

Pseudospectral model for hybrid PIC Hall-effect thruster simulation

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Abstract: Design of efficient Hall-effect thrusters (HETs) is strongly dependent on understanding of electron transport throughout these devices. Among the various mechanisms are proposed to account for enhanced electron transport in the near-field plume of HETs are turbulent fluctuations in the plasma. Since experimental investigations have shown that there is significant energy in azimuthal oscillations of the plasma, it is possible that these azimuthal oscillations in the presence of a radial magnetic field could be the cause of significant axial transport. This paper presents the initial development of a pseudospectral azimuthal-axial hybrid-PIC HET code which is designed to explicitly resolve and filter azimuthal fluctuations in the electrostatic potential. Although development is still far from complete, progress has been made in implementing the electrostatic potential solver. Through significant effort, including the use of both numerical limiters and a smooth fluid neutral description, stable discharges have been demonstrated and interim results are presented.

Nomenclature

E	= magnitude of electric field
B	= magnitude of magnetic field
$\vec{E}$	= electric field
$\vec{B}$	= magnetic field
T_e	= electron temperature
p	= electron pressure
T_n	= neutral temperature
m_n	= neutral mass
n_n	= neutral density
n_e	= electron density
n_i	= ion density
k_i	= ionization rate
k_B	= Boltzmann constant
e	= elementary charge
ν	= electron momentum exchange collision frequency

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$\vec{j}_e$	= electron current density
$\vec{j}_i$	= ion current density
μ	= scalar electron mobility
$\mu_{\perp}$	= perpendicular electron mobility
$\mu_{\wedge}$	= electron mobility perpendicular to both E and B
ϕ	= electrostatic potential
m_e	= electron mass

I. Introduction

The primary challenge in HET simulation, as with most magnetized plasma devices, is the need to accurately model the transport of electron across magnetic field lines. The presumed mechanisms for this type of transport, known as cross-field electron transport, in HETs are a combination of volumetric electron momentum exchange collisions, electron-wall collisions, and field fluctuations. The first mechanism refers to the idea that when an electron undergoes a collision, it can abruptly shift its guiding center and thus accomplish net motion against the magnetic field. These collisions can include both electron-ion and electron-neutral collisions, although for most relevant HET plasma conditions, the electron-neutral collisions dominate. The second mechanism, electron-wall collisions, presumes that the interaction between an electron and the device walls is the equivalent to a scattering collision. Finally, the third mechanism refers to the family of field fluctuations (both resolved and unresolved) which, especially in the presence of magnetic fields and fluctuating densities, can lead to net transport effects. The most popular reduced model in HET simulation for unresolved field fluctuation effect is the Bohm diffusion (or Bohm transport) model.

Traditional computational models for HETs fall largely into two categories - full-PIC and hybrid-PIC. While full-PIC is highly desirable in that it actually resolves nonequilibrium behavior for the electron distribution, hybrid-PIC is the far more popular approach as it removes the strict need to resolve high frequency plasma characteristics such as the electron plasma frequency and Debye length. A common feature of most existing hybrid-PIC codes is the treatment of the electrons as a fluid in local thermodynamic equilibrium. This allows for the formulation of an electrostatic solver, based on current conservation, which relies heavily on the details of the relationship between the forcing terms (electric and pressure forces) and the resulting electron current - i.e. the key to the solver is the accuracy of the electron mobility model.

The most popular hybrid-PIC codes in common use, HPHall,¹ relies on this quasi-1D current conservation approach and resolves the radial-axial plane. The formulation explicitly relies on zero derivatives for all quantities in the azimuthal direction. Experimental observations, including Ellison,² McDonald³ and Sekerak,⁴ have clearly shown that at readily observable physical and timescales (centimeters and kilohertz), this assumption is not true. Indeed, estimates by MacDonald indicate that a significant fraction of the total discharge energy can be accounted for in azimuthal structures with fairly small wavenumber (corresponding to low order azimuthal modes). For this reason, it seems promising to try to resolve these structures computationally to assess their contribution to overall electron transport in HET operation.

This paper attempts to address the role of resolved field fluctuations in the azimuthal direction as a means for promoting electron transport in a hybrid-HET code. To study this problem, an axial-azimuthal hybrid-PIC HET code is under development, initially with a reduced set of physics. In particular, dynamic ionization is ignored through the use of imposed electron temperature profiles. Pioneering work in axial-azimuthal simulation has been performed by Coche⁵ (full-PIC) and Lam and Fernandez⁶ (hybrid-PIC). This work follows the example of Lam and Fernandez but substitutes a spectral description in the azimuthal direction to more naturally resolve oscillations in the plasma.

II. Computational Model

The code developed for this paper is a 2D hybrid-PIC code which resolves an axial-azimuthal plane along the centerline of the HET. As with traditional hybrid-PIC simulations, the ion description (singly charged

xenon only) is with PIC and the electron description is as a fluid with the same density as the ions; however, to avoid the impact of statistical noise in the neutral description on the mobility tensor, the neutrals are modeled with a single temperature (300 K) fluid description rather than the particle description commonly used in other hybrid-PIC HET codes.

A. Electrostatic Potential Solver

Crucially, the electrostatic potential solver is based on the same general current conservation laws as HPHall, but it does not rely on any corrections to the electron mobility with tunable model parameters. The foundation of electrostatic potential solver is current conservation throughout the device which can be written more as:

$$\nabla \cdot (\vec{j}_i + \vec{j}_e) = 0 \quad (1)$$

Assuming that the time derivative of the ion current density is zero, we can replace the divergence of a ion current density with a scalar ionization term to get the overall current conservation equation.

$$\nabla \cdot \vec{j}_e = k_{ioniz} n_e n_n e \quad (2)$$

To get the electron current density as a function of the electrostatic potential (and other driving forces), we begin with a Generalized Ohm's Law description based on the steady state electron momentum equation where $p = n_e k_B T_e$ and $\mu = e/m_e \nu$

$$\vec{j}_e + \mu \vec{j}_e \times \vec{B} = \mu n_e \vec{E} + \mu \nabla p \quad (3)$$

Expanding this results and performing some arithmetic results in the following expression for the electron current density:

$$\vec{j}_e = \vec{\mu} \vec{F} \quad (4)$$

where:

$$F_x = \mu n_e E_x + \mu \frac{\partial p}{\partial x} = -\mu n_e \frac{\partial \phi}{\partial x} + \mu \frac{\partial p}{\partial x} \quad (5)$$

$$F_y = \mu n_e E_y + \mu \frac{\partial p}{\partial y} = -\mu n_e \frac{\partial \phi}{\partial y} + \mu \frac{\partial p}{\partial y} \quad (6)$$

$$F_z = \mu n_e E_z + \mu \frac{\partial p}{\partial z} = -\mu n_e \frac{\partial \phi}{\partial z} + \mu \frac{\partial p}{\partial z} \quad (7)$$

and

$$\vec{\mu} = \frac{1}{1 + \mu^2 B_x^2 + \mu^2 B_y^2 + \mu^2 B_z^2} \begin{bmatrix} 1 + \mu^2 B_x^2 & -\mu B_z + \mu^2 B_x B_y & \mu B_y + \mu^2 B_x B_z \\ \mu B_z + \mu^2 B_x B_y & 1 + \mu^2 B_y^2 & -\mu B_x + \mu^2 B_y B_z \\ -\mu B_y + \mu^2 B_x B_z & \mu B_x + \mu^2 B_y B_z & 1 + \mu^2 B_z^2 \end{bmatrix} \quad (8)$$

1. Simplifications

To make this model computationally tractable, a number of critical assumptions are now made. First, it is assumed that this is purely an axial-azimuthal model, so there is no conservation equation in the z-direction (Eq. 7). Next, the magnetic field is assumed to everywhere exist only in the z-direction. This changes Eq. 8 from a 3x3 to a 2x2 matrix with the following structure:

$$\vec{\mu} = \begin{bmatrix} \frac{1}{1+\mu^2 B^2} & \frac{-\mu B}{1+\mu^2 B^2} \\ \frac{\mu B}{1+\mu^2 B^2} & \frac{1}{1+\mu^2 B^2} \end{bmatrix} = \begin{bmatrix} \mu_{xx} & \mu_{xy} \\ \mu_{yx} & \mu_{yy} \end{bmatrix} = \begin{bmatrix} \mu_{\perp} & -\mu_{\wedge} \\ \mu_{\wedge} & \mu_{\perp} \end{bmatrix} \quad (9)$$

Substitution of the above components into Eq. 4 then into Eq. 2 and some rearrangement leads to the following form:

$$\begin{aligned}
& \frac{\partial}{\partial x}(\mu_{\perp}\mu en_e \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial x}(\mu_{\wedge}\mu en_e \frac{\partial \phi}{\partial y}) \\
& + \frac{\partial}{\partial y}(\mu_{\wedge}\mu en_e \frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial y}(\mu_{\perp}\mu en_e \frac{\partial \phi}{\partial y}) = \\
& \quad + \frac{\partial}{\partial x}(\mu_{\perp}\mu \frac{\partial p}{\partial x}) - \frac{\partial}{\partial x}(\mu_{\wedge}\mu \frac{\partial p}{\partial y}) \\
& + \frac{\partial}{\partial y}(\mu_{\wedge}\mu \frac{\partial p}{\partial x}) + \frac{\partial}{\partial y}(\mu_{\perp}\mu \frac{\partial p}{\partial y}) + k_i n_e n_n e
\end{aligned} \tag{10}$$

Applying the chain rule, moving the cross terms involved with the electrostatic potential to the RHS as a source, and making the substitutions of $\widetilde{\mu_{\perp}} = \mu_{\perp}\mu en_e$ and $\widetilde{\mu_{\wedge}} = \mu_{\wedge}\mu en_e$, reveals the final form:

$$\begin{aligned}
& \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = \\
& - \frac{\partial \ln(\widetilde{\mu_{\perp}})}{\partial x} \frac{\partial \phi}{\partial x} + \mu B \frac{\partial \ln(\widetilde{\mu_{\wedge}})}{\partial x} \frac{\partial \phi}{\partial y} - \mu B \frac{\partial \ln(\widetilde{\mu_{\wedge}})}{\partial y} \frac{\partial \phi}{\partial x} - \frac{\partial \ln(\widetilde{\mu_{\perp}})}{\partial y} \frac{\partial \phi}{\partial y} \\
& + \frac{1}{\widetilde{\mu_{\perp}}} \frac{\partial}{\partial x}(\mu_{\perp}\mu \frac{\partial p}{\partial x}) - \frac{1}{\widetilde{\mu_{\perp}}} \frac{\partial}{\partial x}(\mu_{\wedge}\mu \frac{\partial p}{\partial y}) + \frac{1}{\widetilde{\mu_{\perp}}} \frac{\partial}{\partial y}(\mu_{\wedge}\mu \frac{\partial p}{\partial x}) + \frac{1}{\widetilde{\mu_{\perp}}} \frac{\partial}{\partial y}(\mu_{\perp}\mu \frac{\partial p}{\partial y}) \\
& \quad + \frac{k_i n_e n_n e}{\widetilde{\mu_{\perp}}}
\end{aligned} \tag{11}$$

2. Pseudospectral representation

To directly capture the azimuthal modes (which in this case are oriented in the x-direction), the following approximation is used for the electrostatic potential (which also happens to be the same form as a DFT):

$$\phi(x, y) = \frac{1}{N} \sum_{k=0}^{N-1} \hat{\phi}_k(y) e^{\frac{ikx}{L_x}} \tag{12}$$

Where $N * k = L_x$. The boundary conditions are straightforward since $\phi(x, 0) = V_{anode}$ and $\phi(x, L_y) = V_{cathode}$ implies that there are only DC components (k=0 mode) of the full Fourier expansion at the anode and cathode boundaries.

$$\hat{\phi}_k(0) = \begin{cases} V_{anode} = 300V & \text{if } k = 0 \\ 0 & \text{if } k \neq 0 \end{cases} \tag{13}$$

and

$$\hat{\phi}_k(L_y) = \begin{cases} V_{cathode} = 0V & \text{if } k = 0 \\ 0 & \text{if } k \neq 0 \end{cases} \tag{14}$$

This formulation solves for the Fourier coefficients of the approximation to ϕ rather than to ϕ itself. During an iteration, the RHS of Eq. 11 is evaluated in physical space then a FFT is applied to the RHS of Eq. 11 in the x-direction at each z location to move the solution to frequency space. This provides N_y sets of N_x Fourier coefficients. The LHS of Eq. 11 is treated as a finite difference scheme (j being the spatial index in the y-direction) for the Fourier coefficients which leads to N sets of tridiagonal matrix inversions of the form:

$$-k^2 \hat{\phi}_{k,j} + \frac{\hat{\phi}_{k,j+1} - 2\hat{\phi}_{k,j} + \hat{\phi}_{k,j-1}}{\Delta y^2} = \widehat{RHS}_{k,j} \tag{15}$$

3. Recovering electron velocity

Recovering the individual velocity components of the electrons is fairly simple, since:

$$\vec{j}_e = -en_e\vec{u}_e \quad (16)$$

This leads to the formulas:

$$\begin{aligned} u_{e,x} &= \mu_{\perp}F_x - \mu_{\wedge}F_y \\ &= -\mu_{\perp}\mu E_x - \frac{\mu_{\perp}\mu}{en_e}\frac{\partial p}{\partial x} + \mu_{\wedge}\mu E_y + \frac{\mu_{\wedge}\mu}{en_e}\frac{\partial p}{\partial y} \end{aligned} \quad (17)$$

and

$$\begin{aligned} u_{e,y} &= \mu_{\wedge}F_x + \mu_{\perp}F_y \\ &= -\mu_{\wedge}\mu E_x - \frac{\mu_{\wedge}\mu}{en_e}\frac{\partial p}{\partial x} - \mu_{\perp}\mu E_y - \frac{\mu_{\perp}\mu}{en_e}\frac{\partial p}{\partial y} \end{aligned} \quad (18)$$

B. Neutral Flow Solver

Neutral advection is performed using a high-order semi-Lagrangian advection scheme developed by Qiu.⁷ In addition to the semi-Lagrangian advection, a simple Knudsen diffusion model, shown in Eq. 19, is applied to the neutral population. In practice, given the timescale of the simulation, this is a very minor correction on the neutral density and has minimal impact on the evolution of the solution.

$$\frac{\partial n_{Xe}}{\partial t} = -D_{Kn}\nabla^2 n_{Xe} \approx -v_{th}L_{channel}\nabla^2 n_{Xe} \quad (19)$$

III. Implementation

The basic geometry of the simulation is 10 cm in the θ -direction (representing the azimuthal channel dimension) and 4.5 cm in the z-direction (representing the axial channel dimension). The underlying computational grid is divided into 1 mm segments in the x- and y-directions and there is a single cell of height 2 cm in the z-direction. The prescribed magnetic field does not account for inductive effects and remains constant through the simulation. Further, there is no evolution equation for the electron temperature but it maintains the shape prescribed at the start of the simulation. Given this lack of a self-consistent electron energy solver, it is only necessary to resolve the ion timescale motion so a timestep of 50 ns was used throughout the simulation. The initial conditions chosen for each are shown in Fig. 1. The model used to evaluate the ionization rate are from Appendix E of Goebel.⁸

1. Particle boundary conditions

A constant boundary condition of 25 mg/s and $n = 3e19/m^3$ of Xe at 300K with an inflow velocity of 1911 m/s is used to represent neutral injection at the anode corresponding to the 5 mg/s case described by Coche⁵ for a 2cm wide segment in the θ -direction. Because that work provides neither inflow velocity or equivalent channel thickness for the 2D model, it is unclear whether this flow-rate is 5x that of their work with the 5mg/s number implied for the full annulus rather than the segment. To avoid regions of zero electron density, a similar boundary condition is used to inject a small amount of Xe^+ into the solution at anode - this seed population is sampled from a reservoir with a density of $1E18\ 1/m^3$, a temperature of 11605 K and an inflow drift velocity of 1911 m/s. Periodic particle boundary conditions are used in the θ -direction. In the radial direction, specular reflection for the neutrals and recombination (to a surface temperature of 300 K) of the ions were used. A novel particle merge/splitting algorithm was also investigated to constrain the total number of macroparticles in the simulation - details of this work are provided in a companion paper.⁹

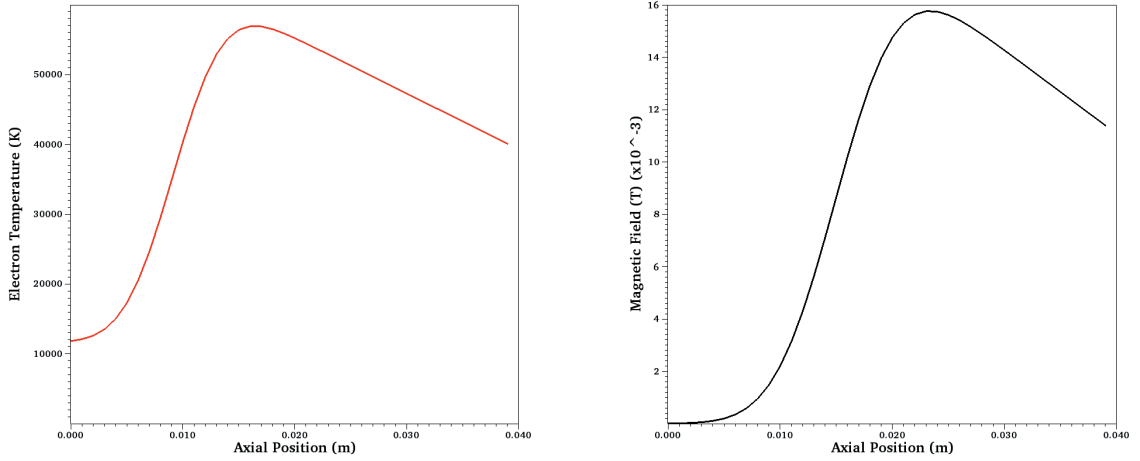


Figure 1. Imposed electron temperature and magnetic field

2. Solution methodology

To account for the fact that the electrostatic potential in Eq. 11 appears on both the left-hand side (as the solution variable) and right-hand side (as a source term) of the equation, a fixed point iterative solve is used to converge the solution at each iteration. For the terms in the right side of the equation, simple finite-difference evaluations were used. In the future, θ -derivatives should also be calculated in frequency space to improve accuracy, but with the square spatial cells used in this work, improved accuracy in only a single direction would have a minor impact on the overall error while dramatically increasing the complexity. Though spectral accuracy is lost, the pseudospectral solve allows for single-step solution across space for a given right hand side enabling rapid convergence of the fixed-point iteration.

Though this iteration as described was successful for non-ionizing cases, the iteration would diverge when the $\partial \ln(\widetilde{\mu}_{\perp})/\partial y$ term exceeded a magnitude of approximately 1.0 as is the case in regions of steep ionization gradient. To stabilize the solver, an ad-hoc arctangent limiter shown in Equation was applied to the perpendicular log mobility gradient terms multiplying the electric field in the RHS. Once limited, only a few iterations were typically needed to bring the L_2 residual down to an acceptable tolerance as shown in the results section. The impact on the solution of the limiter will be assessed in future work, but presumably if the physical gradients were sufficiently resolved, the log of the gradient could be made arbitrarily small. Unfortunately, the particle noise is also inversely related to the cell size which can also cause the term to become large. The impact of the limiter on the solution is left to future work.

$$\left. \frac{\partial \ln(\widetilde{\mu}_{\perp})}{\partial y} \right|_{\text{limiter}} \approx \frac{1}{\pi \Delta y} \text{atan} \left(\frac{\pi}{2} \ln(\widetilde{\mu}_{\perp}(y + \Delta y)/\widetilde{\mu}_{\perp}(y - \Delta y)) \right) \quad (20)$$

The code is single-threaded and requires only standard desktop computing resources, but uses the FFTW compatible interface to the cuda accelerated cuFFT library¹⁰ for the spectral field solve. In the spectral solve, both boundary conditions and the right hand side source terms are de-aliased using the 2/3rd dealiasing rule.¹¹

IV. Results

Considerable effort was expended to demonstrate that this code could be run stably for even a short period of time. Once the mobility gradient was limited, the solution remained stable over a wide range of parameters. Below shows the fixed-point iteration cycle output for the 300th iteration corresponding $t = 15\mu\text{s}$, as a representative example using the criteria $\|(\Phi^n - \Phi^{n-1})\|_{L^2} < 1.0\text{e-}02$ shown in Table 1.

Fig. 2 shows the time evolution of the solution. After an initial startup transient due to inconsistency be-

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Iteration 300: Time=1.500005e-05 dt=5.000000e-08 [Wall Clock:3770.176944]
NORM: 3.953806e-01
NORM: 4.586822e-01
NORM: 2.932743e-01
NORM: 5.065295e-02
NORM: 1.004307e-01
NORM: 5.369610e-02
NORM: 3.419605e-02
NORM: 3.912887e-02
NORM: 6.203489e-03

Iteration 301: Time=1.505005e-05 dt=5.000000e-08 [Wall Clock:3782.982616]

```

Table 1. Pseudo-spectral fixed-point iteration for electrostatic potential.

tween the initial neutral density and steady solution, the discharge becomes quite stable in time. Relatively little variation in the solution after approximately $t = 15\mu s$ was observed in runs as far out as $200\mu s$. The lack of an observed breathing mode is attributed to the constant imposed temperature profile used in place of solving the electron energy equation, but confirmation of this observation is left to future work studying the full coupled system.

As the solution transient clear the domain after approximately $15\mu s$, Fig. 3 shows Ions and neutral densities in the $\theta - z$ plane where the anode is represented by the bottom surface and cathode by the top. The ionization front depletes the neutral population, but never attains the density of the original distribution because they are rapidly accelerated out of the domain by the electric field. The results show little structure in the θ -direction which probably aids in the progression towards completely stable plasma discharge. The coupling of field to ion density alone appears to not break the symmetry of the problem. Once the energy equation is included in the model, it will be interesting to see if azimuthal structure will be recovered due to the rapid ionization quenching the electron temperature locally.

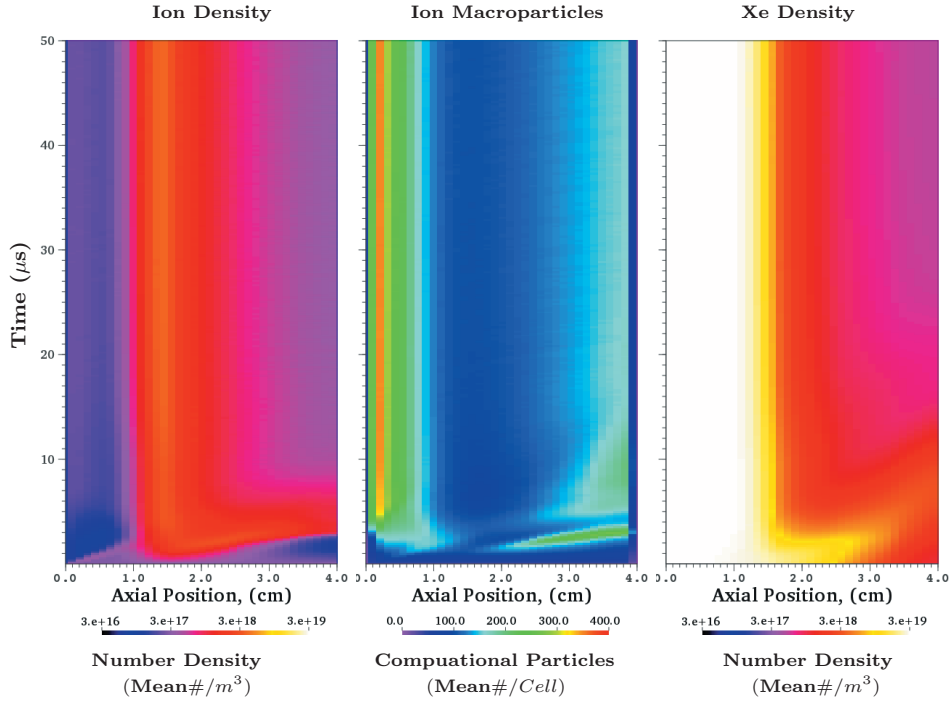


Figure 2. PIC ion densities, macroparticle counts, and neutral Xe densities. Data is averaged over θ -direction and plotted over time.

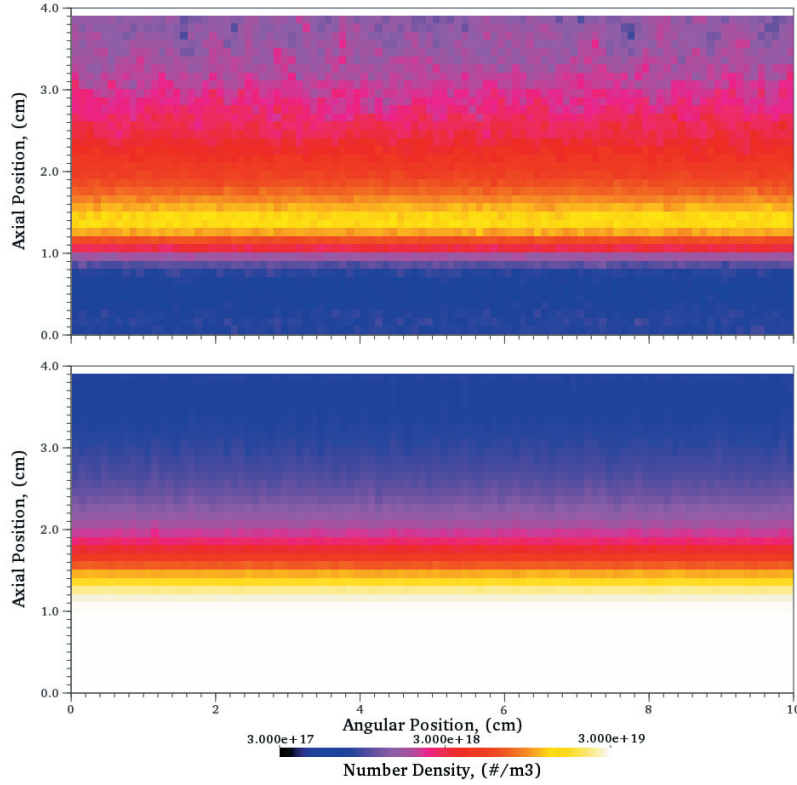


Figure 3. Ion (top) and neutral Xe (bottom) densities at $t = 15\mu s$. Mean flow is from bottom (anode) to top (cathode).

V. Conclusions and Future Work

These results represent a preliminary investigation into a pseudospectral axial-azimuthal hybrid-PIC methodology for a Generalized Ohm's law solver. Initial development required reliance on numerical artifacts (artificial limiters on some source terms for the electrostatic potential solver) to achieve a stable solution. Not surprisingly, without a coupled energy (electron temperature) equation, this effort was unable to produce characteristic breathing mode oscillations.

Significant future work is anticipated for this effort. In addition to the clear need to incorporate a coupled electron energy equation, the impact the ad-hoc limiter must also be investigated. It is unclear whether this limiter will continue to be necessary or whether a similar effect can be accomplished with a more physically motivated wall-loss terms in the energy equation. Nevertheless, this work represents an important initial step towards a new research tool to better understand the plasma processes in HET discharges.

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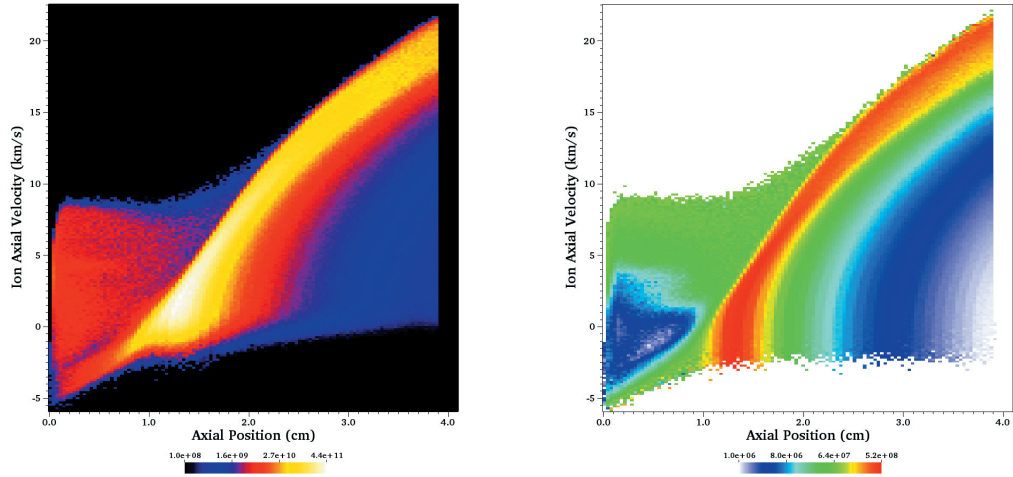


Figure 4. Axial velocity distribution (VDF). Left shows ion VDF bin density and right shows bin averaged macroparticle physical to computational weight ratio.

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