A PIC-DSMC APPROACH FOR ION OPTICS SIMULATIONS

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Abstract

An in-house code is implemented to simulate ion thruster accelerator grids which are utilized to generate thrust. The investigated grid system consists of a screen and an accelerator grid. A static potential difference of 1000 V is applied between the grids which are separated by a few millimeters. The electric field is calculated by solving the Poisson's equation for electric potential throughout the investigated domain. The domain is divided into cells in three dimensions, and Particle-in-Cell (PIC) method is applied to handle ions and neutrals which are represented with macroparticles in the system. Ions and neutrals are tracked with the Leapfrog method. Neutral-neutral and neutral-ion elastic collisions along with neutral-ion charge-exchange (CEX) collisions are incorporated into the model according to the Direct Simulation Monte Carlo (DSMC) method. The code is implemented using C++ programming language and the implementation benefited greatly from the object-oriented design. The results are compared with the experimental results from the literature.

Problem & Model

The equation solved to evaluate the electric potential distribution throughout the domain is the well known Poisson's equation:

$$\nabla^2\phi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2} + \frac{\partial^2\phi}{\partial z^2} = -\frac{\rho_{ch}}{\varepsilon_0}$$

After the electric potential and the electric field is evaluated, the ions move according to the force applied on them. The particle motion is performed with the commonly used Leapfrog algorithm. According to this method, for each macro particle the following equations are valid:

$$\mathbf{r}_i = \mathbf{r}_{i-1} + \mathbf{v}_{i-\frac{1}{2}}\Delta t$$

$$\mathbf{v}_{i+\frac{1}{2}} = \mathbf{v}_{i-\frac{1}{2}} + \mathbf{a}_i\Delta t$$

$$\mathbf{v}_{\frac{1}{2}} = \mathbf{v}_0 + \mathbf{a}_0\frac{\Delta t}{2}$$

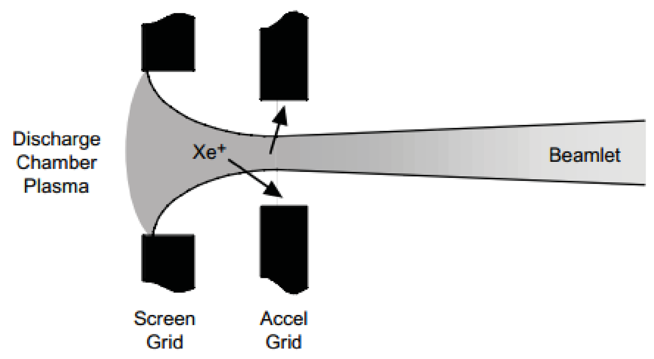


Figure: Representation of a beamlet through a screen and an acceleration grid [1]

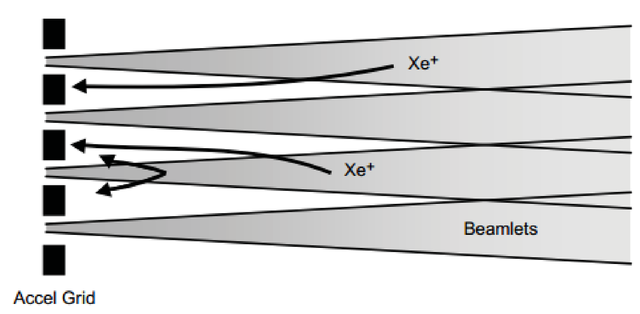


Figure: Representation of overlapping beamlets from multiple grid openings [1]

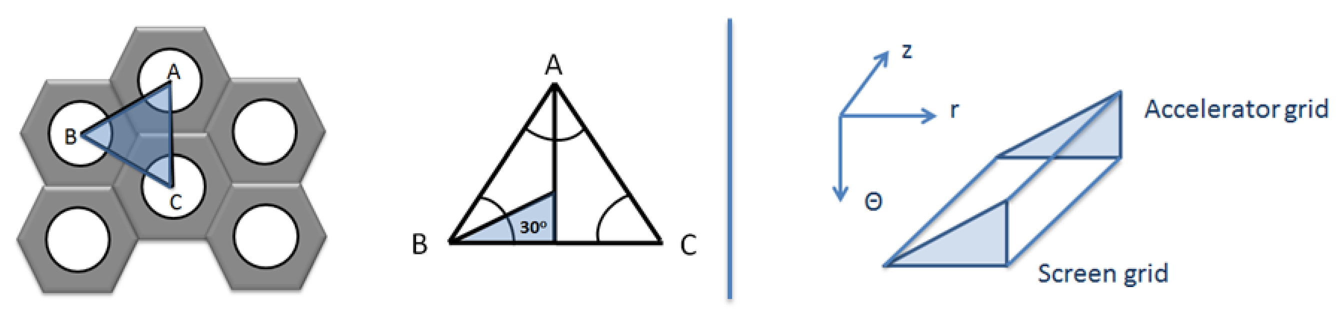


Figure : Ion grids geometry and the solution domain to be used in our case and presented with the introduction of the igx ion optics code

Algorithm & Numerical Method

Poisson's equation that is used to evaluate the electric potential results in a pentadiagonal coefficient matrix when it is discretized with the second order finite differencing. The resulting matrix is solved with ILU-preconditioned GMRES solver.

The negative of the gradient of the electric potential yields the electric field which applies the electric force on the charged particles.

Particle initialization is performed according to the assumption that particle velocities are distributed according to Maxwellian. Two particle species used in this work are ions and neutrals as stated before. Ions have a drift velocity, which is equal to the Bohm velocity in axial direction (2) whereas neutrals move within the grid region without any directed velocity (1). But their initial velocity is always taken positive in the axial direction.

Collisions between particles are handled with the conventional DSMC approach, so that particles in a particular cell collide only with the ones in that cell. In our model there are ion and neutral particles. The collisions that can occur are as follows:

- Elastic collisions between neutrals
- Charge-exchange (CEX) collisions between ions and neutrals

In collision mechanics, the collision frequency (3) is proportional to three variables. These are the densities of the collision partners, the relative velocity of the colliding particles and the collision cross section.

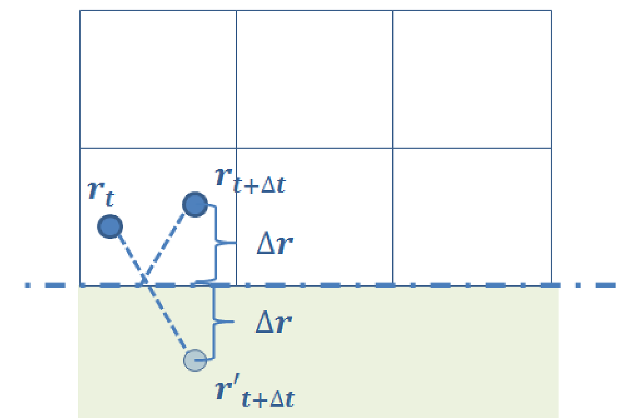


Figure: Radial centerline reflection

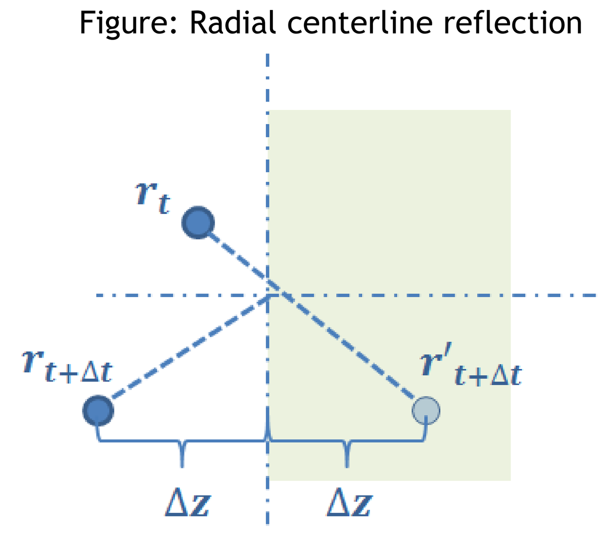
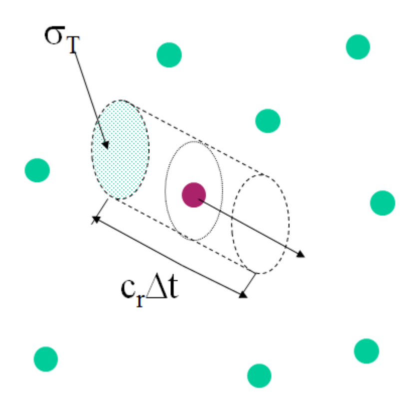


Figure: Axial reflection from grids



$$f_v(v_i) = \sqrt{\frac{m}{2\pi kT}}exp\left[-\frac{mv_i^2}{2kT}\right] \quad (1)$$

$$f_v(v_i) = \sqrt{\frac{m}{2\pi kT}}exp\left[-\frac{m(v_i-a_i)^2}{2kT}\right] \quad (2)$$

$$\nu = nc_r\sigma \quad (3)$$

Figure: Representation of the effective volume swept by a moving particle

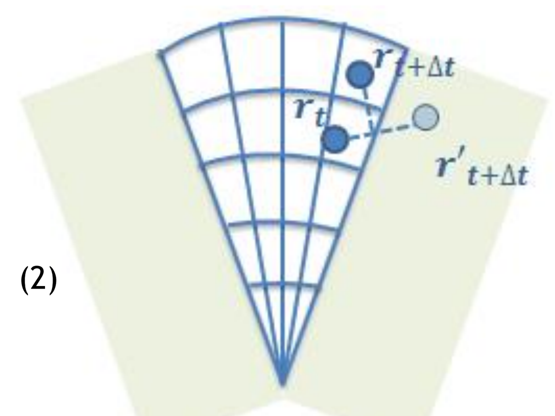


Figure: Reflection from azimuthal grids

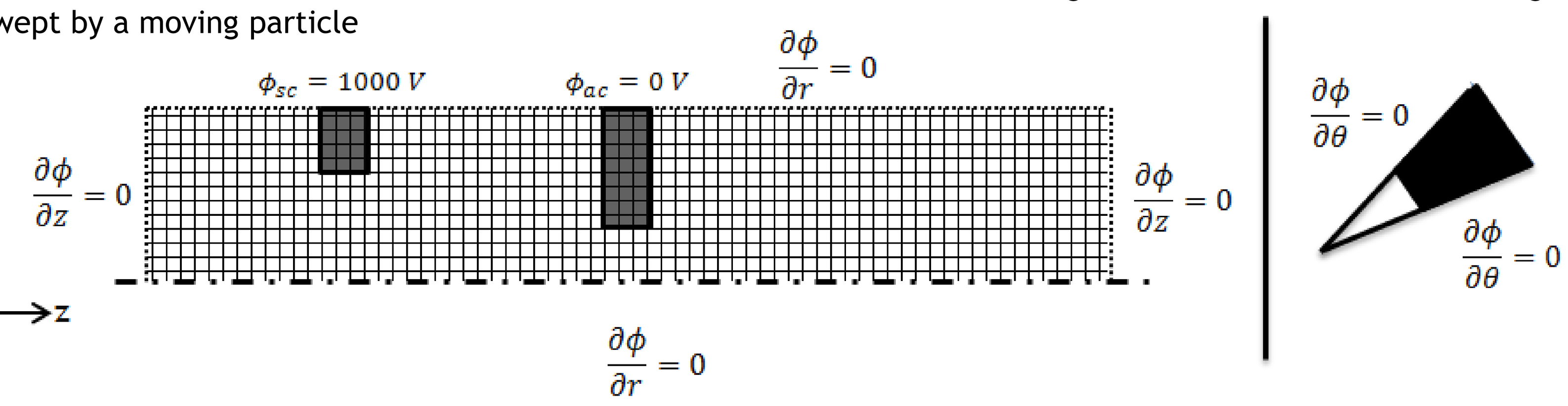


Figure: Boundary conditions for our solution domain

Results

The simulated accelerator grid configuration is obtained from the literature [2]. The boundary conditions are formulated as follows:

- Upstream (plasma chamber) electron temperature: 1.5 eV
- Upstream electric potential: 2266 V
- Downstream (plume) electric potential: 0
- Accelerator grid potential: -400 V
- Screen grid potential: 2241 V

The resulting electric potential field is depicted in Figure on the far right.

Reducing the computational time and increasing the code efficiency

The physical model leads to the following challenges:

- Neutrals are slow compared to ions that are accelerated by the electric field.
- The physical domain under investigation is very short compared to the velocities of particles, which require very small time steps.
- For the Poisson's equation solver, there is a minimum amount of cells required to obtain a convergent solution

To overcome these challenges, an optimization routine has been developed. The routine calculates:

1. **Maximum ion velocity** by taking the potential drop into account in addition to the Bohm velocity
2. The **time step** with a predetermined number of incoming ions and macroparticle factor
3. The **mesh size** yielding from the calculated time step in step 2.

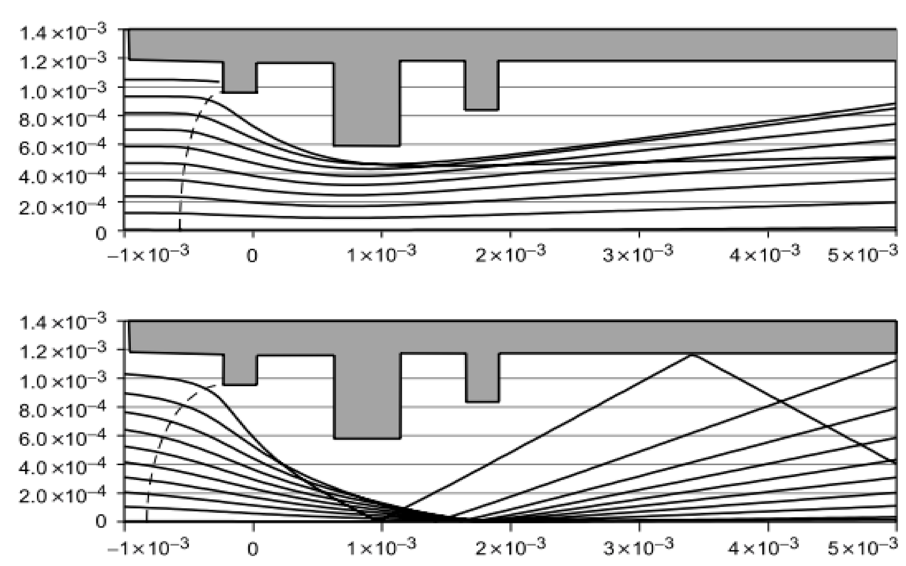
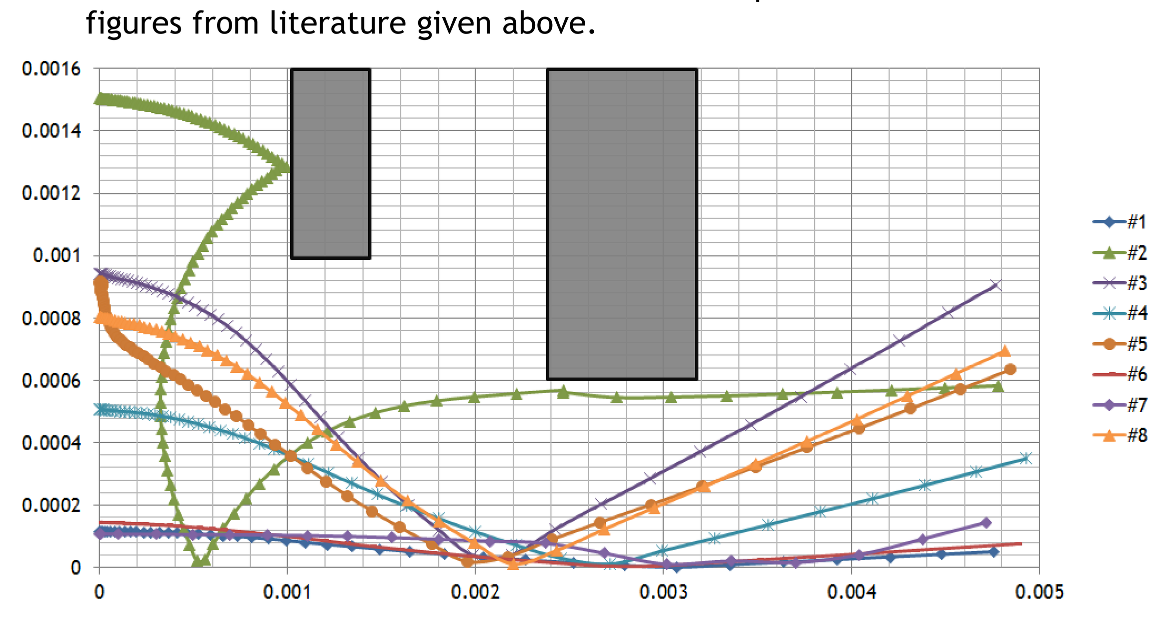


Figure: Example ion trajectories [1]

Another aim of this study is to obtain ion trajectories similar to the first figure above. The second figure results from high electric potential gradient between grids and it is described as an undesired result. Below, there is an ion trajectory figure obtained from the PIC-DSMC code for a comparison with the figures from literature given above.



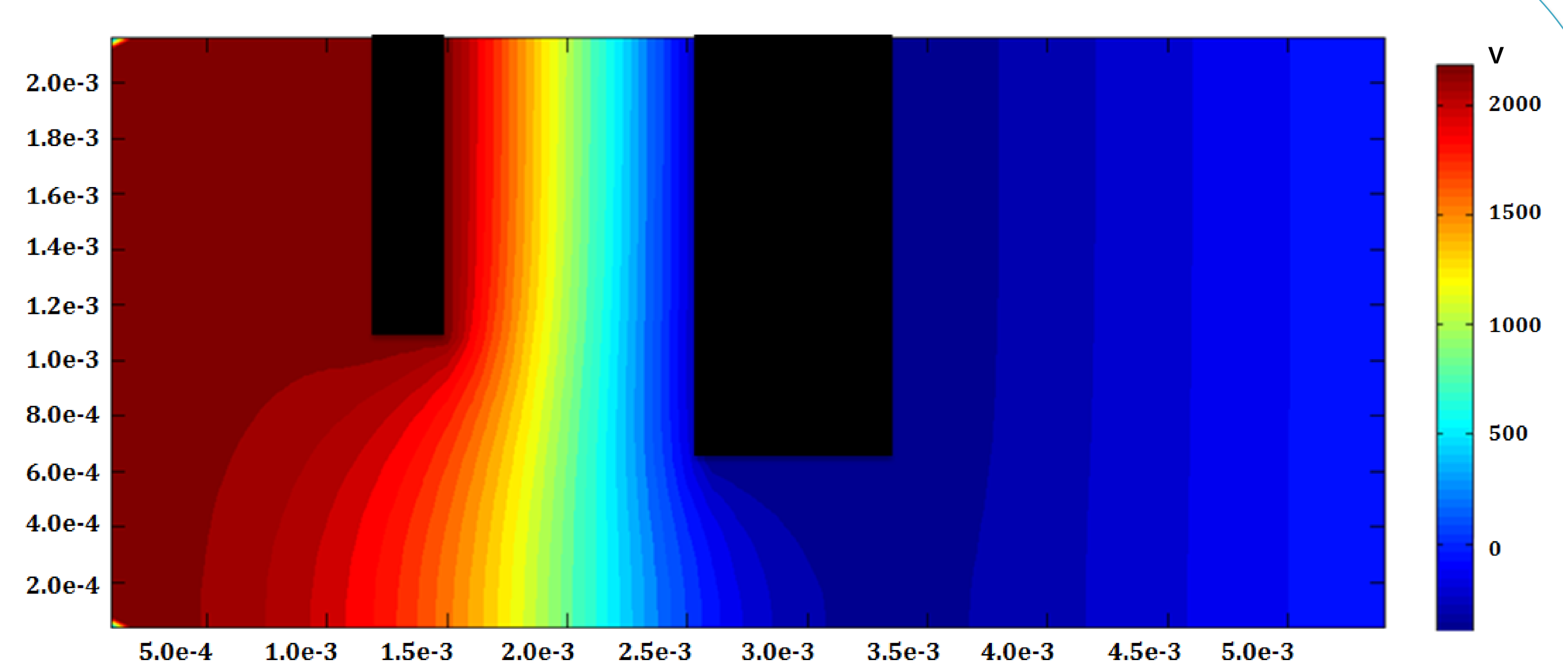


Figure: Electric potential distribution while no ions are present in the domain

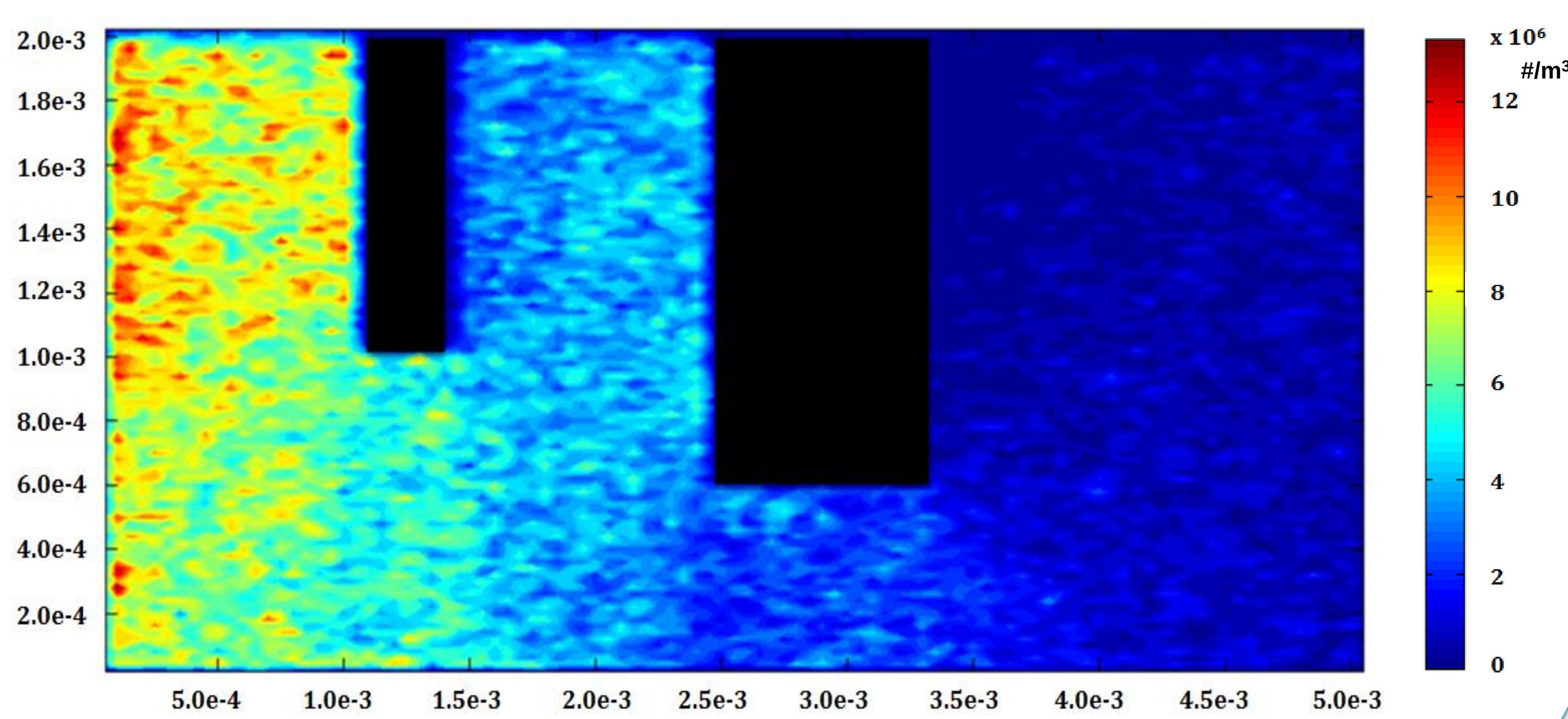


Figure: Neutral number density

[1]: Goebel, D. M. and I. Katz, Fundamentals of Electric Propulsion - Ion and Hall Thrusters, JPL Space Science and Technology Series, 2008.

[2]: Farnell,C., "Performance and Lifetime Simulation of Ion Thruster Optics,"Ph.D. Dissertation, Colorado State University, Colorado, USA, 2007

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