Magnetic Mirror Effect in Magnetron Plasma: Modeling of Plasma Parameters

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Capstone Project Presentation

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Abstract

- The objective of our study is to understand the magnetic mirror configuration that is ideal in in a magnetic plasma trap chamber which can be used in Magnetron sputtering . Particles in a plasma have different speeds depending on the initial distribution which is based on parameters like the plasma temperature. The speeds of particles change depending on the electric and magnetic fields. Based on the magnetic mirror effect, one can determine which particle (having certain velocities) can escape the magnetic trap and which of those are reflected. The less the particles escape the magnetic trap, the more of the flux is used in forming coatings and less of the ionized gas is wasted. This is very useful in understanding the required gas supply and rate of deposition.

- The model used in the project is mostly similar to the single particle model, where in a collection of particles, each particle evolves under the influence of the electric and magnetic fields set up by the apparatus; governed by the Lorentz force. However, we incorporate a little bit of the Kinetic theory in that we are interested in different initial velocity distributions for particles in the plasma and how the velocity distribution changes over time. To achieve this in a simulation, the Lorentz force equations are discretized and then solved using the Boris Algorithm; a standard algorithm for simulating charged particles in electric and magnetic fields.

Introduction

- A magnetic mirror configuration is important in a magnetic plasma trap chamber such as that used in Magnetron sputtering. Particles in a plasma have different speeds depending on the initial distribution which is based on parameters like the plasma temperature. The speeds of particles change depending on the electric and magnetic fields. Based on the magnetic mirror effect, one can determine which particle (having certain velocities) can escape the magnetic trap and which of those are reflected. The less the particles escape the magnetic trap, the more of the flux is used in forming coatings and less of the ionized gas is wasted. This is very useful in understanding the required gas supply and rate of deposition.

- The kinetic energy and the magnetic moment of a charged particle in a magnetic field are conserved if there are no external sources. If the magnetic field has a gradient, the component of the velocity of the particle parallel to the magnetic field changes and might decrease to zero and increase in the opposite direction: which is observed as the particle being reflected. This setup is important to understand and control how the ions are contained in and lost from a magnetron sputtering chamber.

Literature Review

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Title of the paper	Journal & Year	Authors	Description/Remarks
Introduction to plasma physics and controlled fusion	New York: Plenum press, 1984	Chen, F. F	We studied basic plasma physics including the single particle model and kinetic theory described in the technical specification section.
A 4th-Order Particle-in-Cell Method with Phase-Space Remapping for the Vlasov–Poisson Equation	SIAM Journal on Scientific Computing, 39(3), B467-B485. (2017)	Myers, A., Colella, P., & Straalen, B. V.	We studied about the general particle in cell methods used in plasma physics simulations
Why is Boris algorithm so good?	Princeton Plasma Physics Laboratory, PPPL-4872 (April, 2013)	Qin, H., Zhang, S., Xiao, J., & Tang, W. M.	We studied about the Boris algorithm, based on which our particle update strategy is based.
Introduction to nuclear fusion	Seoul National University Open Courseware. (2017)	Na, Yong-Su	We learned about the magnetic mirror effect from the lecture notws.

Gaps in the Literature

- It would take a number of courses on plasma physics to fully understand the current research methods in plasma physics. In the interest of time, we have studied some simple setups; so that we can setup well functioning plasma configuration during the course of the project and study some aspects that we are interested in.
- The forefront of research in plasma physics concerns complicated devices like Magnetic Confinement Fusion, or Quantum Optic systems. Most research in surface engineering focuses on the properties of coatings obtained and parameters of plasma used; in processes that use plasma. In our project, we would like to set up a simple plasma simulation that can help us study smaller devices like the one available in the School of Mechanical Engineering; where we can control a small flux of particles by tuning the electric and magnetic fields.
- This section describes, how we construct a simple easy to use, plasma simulation system; which is yet to be functional.

Gaps in the Literature-Contd.

Particle in Cell Methods

Particle in a cell methods are used to simulate the kinetic theory of plasma. A simple strategy used for particle in cell plasma simulation based on strategies as outlined in the paper and the slides we studied involves the following steps:

1. **Sampling and Initialization**

The initial positions and velocities of particles in the plasma are sampled from a distribution, or based on some strategy.

2. **Action of fields on the particles** The particles move under the influence of electric and magnetic fields as described by the Lorentz force.

3. **Particle deposition**

In this step, charged particles are deposited on the grid defined by the mesh, and the charge density i and the current density J_i generated by the deposited particles is computed. One strategy outlined in the paper defines charge deposition as following. $x_i = (i + 1/2)\,\Delta x$, $i \in Z$ D define the grid. A second order deposition can be achieved by

$$\varrho_i = \sum_p \left(\frac{q_p}{V_i}\right) \mathbf{W_2} \left(\frac{\boldsymbol{x_i} - \boldsymbol{x_p}}{\Delta x}\right)$$

Gaps in the Literature-Contd.

where $V_i = \Delta x$ D is the volume of the cell i and W2 (x) is a D-dimensional interpolating function defined in the paper. In simple models, the current density J_i is often not used.

4. Fields generated by particles

In this step, the electric and magnetic fields generated by the charge density and current density are computed. The paper discussed uses Poisson equation to compute the electric field generated by the charge distribution and neglects the magnetic field generated. However, in high performance simulations like that outlined in the slides we studied, the full set of Maxwell's equations are used to compute the electric and magnetic fields generated by the particles.

5. Force on particles

In this step, the force on the particles due to the electric and magnetic fields are computed. Most simulations like the one outlined in the paper; because they compute the electric and magnetic fields generated by the deposited particles, are able to describe the interaction of each particle with the electric and magnetic fields generated by other particles in the plasma, and hence capture the particle-particle dynamics.

6. Action of the force on particles

Step 2 is repeated to move the particles under the influence of the electric and magnetic fields. A flow-chart for the simulation based on a similar strategy outlined in the slides is presented below

Gaps in the Literature-Contd.

Simulation Flow-Chart

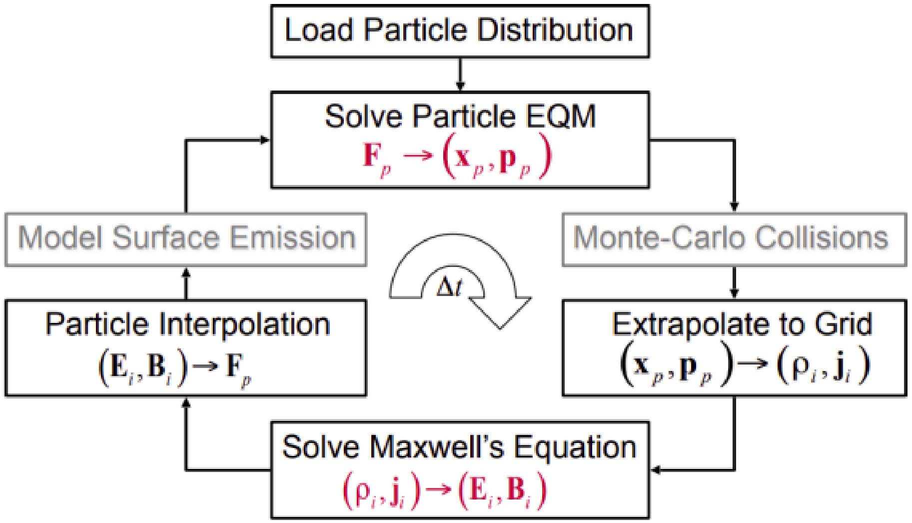


Figure 2: Flowchart for PIC methods.

Problem Definition

Our approach is similar to and differs from the general procedure outlined for Particle in Cell methods, in the following ways:

1. **Sampling and Initialization**

   Similar This step is similar to the first step in general PIC methods. We sample the initial positions and velocities of the particles based on some strategies like sampling from the Maxwell-Boltzmann distribution or uniform initialization strategies described in Methodology.

2. **Action of fields on the particles**

   Similar This step is similar to the second step in general PIC methods. We update the positions and particles of the particles according to the Boris Algorithm, based on the Lorentz force; as described in Methodology.

3. **Particle deposition**

   Skipped We skip this step in our approach for reasons described in the next step.

4. **Fields generated**

   Different As discussed earlier; when discussing the model used in the project, in devices such as those used in surface engineering processes, it is often the case that the electric and magnetic fields generated by the apparatus are far more stronger than those generated by the particles. So it is reasonable to assume that the fields generated by the particles are negligible compared to the fields generated by the apparatus. While general PIC methods compute fields generated by particles in the plasma, we only used fields generated by the apparatus. Since we neglect the fields generated by the particles in the plasma, we can skip depositing particles in the grid; which would be the third step of general outline of PIC methods. This makes our model simpler and easier to work with, evaluate and understand. We define the fields generated by the apparatus or field configurations based on analytic configurations and move the particles in the plasma under their influence. This is later described in methodology.

Problem Definition

5. Force on particles

Skipped As we do not compute the electric and magnetic fields generated by the particles, this step is skipped and the action of the electric and magnetic fields created by the apparatus is done directly in step 6.

6. Action of the fields on particles

Similar to the sixth step of general PIC methods, we repeat step 2 to move the particles under the influence of electric and magnetic fields created by the apparatus.

Our approach can be summarized in the following set of steps: Do for each batch of particles in the plasma stream:

1. Sampling and Initialization Kinetic Theory

2. Definition of fields Apparatus If required use a different field to simulate control of the apparatus, for example: changing the voltage of the electrode; changing the electric field. Do for certain number of time steps:

ˆParticle update based on Lorentz force Single particle dynamics

3. Remove particles

Surface Engineering process Particles are either absorbed to form a coating or exit the plasma chamber. The details are described later in methodology. The steps of our approach as described help us define our objectives as discussed in the following section

Objectives

The objectives of the project are based on our approach to the problem as described in problem definition:

1. **Single Particle Method**
   To simulate charged particles that evolve under the influence of electric and magnetic fields; as governed by the Lorentz force.
2. **Field Configurations**
   To simulate a few different configurations of electric and magnetic fields- some describing apparatus like coils; some describing analytic expressions for fields and to study the different evolution of particles.
3. **Kinetic Theory**
   To study different initial velocity distributions and how the velocity distribution of particles changes as the particles evolve. Parameters like the Plasma temperature are to be studied under this topic.
4. **Analysis**
   To analyze different batches or collections of particles, subjected to different field configurations.

Methodology

1. **Particle Evolution**
   Single particle dynamics As discussed earlier, we evolve individual particles in the plasma with the Lorentz force. To achieve this in a simulation, the Lorentz force equations are discretized and then solved using the Boris Algorithm; a standard algorithm for simulating charged particles in electric and magnetic fields.
2. **Lorentz Force**
   The equations of motion for a charged particle under the influence of Electric and Magnetic fields is described by the Lorentz Force in the S.I. units as

$$\frac{d\boldsymbol{v}}{dt} = \frac{q}{m}\left(\mathbf{E} + \boldsymbol{v} \times \mathbf{B}\right)$$

as discussed earlier in equation (1); along with the expression for the velocity

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v} \qquad (2)$$

These equations are discretized to obtain

$$\frac{\boldsymbol{v}_{k+1} - \boldsymbol{v}_k}{\Delta t} = \frac{q}{m}\left[\mathbf{E}_k + \frac{(\boldsymbol{v}_{k+1} + \boldsymbol{v}_k)}{2} \times \mathbf{B}_k\right] \qquad (3)$$

Methodology

3. Boris Algorithm

The discretized Lorentz equations may be solved using the Boris Algorithm, as we do in this project. The Boris Algorithm splits equation (6.1.2) into three equations.

$$\frac{\boldsymbol{v}^- - \boldsymbol{v}_k}{(\Delta t/2)} = \frac{q}{m}\mathbf{E}_k \qquad or \qquad \frac{\boldsymbol{v}^- - \boldsymbol{v}_k}{\Delta t} = \frac{1}{2}\frac{q}{m}\mathbf{E}_k$$

which is often called the first half of the electric pulse.

$$\frac{\boldsymbol{v}^+ - \boldsymbol{v}^-}{\Delta t} = \frac{q}{m}\left(\frac{\boldsymbol{v}^+ + \boldsymbol{v}^-}{2}\right)\mathbf{B}_k$$

which is often called rotation by the magnetic field.

$$\frac{\boldsymbol{v}_{k+1} - \boldsymbol{v}^+}{(\Delta t/2)} = \frac{q}{m}\mathbf{E}_k \qquad or \qquad \frac{\boldsymbol{v}_{k+1} - \boldsymbol{v}^+}{\Delta t} = \frac{1}{2}\frac{q}{m}\mathbf{E}_k$$

which is often called the second half of the electric pulse.
Adding equations (5), (6) and (7) gives

$$\frac{\boldsymbol{v}_{k+1} - \boldsymbol{v}_k}{\Delta t} = \frac{q}{m}\left[\mathbf{E}_k + \frac{(\boldsymbol{v}^+ + \boldsymbol{v}^-)}{2} \times \mathbf{B}_k\right]$$

which is almost the discretized Lorentz equation , except that $(\boldsymbol{v}^+ + \boldsymbol{v}^-)$ is substituted for $(\boldsymbol{v}_{k+1} + \boldsymbol{v}_k)$. However, subtracting equation from equation gives $(\boldsymbol{v}^+ + \boldsymbol{v}^-) = (\boldsymbol{v}_{k+1} + \boldsymbol{v}_k)$, giving the discretized Lorentz equation . This means that the Boris algorithm is equivalent to the discretized Lorentz equation.

Methodology

The equations can be written slightly different as

$$
\begin{aligned}
\boldsymbol{v}^- &= \boldsymbol{v}_k + q'\mathbf{E}_k \\
\boldsymbol{v}^+ &= \boldsymbol{v}^- + 2q'\left(\boldsymbol{v}^- \times \mathbf{B}_k\right) \\
\boldsymbol{v}_{k+1} &= \boldsymbol{v}^+ + q'\mathbf{E}_k \\
\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \Delta t \;\; \boldsymbol{v}_{k+1}
\end{aligned}
\tag{8}
$$

4. **Particle Sampling-** kinetic theory

As discussed earlier, kinetic theory of plasma uses density function and its evolution to describe a plasma. We pointed out that we will be using some aspects of kinetic theory in our project; in that we will initialize the batches (collections) of particles based on certain distributions. This will allow us to study parameters like the plasma temperature, in our project.

5. **Maxwellian distribution**

One important density function often used in the kinetic theory of plasma is the Maxwell Boltzmann distribution often called the Maxwellian which has the density function

$$\widehat{f_M} := \hat{f}(\boldsymbol{x}, \boldsymbol{v}, t) = \left(\frac{m}{2\pi KT}\right)^{\frac{3}{2}} \exp\left(-\frac{v^2}{v_{th}^2}\right) \tag{9}$$

where

$$v_{th}^2 = \frac{2KT}{m}$$

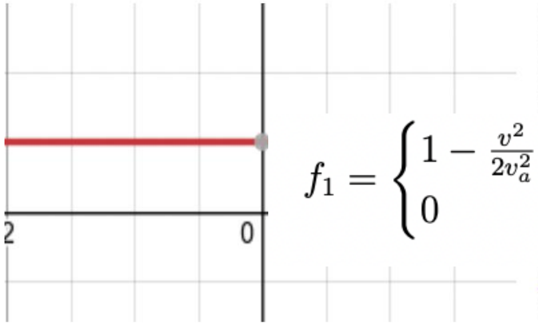
Some features of the Maxwellian are:

$$v_{rms} = \sqrt{\frac{3KT}{m}}, |\bar{v}| = 2\sqrt{\frac{2KT}{\pi m}}, |\bar{v_z}| = \sqrt{\frac{2KT}{\pi m}}, \bar{v_z} = 0$$

Methodology

6. **Parabolic distributions**

We are also interested in defining other density functions to do the sampling. The simplest density function to try would be to have all particles have the same velocity i.e. a Dirac delta function distribution. Another simple distribution would be a uniform distribution between two velocities, where a particle is equally likely to have any velocity in the range.



$$f_1 = \begin{cases} 1 - \frac{v^2}{2v_a^2} & -v_a \leq v \leq v_a \\ 0 & else \end{cases}$$

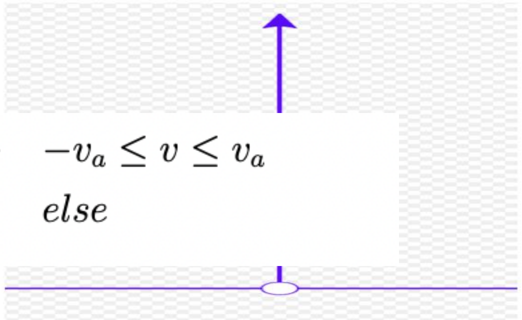


Figure 3: f_0 Figure 4: f_δ

Functions that look like f0 might define he uniform distribution while functions like fδ might describe the Dirac delta distribution. The figure for f0 was generated using desmos graphing calculator while the figure for fδ was snipped from the image in wikipedia for the Dirac delta function. We define initialization strategies based on uniform and Dirac delta distributions in our simulations. Parabolic functions in a given range also seem like interesting distributions and yet simple to work with. After some trial and error, two functions that seem interesting are:

$$f_1 = \begin{cases} 1 - \frac{v^2}{2v_a^2} & -v_a \leq v \leq v_a \\ 0 & else \end{cases}$$

Methodology

7. **A justification for Parabolic density functions - Vlasov equation**

One good exercise is to check what happens when plugging in ˆf1 , ˆf2 and fM in the collisionless Vlasov equation. As discussed earlier Kinetic theory of plasma describes the system with a density function. The dynamics of the plasma is described by the changing of the density function. Earlier, Boltzmann equation was discussed as an equation used to describe this dynamics. Vlasov equation is an instance of the collisionless Boltzmann equation discussed earlier; where it is assumed that the particles do not interact with each other, and the force exerted on the particles is described by the Lorentz force. The Vlasov equation is written as:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f + \frac{q}{m} (\mathbf{E} + \boldsymbol{v} \times \mathbf{B}) \cdot \partial_{\boldsymbol{v}} f = 0$$

For the Maxwellian function the equation now becomes,

$$\left(\frac{m}{2\pi KT}\right)^{\frac{3}{2}} \exp\left(\frac{-v^2}{v_{th}^2}\right)\left(\frac{-2}{v_{th}^2}\right)\left[v_x\left(E_x + v_y B_z - v_z B_y\right) + v_y\left(E_y + v_z B_x - v_x B_z\right) + \right.$$

$$\left. v_z\left(E_z + v_x B_y - v_y B_x\right)\right] = 0$$

which gives

$$v_x E_x + v_y E y + v_z E_z = 0$$

which can also be written as

$$\boldsymbol{v} \cdot \mathbf{E} = 0$$

Methodology

In the range $v \in \mathbb{R} \backslash [-v_a, v_a]$ the equation becomes $0 = 0$ which is trivial. The equation becomes undefined for $v = v_a$ and $v = -v_a$ but we can ignore that for now. In the interesting range of $v \in (-v_a, v_a)$, the equation becomes

$$\frac{1}{4v_a^3}\left(\frac{-2}{2v_a^2}\right)\left[v_x\left(E_x + v_y B_z - v_z B_y\right) + v_y\left(E_y + v_z B_x - v_x B_z\right) + v_z\left(E_z + v_x B_y - v_y B_x\right)\right] = 0$$

for $\hat{f}_1$ and

$$\frac{1}{12v_a^3}\left(\frac{2}{2v_a^2}\right)\left[v_x\left(E_x + v_y B_z - v_z B_y\right) + v_y\left(E_y + v_z B_x - v_x B_z\right) + v_z\left(E_z + v_x B_y - v_y B_x\right)\right] = 0$$

for $\hat{f}_2$ which both give the same equation as $\widehat{f_M}$

$$v_x E_x + v_y Ey + v_z E_z = 0 \qquad or \qquad \boldsymbol{v} \cdot \mathbf{E} = 0$$

Methodology

8. **A justification for Parabolic density functions - Magnetic mirror**

So an approximation $\left\langle \frac{v_x^2+v_y^2}{v_x^2+v_y^2+v_z^2} \right\rangle = \frac{\langle v_x^2+v_y^2 \rangle}{\langle v_x^2+v_y^2+v_z^2 \rangle} + c_0$ can be done where c_0 is an error term.

For $\widehat{f_M}$, $\langle v_x^2+v_y^2 \rangle = \frac{2KT}{m}$ and $\langle v_x^2+v_y^2+v_z^2 \rangle = \frac{3KT}{m}$ so

$$\langle sin^2\theta \rangle = \left\langle \frac{v_\perp^2}{v^2} \right\rangle = \left\langle \frac{v_x^2+v_y^2}{v_x^2+v_y^2+v_z^2} \right\rangle = \frac{\langle v_x^2+v_y^2 \rangle}{\langle v_x^2+v_y^2+v_z^2 \rangle} + c_0 = \frac{2}{3} + c_0$$

For $\hat{f}_1$, $\langle v_x^2+v_y^2 \rangle = \frac{22}{45} v_a^2$ and $\langle v_x^2+v_y^2+v_z^2 \rangle = \frac{11}{15} v_a^2$ so $\langle sin^2\theta \rangle = \frac{2}{3} + c_0$ and

For $\hat{f}_2$, $\langle v_x^2+v_y^2 \rangle = \frac{98}{135} v_a^2$ and $\langle v_x^2+v_y^2+v_z^2 \rangle = \frac{49}{45} v_a^2$ so $\langle sin^2\theta \rangle = \frac{2}{3} + c_0$

$\hat{f}_1$ and $\hat{f}_2$ behave similar to $\widehat{f_M}$ when plugged into the expression for $\langle sin^2\theta \rangle$.

Since $\hat{f}_1$ and $\hat{f}_2$ behave similar to $\widehat{f_M}$ when plugged into the Vlasov equation and the expression for $\langle sin^2\theta \rangle$, it seems that $\hat{f}_1$ and $\hat{f}_2$ are nice distribution functions to work with.

Methodology

9. **Fields**

In order to define the plasma chamber and hence the control on the plasma, we are interested in defining a few different electric and magnetic field configurations. We have a few different field configurations in mind. For the electric field, as of now we have 2 field configurations:

1. **Uniform electric field**

   The electric field has the same value everywhere. It is a very simple configuration to think about and use.

2. **Electric field due to an electrode**

We describe the electrode in the following way: Every particle sees the electrode create an electric field created by a pair of capacitor plate at a distance taken only in the x-y plane. This is to say that every point on the electrode; now assumed to be a line along the z-direction, creates an electric field like that created between a pair of capacitor plates, if there is a particle at the same z-coordinate as that point. So currently we use the expression $E = V \cdot dr$ where dr is a vector whose z-coordinate is zero.

10. **Running different batches**

As discussed earlier we would like to describe different batches of particles, so as to model plasma streams; where the particles are sent into the chamber based on different initialization strategies. The particles are then evolved based on the Boris algorithm. We would then remove the particles to simulate particles exiting the chamber, or being absorbed to form coatings as in different surface engineering processes like Magnetron Sputtering.

Work carried out so far

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The simulation is programmed in jupyter notebook files (.ipynb extensions) that run python and markdown.

The notebooks are available in the following Github repository, in the notebooks folder.

GitHub repository: https://github.com/18BME2104/MagneticMirror

Algorithm Outline

Different aspects of the program are discussed based on the different notebooks (ipynb files) that describe them.

Required functionalities and Files:

1. Constants - constants.ipynb
2. Particle - particle.ipynb
3. Electric and Magnetic fields - field.ipynb
4. Particle initialization - sampling.ipynb
5. Updating the particles - step.ipynb
6. Batches of updates - run.ipynb
7. Plotting - plot.ipynb

Work carried out so far

1. **Constants - constants.ipynb**

The constants.ipynb notebook describes some constants useful in the program. Some useful constants are e (electron charge) me (electron mass), charges and masses of ions in the plasma, a.m.u (atomic mass unit), N_A (Avogadro's number), ϵ_0 (permittivity of vacuum), μ_0 (permeability of vacuum), K or k_B (Boltzmann's constant), etc.

2. **Particle - particle.ipynb**

The particle.ipynb notebook describes the state of a particle; its position, velocity, mass, charge, name, and optionally acceleration (which is set to 0 as default if it is not required to track the acceleration of a particle) as of now.

Currently the Boris algorithm as discussed earlier, is an update strategy defined to update the state of a particle. Other strategies could be defined in new functions in the class. However, Boris algorithm is good enough for us to get started.

Electric and Magnetic fields - field.ipynb

Electric and Magnetic field configurations described in **field.ipynb**.

Currently **Uniform Electric field** and the **Radial Electric field** (the field depends on the particle's position) created by an electrode are available to set up electric fields. Uniform Magnetic field and Magnetic field created by a Helmholtz coil and that by two Helmholtz coils are available

•

Work carried out so far

4. Particle initialization - sampling.ipynb

The initial positions and velocities of the particles play an important role in the evolution of their state under the influence of electric and magnetic fields. The initial distribution of positions and velocities define where the particles start in the setup (or lab apparatus); for example where they are injected into a sputtering chamber through valves, and what velocities they start with; for example what potential they are accelerated through or what parameters were used for the pumps used to pump the particles in.

5. **Updating the particles - step.ipynb**

The Step class is concerned with **initializing particles**, **defining the fields**, and **updating the states of the particles** (positions and velocities) under the action of electric and magnetic fields
To use sampled positions and velocities that have been saved in csv files, some reading functionality is useful to load these positions and velocities to be used during initialization.

Work to be done

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Work on the constants.ipynb, particle.ipynb, fields.ipynb and sampling.ipynb has been done to a certain extent. Basic work on step.ipynb has been done. However, we could modify functionalities defined here and add other definitions as work on run.ipynb progresses, so that everything works well together. Other functionalities that could be added are:

1. **Sampling** : Sampling strategies based on parabolic density functions discussed earlier are yet to be defined. New sampling strategies such as one initializing particles with the same Kinetic energy; as would happen if particles (of possibly different species) were accelerated through the same potential difference, could be defined.
2. **Fields** : New field configurations could be defined. We could also modify existing field configuration like the Electric field due to an electrode; if we find a different expression to describe it better, or if the current expression does not work well. However, we do not yet have a plasma simulation running. The major portion of the work to be done to achieve this includes working on the run.ipynb notebook. To be able to understand the simulation; to check if works correctly and to understand the plasma behavior, we also need to define functionalities to plot different parameters like particle positions and velocities. These functionalities will be defined in plot.ipynb notebook, which can be imported into ryn.ipynb and step.ipynb notebooks to plot these quantities when the simulation is running, or from saved data

Gant Chart (Work plan)

Milestones in the project phase

- Milestone 1 **Algroithm start**
  Week 3 - **Achieved**
- Around week 3 we had some understanding of basic plasma physics and so started working on how to formulate the problem as an algorithm. (Before review 1)
- Milestone 2 **Simulation running**
  Week 9 - **Expected** We expect to have the simulation running around week 9 of the project. This will allow us to have some preliminary results and understanding of our model, by re- view 2. (Before review 2)
- Milestone 3 **Study and understanding** Week 15 - **Expected** We intend to perform study on plasma using our algorithm and improve our un- derstanding of a plasma and how to control and study a plasma system before the end of the project. (Before review 3)

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