions of the HPRF experiment is very low, 2.9×10^4 m/s.
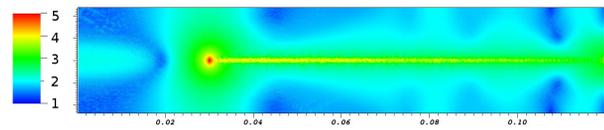
Figure 3: Logarithm of the electric field magnitude [log V/m] in the longitudinal slice of HPRF test cell during the propagation of the proton beam.

RESULTS AND DISCUSSION

We have performed simulations of the entrance of 200 MeV proton beam into the HPRF test cell filled with the hydrogen gas with the density of 10^{21} $1/cm^3$ at the pressure of 200 bar and the generation and short time scale dynamics of plasma. Each proton generates on the order of 1000 electron-ion pairs per 1 cm travel distance. Accelerated by the external field, electrons and ions practically instantaneously reach the equilibrium drift velocity defined by their collisions with neutral molecules. Unlike in simulations with preset initial distributions of positive and negative charges in vacuum shown in Figure 2, the self consistent simulation of the plasma formation and evolution in high density gas demonstrates very weak wake fields induced by the proton pulse. The 2D distribution of the magnitude of the electric field is shown in Figure 3.

CONCLUSIONS AND FUTURE WORK

We have developed a parallel electromagnetic code SPACE that combines the PIC method for particles with atomic physics. Simulations of the generation of plasma by the 200 MeV proton beam in the hydrogen filled RF test cell and the short time scale dynamics of plasma and induced wake fields have been performed. Simulations demonstrated insignificant strength of wake fields. In the future, we will perform simulations involving electronegative ions using the SPACE code. We will complete implementation of a multiscale approach in SPACE that allows simulations of both short (picosecond) and long (microsecond) time scale processes in plasma, and conclude on plasma effects in a practical RF cavity.

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