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Adrian Wheelock
David L. Cooke
Nicholas A. Gatsonis*

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COMPUTATIONAL MODELING OF ION BEAM-NEUTRALIZER INTERACTIONS IN TWO AND THREE DIMENSIONS

Adrian Wheelock* and David L. Cooke†
Air Force Research Laboratory, Space Vehicles Directorate, Hanscom AFB, MA 01731

Nikolaos A. Gatsonis‡
Mechanical Engineering Department, Worcester Polytechnic Institute, Worcester, MA 01609

The fact that ion beams readily neutralize given a source of electrons is well known, but the physics behind that process are not. As electric propulsion devices move into the micro and macro regimes with colloids, FEEPs, and large arrays of thrusters, the interactions between the neutralizer and the thruster are under examination. Simulations using 2D and 3D Particle-in-Cell (PIC) codes are presented, detailing starting and steady state interactions between an ion beam and electron beam. It is shown that the starting conditions require detailed current coupling to propagate normally. Steady state simulations show robust behavior regardless of ion or electron currents. Further investigation of steady state reveals no mechanism for imparting ion beam bulk velocity to electrons.

Introduction

Ion beam neutralization during operation of electric propulsion devices requires both current and charge density matching with an emitted electron beam. This current coupling is easily accomplished in reality, yet the exact process remains unknown. Currently the neutralization process is described through an "effective collision frequency" that binds electrons to the ion beam. As electric propulsion becomes more prevalent in space missions, this question garners significant importance. Proper modeling of current coupling and neutralization will enable development of low-current neutralizers and optimization of neutralizers for micropropulsion devices. Explanation of the effective collision frequency also has bearing on space instrument calibration, electrodynamic tethers, and ionospheric research.

In the early years of electric propulsion research, the neutralization question was one of the fundamental issues for successful development of this promising technology. A dense ion beam requires space charge neutralization to avoid a potential barrier that can divert or reflect the beam. The vehicle on which the thruster operates needs current neutrality to avoid unwanted charging. In the context of collisionless plasma theory, achieving both current and charge neutrality with the same source of electrons appears to be nearly impossible owing mostly to the large difference in mass between electrons and the ions. For example, define the ion flux, $F_i = N_i v_i$, and the net electron flux, $F_e = \frac{1}{4} N_e v_{eth}$, where N is density, v is velocity, i and e are ion and electron subscripts and eth designates the electron thermal velocity for an idealized electron source. Equal density and flux requires $v_{eth} = 4v_i$. A 1 keV Xenon beam has v_i=38,000 *m/s* so a matching electron velocity requires a source temperature of about 0.05 eV. A challenging, but not impossible number, but a collisionless analysis suggests that detailed balancing is required, whereas real systems quite easily achieve 'beam coupling.' Of course a higher temperature, lower density electron source will lead to a positive potential well that does trap electrons, but then the theory must explain by what process the trapped electrons shed energy so as to actually fill the well. Another observation, presented in more detail below, is that when ion beams and neutralizers are operated in conducting vacuum tanks, the currents are closely coupled even though the grounding tank eliminates the charge accumulation that could provide feedback for current balance so it appears that one or more plasma mechanisms must be responsible for this collective phenomena -- charge and current neutrality – which we hereafter call current coupling.

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* Electronics Engineer, Ph.D. candidate WPI, Student Member AIAA
† Tech Advisor, Senior Member AIAA
‡ Associate Professor, Senior Member AIAA

Our immediate goal is to determine if what might be considered standard Particle-In-Cell, PIC, techniques are adequate or if additional treatment is needed to understand and capture the beam coupling process. In this paper we present first a review of neutralization studies. We then present a series of simulations using a 2-D PIC code[1,2,3] as well as the implementation of a 3D PIC/DSMC code.[4,5] These show the dependence of the beam neutralization on beam energy and neutralization current. The simulations presented in this paper serve also as means of validation of the PIC-modules of our PIC/DSMC code under development.

History of EP Neutralization

Possibly first pointed out by L. Spitzer in 1952 [uncited note in Seitz et al. 1961], electric propulsion plumes needed to be properly mixed with electrons or else severe space-charge effects would result. Before the first space tests, serious doubts lingered as to the stability of any neutralization approach to the ion beam created by an electrostatic thruster. The general idea was for neutralization to occur shortly after emission to prevent beam return. However, a lack of understanding as to how the electrons would stay within the beam if injected or even if the neutralization process was unstable to small perturbations brought about significant research activity. Failing to properly neutralize the beam would cause a dramatic reduction in thrust, as a significant portion of the beam would return to the spacecraft. This problem was first addressed by the Ramo-Wooldridge staff in their review of electrostatic propulsion in 1960.[6] Their one-dimensional investigation was admittedly unrealistic enough to provide a satisfactory indication as to the stability and practicality of neutralization.

Over the next few years, many theorists who looked at 1- and 2-D models predicted growing instabilities that could turn the beam back to the spacecraft. Some research pointed towards the possibility of neutralization, such as French[7] and Mirels. (1961)[8] Other work pointed towards potential problems, such as Seitz et al.[9] Some of the earliest computational studies were brought to bear on the problem, and Buneman and Kooyers[10], using a one-dimensional code in 1963, were able to provide a neutralized beam when electrons were injected at energies lower than the directed ion energy and velocities on the same order. Fluctuations in the space charge field provided mixing of the beam. Two years later Wadhwa et al.[11] performed a two-dimensional PIC simulation showing that electrons would oscillate within the beam to allow for neutralization, but theorized the oscillations were not the only mechanism at work. One method suggested was that fluctuations in the space-charge field allowed for entropy increase to mix the electrons, but these fluctuations were not found far downstream of the neutralizer, suggesting a collective cooling mechanism.

The 1964 Space Electric Rocket Test I (SERT I) found that it was quite easy to neutralize ion beams in space using straightforward neutralizer geometry. In a series of tests it was shown that the ion thruster developed thrust at a level indicating complete beam neutralization. After SERT I, proof of concept was achieved and the theoretical discussion of beam neutralization was dropped in favor of engineering new thrusters. Studies after SERT I include evaluations of neutralizer placement[12,13], optimization of the thrusters, and simulations to analyze spacecraft-plume interactions.[14,15] A few numerical simulations of neutralization have been performed recently, including Othmer et al.[16,17,18] using a relativistic 3D PIC simulation and Tajmar and Wang investigating FEEP neutralizer placement.[12] Othmer suggested that electrons reflected from the ends of the beam therefore eventually matching velocities, but this does not explain why current coupling can be observed in a vacuum chamber, where the beam is nominally stationary and bounded. Tajmar was not investigating the coupling effect directly. Work in the nuclear fusion community has recently[19] investigated pulsed plasma beams being neutralized by background plasma, but the high powers and densities involved make a direct connection difficult.

Despite decades of research and the implementation of electric propulsion devices, the detailed process by which an ionized beam is neutralized in space is still unknown. Assorted methods to fit data with theory have been found, but the actual process has yet to be studied in sufficient detail to fully understand the subject. Further, new electric micropropulsion devices such as the FEEP or the colloidal thrusters or large arrays of ion and Hall thrusters are still not guaranteed to behave. We might also desire a means to predict and optimize neutralizer operations. Thus, a simulation technique exhibiting beam coupling is needed. Additionally, results from ion beam neutralization modeling will be applicable to ion beams for instrument calibration, electrodynamic tethers, ionospheric research, and fundamental plasma physics.

Current Coupling Observations in a Vacuum Tank

In order to observe this phenomenon directly, we utilized the JUMBO large vacuum facility (6 foot diameter) at AFRL/Hanscom. A 3-cm IonTech ion source, functionally identical to an electrostatic ion

Table 1: Ion Source Settings

Cathode Current	3.00 A
Discharge Voltage	55.0 V
Accelerator/Beam Current Limit	20 %
Background Pressure	5E-4 Torr

engine, was installed. This source used a hot tungsten wire placed across the beam to provide neutralization, although in a vacuum tank it is not required for operation. The ion source was able to run on a wide variety of gases; for these tests we used nitrogen.

The controller enabled accurate control of beam (extractor) voltage to 1V, neutralizer filament current to 10mA and measurement of beam (extracted) current and neutralizer emission current to an accuracy of 1mA. With other settings shown in Table 1, three tests were performed, one with the beam voltage set to zero, one at 450 V and one at 800 V. In each test, the filament current was increased from zero to 3.50 A, then brought back to zero. The results can be seen in Fig. 1, 2, and 3.

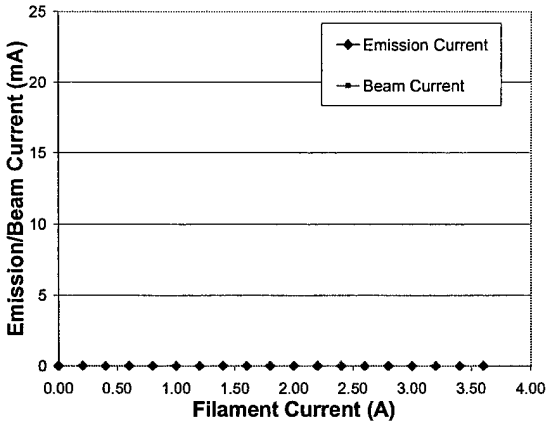

Figure 1: Currents with 0V Beam

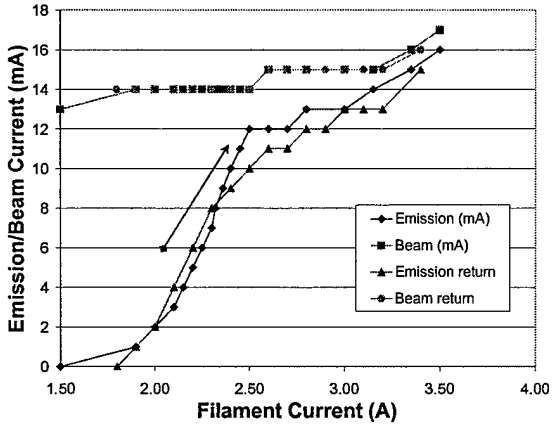

Figure 2: Currents with 450V Beam

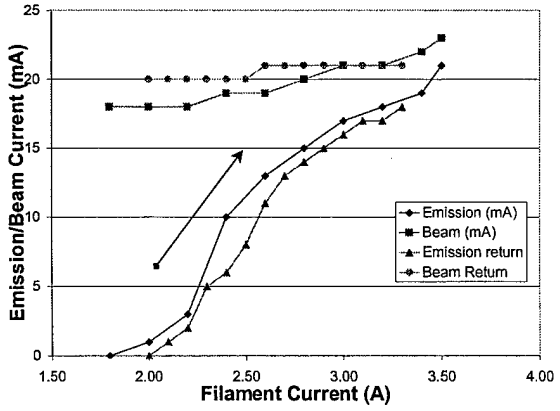

Figure 3: Currents with 800V Beam

As expected, without an ion beam present, even though the filament current was at over 3 A, there was zero emission current. Once a beam was provided, however, the emission current quickly rose to near the beam current, though never quite reached it. The increase in beam current with increasing filament emission current we theorize is due to backstreaming electrons from the filament. The gap between neutralizer and beam current may be due to charge-exchange ions due to the high background pressure at which we operated as well as electrons released from chamber walls partially neutralizing the beam.

Unstructured 3D PIC Code Description

While the majority of our simulations were performed using the code XPDP2,[1,2,3] we have also begun using our 3D PIC/DSMC code[4,5] to examine the problem in a more realistic fashion. We have developed an unstructured grid generator that provides three-dimensional meshes of arbitrary geometry and allows for adaptation of the mesh according to the preliminary solution obtained on an initial grid. The generator is based on Watson's[20] incremental node insertion method, using properties of Delaunay[21] triangulation.

The general procedures for loading and injection used in this work follow Birdsall et al.[22] and Bird.[23]

Integration of the equations of motion of a charged particle are performed by the Boris method[24] as discussed by Birdsall et al.[27] Particles are moved between adjacent cells using a particle-tracing technique.

To formulate a finite volume method for Poisson's equation

$$\nabla^2\Phi = -\frac{\rho}{\varepsilon_o} = -\frac{\sum_{i=1}^{Ni} q_i n_i + q_e n_e}{\varepsilon_o}, \qquad (1)$$

advantage is taken of the Voronoi dual of the Delaunay triangulation to associate an irregular volume to each node on the grid. The Voronoi cell corresponding to each Delaunay node contains the set off points closer to that node than any other, the facets of the Voronoi cell are orthogonal to the lines joining the tetrahedral nodes as shown in Figure 4.

This method reduces Gauss' law for a node-centered finite volume scheme to the standard 2nd order finite-difference method on Cartesian meshes.

In a bounded domain, piece-wise Dirichlet and Neumann boundary conditions specify a solution of Poisson's equation. Since the boundaries of the Delaunay mesh are forced to coincide with the boundaries of the computational domain, boundary condition implementation is straightforward. In the case of a Dirichlet boundary condition, the voltage is placed on the right hand side of the matrix and the corresponding row is zeroed, with a one placed on the diagonal. Fluxes in Neumann boundary conditions are added to the flux formulation for the Voronoi cell corresponding to the boundary node, with the value of the inward normal electric field multiplied by the boundary area added to the right hand side of the node of interest.

In matrix form with boundary conditions as in Fig. 4, Gauss' law is:

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ R_{2,1} & R_{2,2} & R_{2,3} & \cdots & R_{2,N} \\ R_{3,1} & R_{3,2} & R_{3,3} & \cdots & R_{3,N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ R_{N,1} & R_{N,2} & R_{N,3} & \cdots & R_{N,N} \end{bmatrix} \begin{Bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \vdots \\ \Phi_N \end{Bmatrix} = \frac{1}{\varepsilon_o} \begin{Bmatrix} Q_1 \\ Q_2 + \varepsilon_0 E_{N,2} A_{N,2} \\ Q_3 \\ \vdots \\ Q_N \end{Bmatrix} \tag{2}$$

N is the number of nodes in the mesh. The coefficients are determined by

$$\begin{aligned} R_{i,j} &= \sum_{k=1}^{N_{F,i}} \frac{A_{i,k}}{L_{i,k}} \text{ for } i = j, \\ R_{i,j} &= -\frac{A_{i,j}}{L_{i,j}} \text{ if } j \text{ is adjacent to } i, \\ R_{i,j} &= 0 \text{ otherwise} \end{aligned} \tag{3}$$

$A_{i,j}/L_{i,j}$ is the ratio of the area of the Voronoi face $A_{i,j}$ between nodes i and j to the distance between nodes i and j if the nodes $L_{i,j}$. The boundary conditions for node 1 are Dirichlet with potential Φ_0, and node 2 is on a Neumann boundary with inward flux $E_{N,2}A_{N,2}$.

Gauss' law may now be solved by a variety of linear solvers. Our current method uses Jacobi iteration to provide a solution, but this method is quite slow for computationally large problems. Also, the size of the domain we are interested in requires large numbers of particles in a high-resolution mesh, further slowing the computation.

To remedy this issue, we have begun work on parallelizing the code using OpenMP and PETSc[25]. The modular functionality of PETSc allowed us to parallelize only the Poisson solver subroutine without drastic modifications to the rest of the code. As work continues, the parallelization will expand to more of the code until it is a fully parallel program.

As in many math libraries, the careful construction of matrices and vectors is key to utilizing the solvers the library provides. To ensure a standard interface to its solvers, PETSc has native data structures for vectors and matrices, which automatically handle parallel data distribution. Data was required to be translated between Fortran90 vectors and PETSc data structures. These vectors were distributed across the processes, with lower-ranked processes getting any extra rows. Once the data structures were built, they were passed on to the Krylov solver. GMRES[26] was selected from a provided suite of Krylov Subspace solvers using a Jacobi preconditioner.

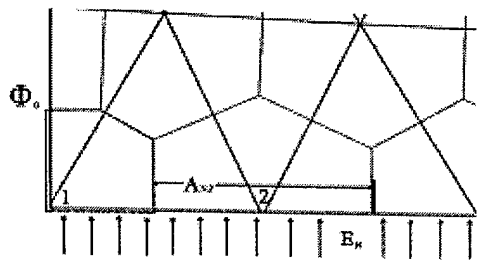

Figure 4: Boundary Conditions in Delauny-Voronoi Dual.

OpenMP was inserted in a variety of simple loops where it would enhance performance. Due to overhead, it may or may not speed up execution. For cases where it would not enhance performance, a compile-time flag can be commented out of the makefile to turn off OpenMP. OpenMP was active for the test case. To validate the parallel code, a simple test case was run for 200 timesteps on a 2x8 Linux cluster and the results compared, as seen in Fig. 5. The results were effectively identical.

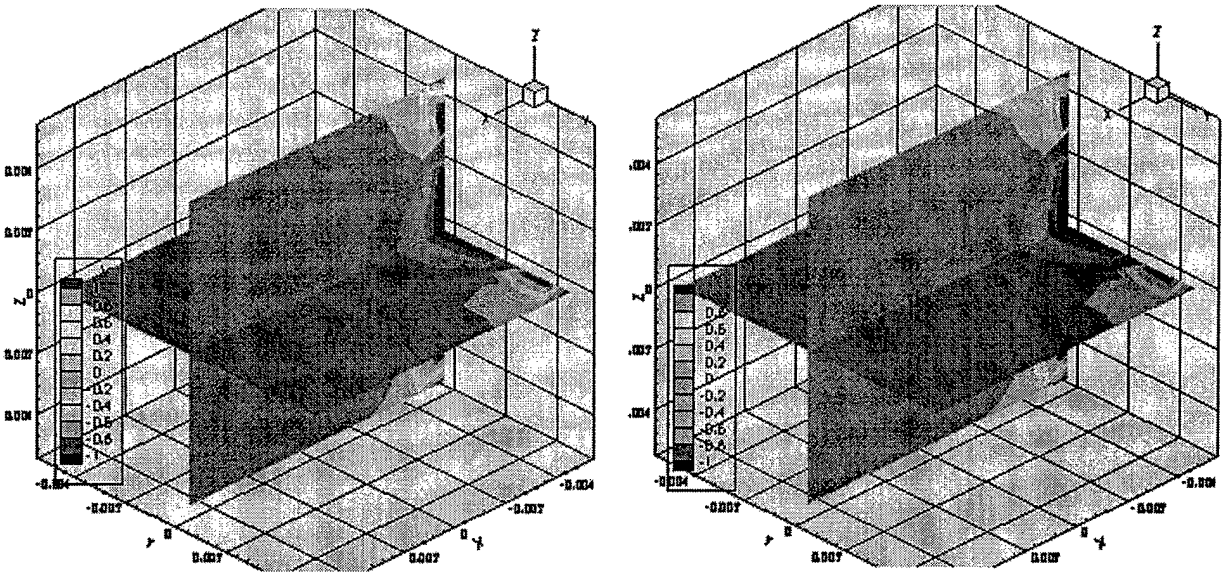

Figure 5: Comparison of ion beam inside annular electron beam at 200 timesteps. Left: GMRES/PETSc Right: Unmodified Jacobi Iteration

Unfortunately, the overhead of the parallelism was unable to speed up the test case. As shown in Fig. 6, the time to perform the test case increased as the number of processors increased. It is likely, however, that these numbers can be improved in more complex simulations and as more of the code begins to use PETSc, so time is not wasted transferring data between PETSc and the rest of the code.

Simulations and Results

In this section, we present the results of a series of 2D and 3D ion beam simulations. As explicit 3-D simulations are computationally intensive, the majority of our results have been achieved using the 2-D code XPDP2.

2-D Results

Previous work by the authors has established that there are two cases that XPDP2 is capable of performing. The "filling" case is that of a beam expanding into a vacuum, while the "chamber" case is a beam propagating across a bounded domain that is grounded. Since current coupling can be observed in a chamber, as demonstrated above, we have recently focused on the "chamber" case. Discussion of the filling case can be found in Wheelock et al.[27]

In the chamber case, if current coupling is modeled by standard PIC, then there should be a preference for

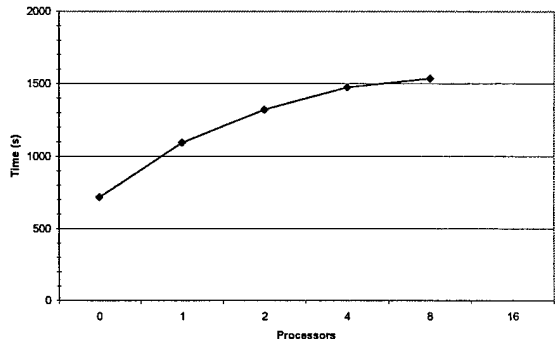

Figure 6: Speedup (Slowdown) of 3-D code. 0 is unmodified case with all speedups activated.

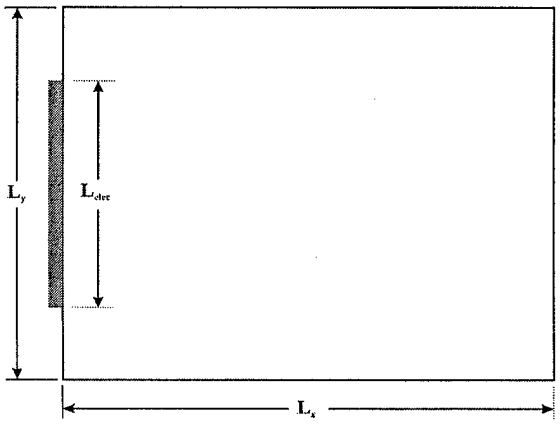

Figure 7: 2-D Simulation Domain

electron flow in the direction of ion flow. Utilizing the ability of computer code to "freeze" the ions, we can determine if there is an effect of ion motion on the electrons. The easiest way to measure this is through the current collected on an electrode on either side. If a bias exists that is created by ion motion, it would be evident by comparing the fraction of electron current leaving each side.

To determine the fraction of electrons leaving the domain on each side, one can develop a simple formula. From current conservation, the current passing through, say, the right electrode is equal to the current from the electron and ion sources as such:

$$I_R = -I_i - I_e^R + f_R^R I_e^R + f_R^L I_e^L \tag{4}$$

where the subscripts denote the ion or electron current with i and e respectively and the collection side for R. Superscripts denote the injection side. Assuming that the fraction of electrons f leaving each side is equivalent for particles emitted from either side, we can simplify 1 to

$$I_R = -I_i - I_e^R + f_R I_e^T \tag{5}$$

where I_e^T is the total electron current emitted from both sides. Since I_e^R is a component of I_e^T, we can define it as $I_e^R = \beta I_e^T$, so β is the fraction of electrons emitted from the right side. Similarly, the electron current is some fraction α of the ion current, so we can define $I_e^T = \alpha I_i$. This allows us to rewrite 2 as

$$I_R = -I_i - \alpha I_i (\beta - f_r) \tag{6}$$

Solving for f_r, we find

$$f_R = \frac{I_R + I_i}{\alpha I_i} + \beta \tag{7}$$

Similarly, we find

$$f_L = \frac{I_L - I_i}{\alpha I_i} + \gamma \tag{8}$$

where $f_R + f_L = 1$ and $\beta + \gamma = 1$. A similar solution for f_R and f_L can be found in the case of frozen ions where no ion current is collected. Full current coupling would be indicated by $f_R = 1$ as all the electrons follow the ions out of the problem on the right side. If there is no preference for either side, the ratio f_R/f_L should scale as the ratio of the areas collecting current. The current on the electrode was calculated and recorded over the duration of the simulation and averaged over the entire simulation period, excepting a brief window at the beginning before the electrons had

Table 2: 2-D Current collection data

Sim #	Ions	β	α	Resolution	f_L	f_R
3.1	Mobile	½	0.9	λD~Δx	0.33	0.59
3.2	Frozen	½	0.9	λD~Δx	0.35	0.61
3.3	Mobile	½	1.0	λD~Δx	0.32	0.67
3.4	Frozen	½	1.0	λD~Δx	0.46	0.49
3.5 e- only	Mobile	½	1.0	λD~4Δx	0.47 0.49	0.50 0.51
3.6 e- only	Frozen	½	1.0	λD~4Δx	0.51 0.45	0.46 0.55

properly mixed.

As seen in Table 2, the currents collected on either side scale approximately with the area of the collecting electrode. Since the trapping of electrons in the well may be due to small-angle coulomb collisions, the resolution was enhanced by a factor of four and the simulations repeated. Again, no preference was shown. Examination of just electrons in the problem rather than the full current to either side similarly showed no preference.

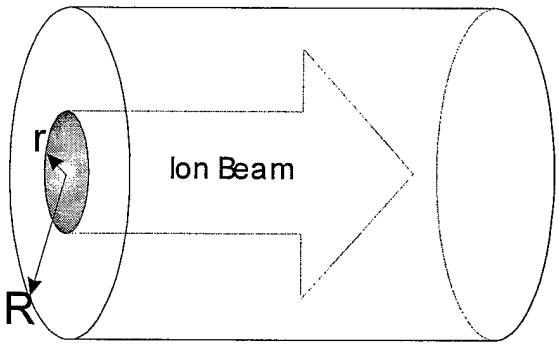

Figure 8: 3-D Simulation Domain

3-D Results

To perform unstructured 3-D simulations with realistic mass ratios requires quite a bit of computational time. The majority of the efforts in this area went into parallelizing the code and attempting to improve the mesh generator.

The 3-D simulation domain is shown in Fig. 8. The cylindrical domain of radius R and length L consists of a circular emission area with radius r where both ions are injected. Around this is an annular emission region of inner radius r2 outer radius r3 where electrons are emitted. While this is unphysical, this easily examined the ability of electrons to move into an ion beam. Future work will include a separate neutralizer.

Due to the longer simulation time required of 3-D runs, only a few simulations were performed for the present work. A domain with $L = R = 0.01$ m was generated with beam injection surface radius $r = 0.002$ m and the electron injection surface between $r_2 = 0.003$ m and $r_3 = 0.004$ m. The background was held at a density of 1E11 while the injected density was 1E15 for both ions and electrons in the first run, and was 5.7E14 for electrons in the second run to match emitted currents. Injected velocity was set to 12122.5 m/s to correspond to a 100eV Xenon beam and 41935.9 m/s to correspond to a 0.01eV electron beam. Injected temperatures were held at 0.1 eV for both ions and electrons. Surfaces on the injector side were set to be solid conductors while the downstream surfaces were free space, allowing particles to exit the simulation.

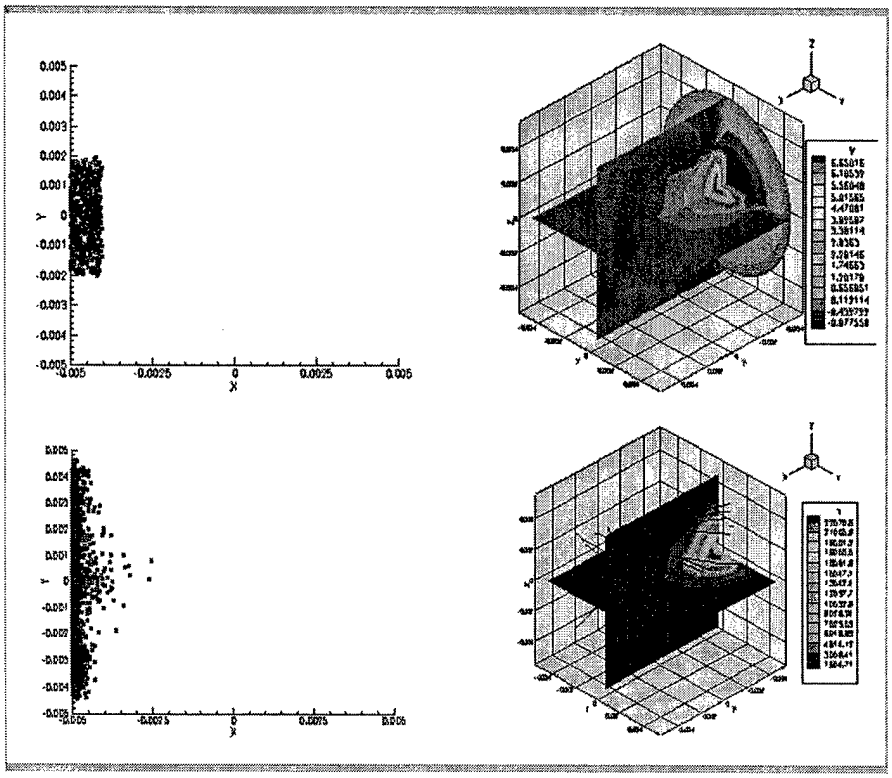

Figure 10: 3-D Simulation results. Left: X-Y phase space for ions (top) and electrons (bottom). Right Top: Potential Right Bottom: Temperature and velocity streaklines.

It can be seen in Fig. 9 that a well forms in the ion beam, drawing the electrons in to maintain quasineutrality. The beam then propagates across the simulation domain, drawing electrons with it.

Conclusions

It can be shown that electrons readily neutralize an ion beam in real life, but this phenomenon is difficult to replicate in PIC. Our efforts to do this have shown that PIC does not produce any tendency for

electrons to couple with the ion beam so both current and density match. Electrons will move to fill the well, but this is not necessarily current coupling. Without a clear coupling in standard collisionless PIC, it is increasingly likely that other factors not currently included in the model are playing important roles, such as collisions and fluctuations.

In the future we hope to expand our investigations into collisions and fluctuations, as well as model a truly 3-D thruster-neutralizer configuration. Experiments will also be designed to investigate neutralizer and ion beam behavior and compared to simulation.

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