

Direct Grid-Based Vlasov Simulation of Collisionless Plasma Expansion of Ion Thruster Plume

Chen Cui*, Yuan Hu[†] and Joseph Wang[‡]

University of Southern California, Los Angeles, CA, 90089-1192, USA

The electron velocity distribution functions in a ion thruster expanding plume has been found to be non-equilibrium. Previous study has identified the plume expansion on axial direction can be analogous to a 1D semi-infinite plasma expansion and a 1D semi-finite plasma expansion on the transverse direction. In this study, a one-dimensional direct grid-based Vlasov simulation is developed and applied on the study of the semi-infinite plasma expansion to overcome the numerical heating introduced by particle method. Electron distribution functions are digested through the process and it is shown to be highly non-equilibrium at first and back to equilibrium status after the expansion is well-established. The heat flux are contained from both kinetic view and fluid view. It is shown the fluid view and kinetic view of heat flux are not similar to each other thus the fluid description of electrons may not be a good choice if the electrons kinetic effects are expected to play a role in the study.

I. Introduction

Electric propulsion devices have the advantages of highly efficient utilization of propellant mass over the traditional chemical rockets. It is considered to be nearly the only choice for the deep space missions, it can also be the workhouse for orbit station keeping and orbit changing. In the many physics problems involved in the electric propulsion devices, plume expansion is given concerns. The plasma beam exhausting from ion thrusters and Hall thrusters will have interactions with spacecrafts and cause terrible contaminations on the instruments carried on spacecrafts. Thus, the study of the electric propulsion plume becomes a crucial project. Among all of the relevant physics problems contracted from the plume, the expansion of a collisionless, unmagnetized plasma expansion into a vacuum is a fundamental one. This problem can be treated as a model problem for many applications including electric propulsion and spacecraft-plasma interactions. For the typical ion and Hall thrusters, the plasma beams can be categorized into mesothermal plasma flow which can be defined as $v_{ti} \ll v_d \ll v_{te}$. In the equation mentioned, v_{ti} , v_d , v_{te} are the ion thermal velocity, beam drifting velocity and electron thermal velocity respectively.

Previous works on the plume study were basically focus on the ion dynamics and the time scale was based on the ion time scale. Due to this reason, the electrons were treated as massless fluid and thus the Boltzmann relationship between the electron density n_e and the potential Φ

$$n_e = n_0 \exp \frac{e(\Phi - \Phi_0)}{T_e} \quad (1)$$

were commonly used in those works. Hybrid Particle-in-Cell simulations were carried out to study the problems and also in theoretical work the relationship mentioned above was also used[1–6], it is clear that in order to make the Boltzmann relationship valid, the electrons should be simplified into an isothermal, equilibrium fluid. However, since in the field of the electric propulsion study the Knudsen number is always in the scope of rarefied flow or even free molecular flow, the collision process will not be the dominate effect and thus it will be hard for the electrons to relax to the equilibrium state, and the isothermal assumptions may also be not valid. In some further studies, polytropic laws are used to study the expansion process. In the work[7, 8], both ions and electrons are treated as particles and the simulation results suggested that the electrons are non-isothermal and showed that only on the ion streamline will the polytropic law $p_e n_e^{-\gamma}$ work:

$$\frac{D}{Dt}(p_e n_e) = \left(\frac{\partial}{\partial t} + v \frac{\partial}{\partial x} \right) (p_e n_e^{-\gamma}) = 0 \quad (2)$$

*Graduate Student, Department of Astronautical Engineering, 854B Downey Way

[†]Ph.D. , Department of Astronautical Engineering, 854B Downey Way

[‡]Professor, Department of Astronautical Engineering, 854B Downey Way

and the γ will approximately be 3 for the planar expansion process. In the recent work from Hu and Wang[9–14], they performed fully kinetic Particle-in-Cell simulations and found that the commonly used isothermal or polytropic equilibrium fluid assumption for electrons may breakdown in some regions of plasma expansion process. In this way, the study of the electrons distribution functions will be important for the study of the macroscopic properties of the plasma expansion process. It has been found in[9, 12] that the plasma plume expansion can be divided into four regions as unperturbed, quasi-steady expansion, self-similar expansion and electron front regions. The unperturbed region is similar to the gas expansion in the gas dynamics. The combination of the forward plume propagation and the backward rarefaction propagation establish the quasi-steady region. And the self-similar region is considered to be similar with the one-dimensional self-similar plasma expansion. The anisotropic electrons will lead the plume to different expansion conditions on the axial and transverse direction. The previous work from Hu and Wang[12, 15] also found that the expansion on the axial direction is similar to the classical one-dimensional semi-infinite plasma expansion and on the transverse direction the expansion process can be like a one-dimensional expansion of a finite plasma. In these cases the electron thermodynamics play a very important role there.

From the previous review it is clear that the study on details of the electron microscopic properties will be helpful for electron macroscopic properties in multiple processes. Fully kinetic studies will be required to resolve the electrons kinetic properties. However, the frequently used particle methods suffer from the numerical heating and numerical noise that will lead to inaccurate predict of velocity distribution function. An alternative way of using the grid-based method can effectively eliminate the numerical noise and can take advantages of the solution methods developed for the numerical partial differential equation(PDE) community[16–19].

The presented study focuses on developing a grid-based Vlasov method to reduce the numerical noise and study the thermodynamics properties of the electrons in the 1D plasma expansion. The rest of this paper will be organized as follows. Section II describes in detail the algorithm and models used in this study and Section III first talks about several classic problems and verify our newly developed code. Then the study on 1D plasma expansion will be presented and discussed. In Section IV, a brief summary and conclusions are presented.

II. Plasma and Simulation Model

The simulation model in this work is a Eulerian grid-based Vlasov simulation code developed at USC. Full Vlasov simulation solves distribution functions directly from the collisionless Boltzmann equation, namely, Vlasov equation:

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_\alpha + \mathbf{a} \cdot \nabla_{\mathbf{v}} f_\alpha = 0 \quad (3)$$

where $f_\alpha(\mathbf{x}, \mathbf{v}, t)$ is the velocity distribution function for species α respectively. Note in this equation the $\mathbf{x}$ and $\mathbf{v}$ formed up the phase space and they are independent orthogonal basis. Thus they need to be treated as individual bin and need to be discretized individually. Since the simulations for this work are performed under the scope of electrostatic scheme, so the acceleration term in the equation 3 can be written as:

$$\mathbf{a} = \frac{F_\alpha}{m_\alpha} = \frac{q_\alpha \cdot \mathbf{E}}{m_\alpha} = \frac{-q_\alpha \nabla \Phi}{m_\alpha} \quad (4)$$

where the Φ is electric potential. In our simulation model the Φ will be self-consistently solved from Poisson equation:

$$\nabla \cdot (\epsilon_0 \nabla \Phi) = -e(Z_i n_i - n_e) \quad (5)$$

where the Z_i, n_i, n_e denotes the charge number and number density for ion species i and number density for electron respectively. The macroscopic quantities can be calculated from different orders moment of the velocity distribution function

$$\langle M_n \rangle = \int_{-\infty}^{\infty} M_n \hat{f} d\mathbf{v} \quad (6)$$

where the M_n denotes for the n -th moments need to be calculated. For example the number density n_α can be evaluated when the $M_n = n_\alpha$. Thus $n_\alpha = \langle n_\alpha \rangle = \int_{-\infty}^{\infty} n_\alpha \hat{f} d\mathbf{v}$. Average velocity, average energy and other species of properties will be found in the same way.

A. Plasma Model and Parameters

All of variables in the simulation model are normalized respect to the electron parameters at initial phase space

$$\left\{ \begin{array}{l} \tilde{\mathbf{x}} = \frac{\mathbf{x}}{\lambda_{D0}} \\ \tilde{t} = t\omega_{pe0} \\ \tilde{m} = \frac{m}{m_e} \\ \tilde{v}_\alpha = \frac{v_\alpha}{v_{te0}} \\ \tilde{n}_\alpha = \frac{n_\alpha}{n_{e0}} \\ \tilde{\Phi} = \frac{\Phi}{k_B T_{e0}} \\ \tilde{f} = \frac{f}{n} \cdot v_{te0} \end{array} \right. \quad (7)$$

where the subscript “0” denotes the values at initial phase space. The Debye length $\lambda_{D0} = \sqrt{\epsilon_0 k_B T_{e0} / n_0 e^2}$, plasma frequency is written as $\omega_{pe0} = \sqrt{n_0 e^2 / \epsilon_0 m_e}$ and the electron thermal velocity at initial phase space is written as $v_{te0} = \sqrt{k_B T_{e0} / m_e}$. In order to evaluate the Mach number of the plasma flow, Mach number need to be defines as $Ma = v_d / C_{s0}$, where the v_d and C_{s0} are the drifting velocity and ion acoustic velocity respectively. C_{s0} is written as $C_{s0} = \sqrt{k_B T_{e0} / m_i}$.

In this work we consider about a one-dimensional semi-infinite plasma expansion model which is analogous to the radial plasma plume propagation. The parameters are chosen to make sure that the plasma satisfies the mesothermal plasma assumption which is a good approach for the ion thruster plasma beam. In order to make the condition $v_{ti} \ll v_d \ll v_{te}$ valid, the following parameters will be chosen in the following simulations: The mass ratio between the ion and electrons are chosen be approximate the real protons to electrons mass ration. That is, $m_i / m_e = 1836.0$. Considering the mesothermal plasma assumption and real case, the temperature ratio between the ions and electrons are set to be $T_{i0} / T_{e0} = 0.01$. Thus the initial ratio of the ion thermal velocity and electron thermal velocity is set to be $v_{ti0} / v_{te0} = \sqrt{(T_{i0} m_e) / (T_{e0} m_i)} = 0.0023$. In order to fulfill the condition of typical ion thruster plume properties, the drifting velocity of the propagation beam is set to be $v_d = 0.1 v_{te0}$. This condition fulfill the mesothermal plasma assumption. Since the conditions are set to be as above, the ion acoustic velocity then becomes $C_{s0} = 0.0233 v_{te0}$ and this will lead to $Ma = v_d / C_{s0} \approx 4.292$.

The plasma in the simulation model are all set to be Maxwellian distribution at the initial moment. Both of the electrons and ions are loaded as a step function respect to the domain spatial length as shown below in the figure 1 and 2. At the initial moment the left half computational domain is set to be loaded with both electrons and ions with a density of $n_\alpha = 1$ and right half is set to be vacuum which means both of the electrons and ions density are set to be 0.

B. Numerical Scheme

Comparing to the traditional particle-based kinetic methods, grid-based direct kinetic methods directly discrete the phase space into mesh and directly resolve the distribution function's value from solving the Vlasov equation. Although the so called Vlasov-Poisson system used in this work is a non-linear one, the Vlasov equation itself is a linear first-order hyperbolic partial differential equation. This is a great advantages for numerical study of the Vlasov equations since there have been a lot of methods developed for this type of methods. Basically the current methods can be divided into two categories, one is splitting the dimensions[16, 20] and the other is unsplitted methods[21, 22]. Semi-Lagrange method is broadly used for first category and time-stepping methods are used for second category. finite difference[23], finite volume[17, 24] and finite element[25] methods are used to discrete the phase space variables. Several previous study in the electric propulsion community have utilized different schemes to study their problems[26, 27].

In our simulation model a positive flux conservative method from Filbet's work[17] is adopted. This scheme ensures the conservation of the flux and average:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} f_h(x) = \Delta x \cdot f_i \quad (8)$$

Also since in the physical phase space the distribution function can never be negative so this scheme also ensure that the positive principle and maximum principle:

$$0 \leq f_h(x) \leq f_\infty, \text{ where } f_\infty = \max_{j \in I} f_j \quad (9)$$

$$f_h(x) \geq 0, f(x) \geq 0 \quad (10)$$

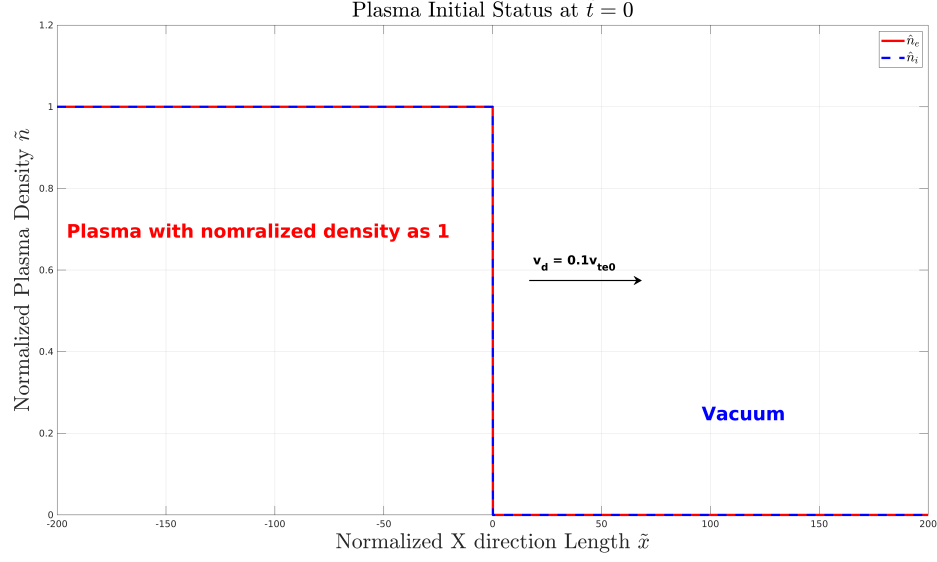


Fig. 1 Plasma Status in the domain at initial moment

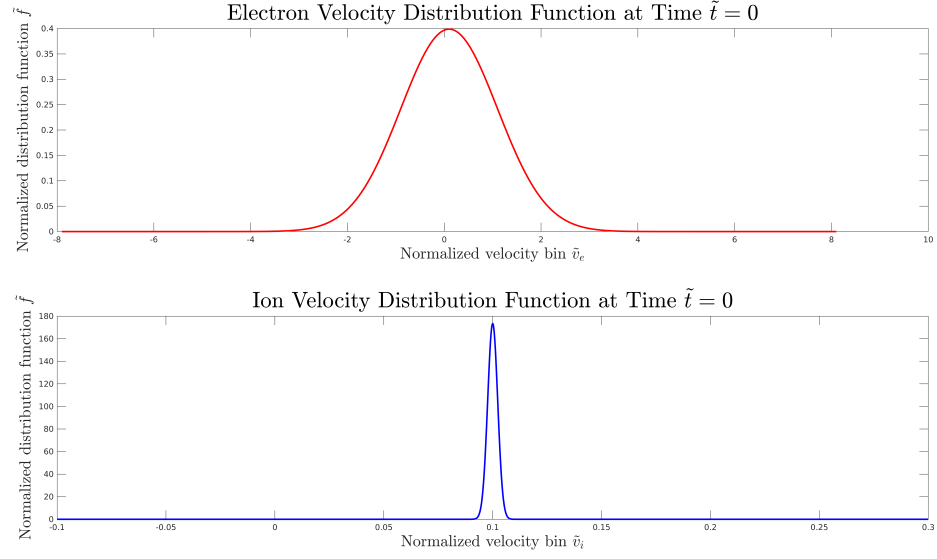


Fig. 2 Distribution Function in the domain at initial moment

Thus the Vlasov equations in this simulation model can be written in this conservative form and then be solved numerically:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} f(t^{n+1}, x) dx = \Psi_{i-1/2}(t^n) + \int_{x_{i-1/2}}^{x_{i+1/2}} f(t^n, x) dx - \Psi_{i+1/2}(t^n) \quad (11)$$

where the Ψ is defined as the numerical flux which is written as:

$$\Psi_{i+1/2}(t^n) = \int_{X(t^n, t^{n+1}, x_{i+1/2})}^{x_{i+1/2}} f(t^n, x) dx \quad (12)$$

In the equation 12, the term $X(t^n, t^{n+1}, x_{i+1/2})$ is the start on time t^n level of a characteristic line with an end as

$x_{i+1/2}(t^{n+1})$. Details of how to construct the numerical flux Ψ can be found in the work by Filbet[17]. In our model we adopted the third order PFC method to preserve the same accuracy with less mesh points and computational costs.

In our presented simulation model, the simulation domain is select to be a one-dimensional spatial space and one-dimensional velocity space phase domain(1D1V). In order to make the plasma expansion process receive no effects from boundary, a fairly large spatial domain is selected to make sure after the simulation process the expansion front is still far from the boundary. The spatial domain length is selected to be $400\lambda_{D0}$, and is discretized into 4000 cells and each cell has a length of $\Delta x = 0.1\lambda_{D0}$. The discretization of the velocity space need to be careful. It is important to choose the velocity limit in the velocity space to avoid the truncation errors. Since in plasma the ions and electrons consist a multi-scale problem, two different velocity bin discretization are chosen for two species. The maximum velocity and minimum velocity for electrons are selected to be $8.1v_{te0}$ and $-7.9v_{te0}$ respectively. The maximum velocity and minimum velocity for ions are selected to be $0.3v_{te0}$ and $-0.1v_{te0}$ respectively. Electrons' velocity space is discretized into 256 cells and thus $\Delta v_e = 0.0625v_{te0}$. Ions' velocity space is discretized into 2000 cells and thus $\Delta v_i = 2 \cdot 10^{-4}v_{te0}$. In order to make our numerical scheme stable, plasma "particles" are not allowed to travel more than one grid cell on both spatial space and velocity space, namely, CFL conditions need to be satisfied.

$$\begin{cases} \frac{v_{max}dt}{dx} \leq 1 \\ \frac{a_{max}dt}{dv} \leq 1 \end{cases} \quad (13)$$

Thus the time step size need to be chosen carefully and in this work it is chosen to be $\Delta t\omega_{pe0} = 0.025$ and the simulation will run until $t\omega_{pe0} = 250$.

Boundary conditions in this work is also essential. Zero Dirichlet boundary condition is given at $x = 0$ and Neumann boundary condition is given at $x = L$ for Poisson equation. Fixed boundary condition are given to both side of the domain for the Vlasov equation to simulate the semi-infinite plasma expansion condition.

III. Results and Discussion

All of the results shown in this part are plotted in the normalized scale if it is not specified. If it is not specified, the simulations' set up are the same as section II.B. This section will be organized as following three parts: III.A: Verification of the code. III.B: Results for Mesothermal Plasma One dimension Expansion. III.C: Discussions.

A. Verification of the model

In order to generate reliable results in the following parts, the code and model need to be verified to be workable and the results need to be physical. Two classical verification examples, Landau Damping and Two-Stream Instability, are performed with our new model and the results are shown in the upcoming sections.

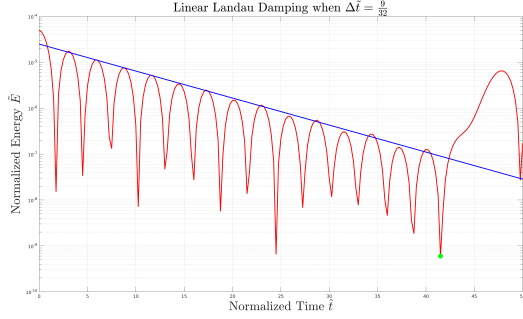
1. Linear Landau Damping

A simulation with the following set is performed under periodic boundary condition to verify the code. Only one species, electron are considered in this simulation. The initial distribution function is given following [17]:

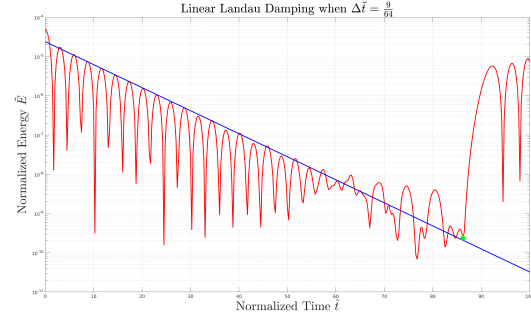
$$\tilde{f} = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\tilde{v}^2}{2}\right) \cdot (1 + \alpha \cos(kx)) \quad (14)$$

where $\alpha = 0.01$ and $k = 0.5$ and $v_{te0} = 1$. The domain is set to be periodic on the spatial domain and set to be cut off on velocity domain. The cut off limit for the velocity domain is set to be: $v_{max} = 4.5v_{te0} = 4.5$, $v_{min} = -4.5v_{te0} = -4.5$. The spatial domain is set to have a length of 4π and is divided into 32 cells. The velocity space is divided into 16, 32, 64 cells respectively. Time step is set to be $\Delta \tilde{t} = \frac{1}{8}$. The plot of $\tilde{E}(t)$ versus of simulation time are shown below as figure 3a and 3b.

As predicted by the theory, the recurrence will happen at time $\tilde{T}_R = 2\pi/(k\Delta\tilde{v})$. Thus it can be easily found that the theory predict time for 32 velocity cells case should be $\tilde{T}_R = 44.86$ and for 64 cells case $\tilde{T}_R = 89.36$. It can be easily found from the simulation results that the recurrence happen near the predicted value. However, we need to note that there will be less stable due to the less accurate electric field near the recurrence points.



(a) $N_v=32$

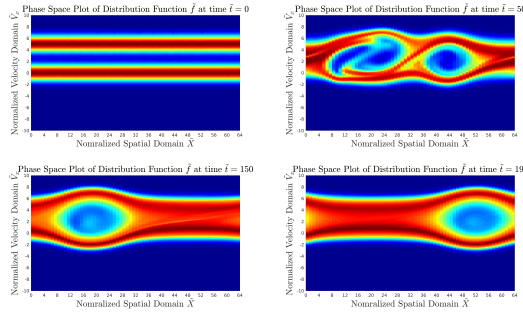


(b) $N_v=64$

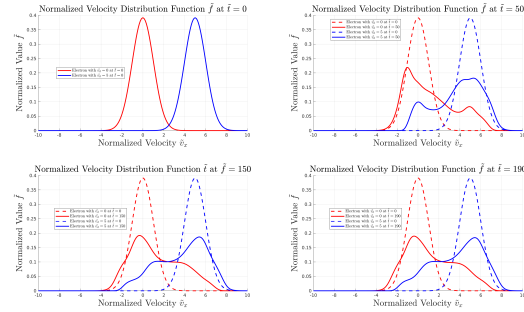
Fig. 3 Linear Landau Damping with Different Velocity Cell Numbers

2. Two-Stream Instability

Another verification example is chosen to be a classical two-stream instability problem. Two populations of particles are included in this simulation. Both of the electrons are set to be in Maxwellian distribution at the start moment. One species is set to be “sit” in peace at the start moment, namely, $\tilde{v}_d = 0$ at $\tilde{t} = 0$. The other species is set to be moving toward the sitting population with a drifting velocity $\tilde{v}_d = 5$ at $\tilde{t} = 0$. Velocity cut off limit for both populations are set to be $\tilde{v}_{\max} = 10$ and $\tilde{v}_{\min} = -10$. Both of two populations’ initial thermal velocity are set to be $\tilde{v}_{te} = 1$. The contour of phase space evolution are shown in figure 4a and the plot for the evolution of distribution functions are shown in figure 4b.



(a) Phase Space Evolution Contour



(b) Velocity Distribution Function Evolution

Fig. 4 Two-Stream Instability

The kinetic energy and electric field energy’s evolution is also a good check point for the system, It is easy to find that after a short time the system reach a “stable” instability status and show a “stable” vortex in the phase space. Energy plot can be found in figure 5.

B. Mesothermal Plasma Expansion

In this part a semi-infinite expansion model is studied. The model is set to have a drifting velocity and satisfy the mesothermal plasma assumption. This can be an abstract model for ion thruster axial plasma plume expansion.

The density of both ions and electrons are digested through the simulation and are shown below as figure 6.

It can be shown from figure 6 that there will be some instability in the front of the expansion at the beginning. However, after some time the instability are passed to the depp back and finally disappear. This will be further discussed in the next section. The Temperature are also digested and plot versus the x direction in figure 7. It can be shown from the figure that the electrons’ temperature level up with the electrons enter the vaccum area as expected. Further discussion on the electrons kinetic properties will be discussed in the next session.

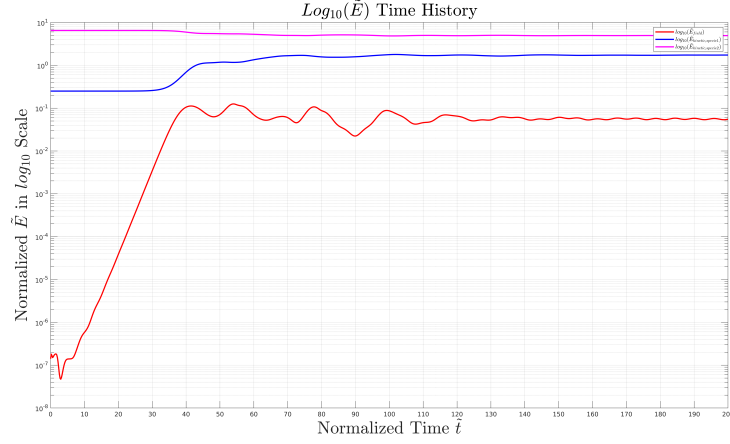


Fig. 5 Energy Evolution History of Two-Stream Instability

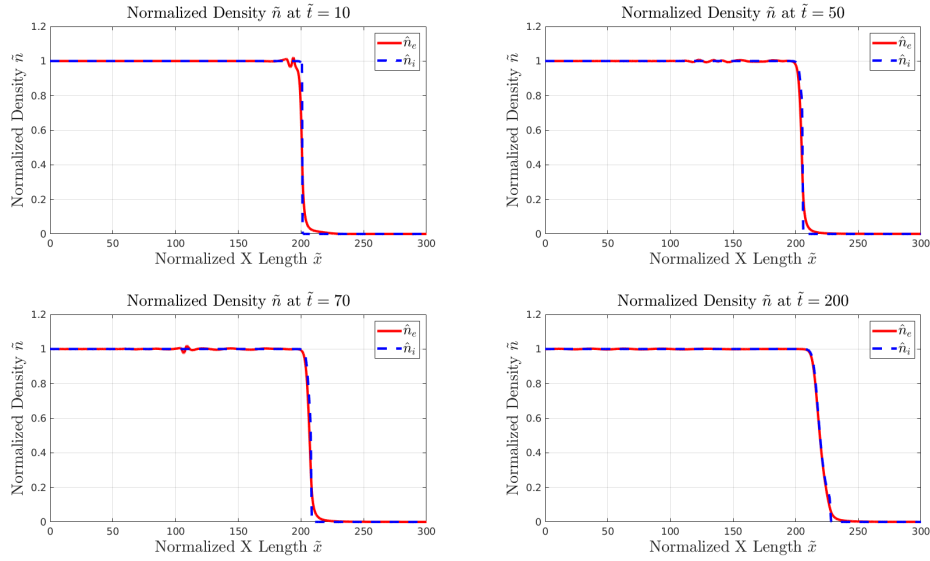


Fig. 6 Density Evolution History

C. Discussion

1. Microscopic Kinetic Properties

It has been mentioned in the previous work[15] that the electrons at the expansion front can be non-equilibrium. It has also been verified in this work that the electrons are non-equilibrium. The phase space contour of the electrons and ions are digested at several time points such as $\tilde{t} = 10, \tilde{t} = 50, \tilde{t} = 70, \tilde{t} = 200$. It can be found in the figure 8 that the phase plot is shown to have non-equilibrium distribution during the expansion process. It can be shown that there will be non-equilibrium electrons propagating from expansion front to the deep back. It can also be shown that due to the higher thermal velocities, electrons will first free flow to the low density area. This will generate a electron-majority area right in front of the expansion front and thus a negative based potential well is established. With the negatively potential well, the ions will be accelerated to a high velocity and thus the filament is shown in the phase space contour. The reason for the filaments in the electron contour need to be further investigated and thus a digest on the distribution function need to be performed.

The local statistical temperature of both ions and electrons are digested directly through taking moments of the

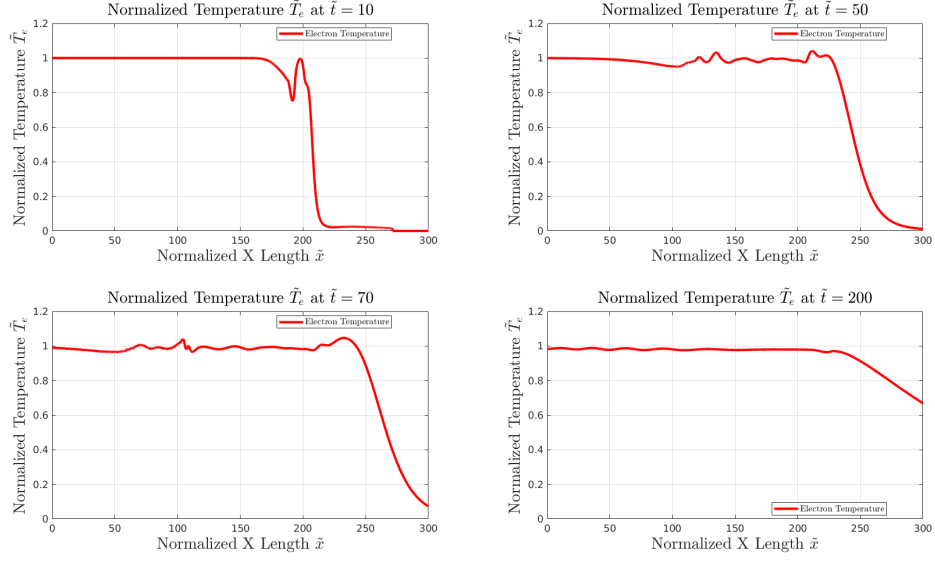


Fig. 7 Temperature Evolution History

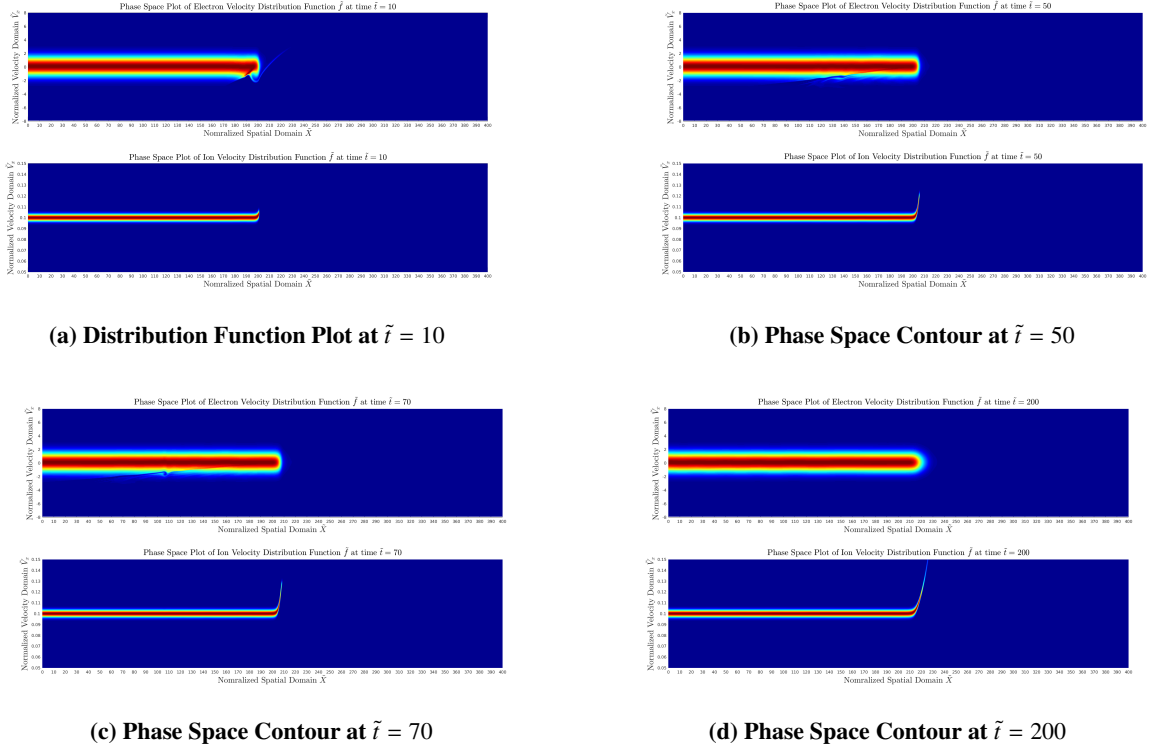


Fig. 8 Phase Space Contour at Different Time Moment

distribution function.

$$\bar{T}_\alpha = \tilde{m}_\alpha \cdot (\langle \tilde{v}^2 \rangle - \langle \tilde{v} \rangle^2) \quad (15)$$

with this local temperature, we can construct the local Maxwellian distribution that the electrons are supposed

to be

$$\tilde{f}_0 = \frac{1}{\sqrt{2\pi}\tilde{v}_{teL}} \exp\left(-\frac{(\tilde{v} - \tilde{v}_{bulk})^2}{\tilde{v}_{teL}^2}\right) \quad (16)$$

where the $\tilde{v}_{teL}$ is the local thermal velocity of electrons and can be written as $\tilde{v}_{teL} = \sqrt{\tilde{T}_e/\tilde{m}_e}$. The bulk velocity, namely, local drifting velocity can also be digested from distribution function and thus can be written as: $\tilde{v}_{bulk} = \langle \tilde{v} \rangle$. With the constructed local ideal Maxwellian distribution function we can thus show the plots as figure 9.

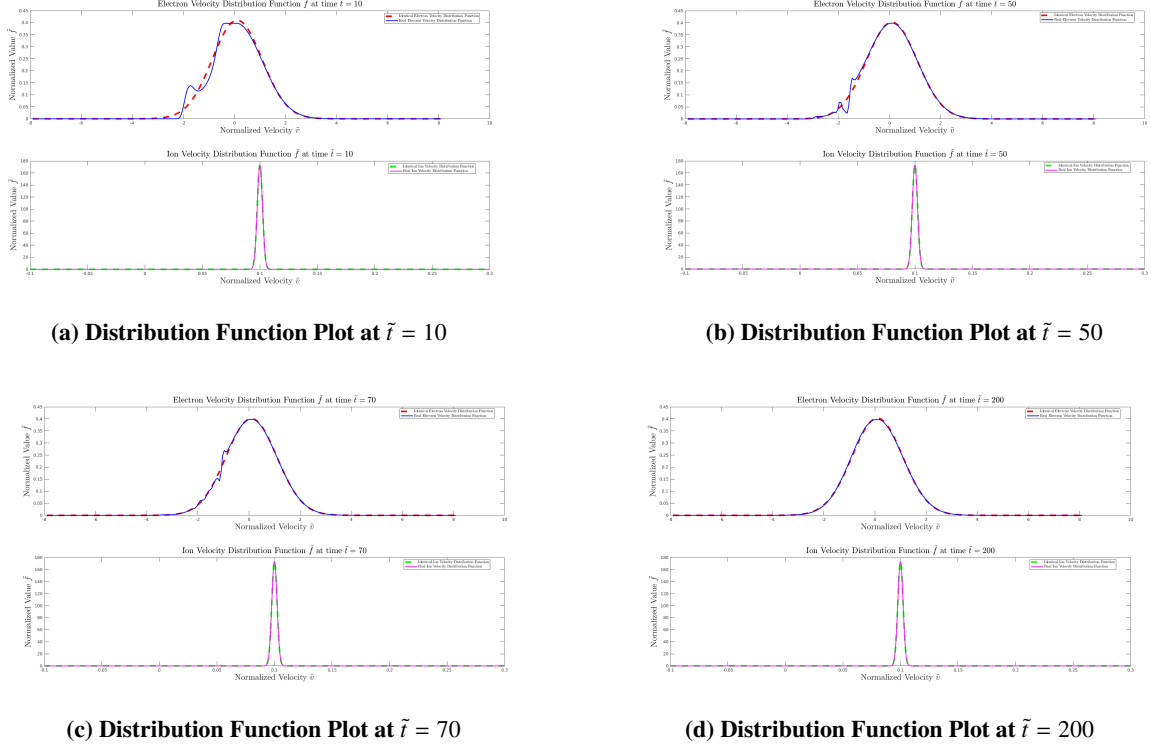


Fig. 9 Distribution Function Plot at Different Time Moment

From the figure 9 we can found that the electron distribution function perform highly-non-equilibrium states at very first process of the expansion. This might because of the high electric field established at the start of expansion. The electrons flow freely into vacuum and they established a electric potential well. However the response of the ions is slow and thus the electric field becomes higher and prevent the electrons to enter it. This can be a explain for the higher electron velocity distribution function value at low-velocity tail. After the expansion process perform for some period the electric potential well is well-established and thus the distribution function of electrons will be back to Maxwellian Distribution.

2. Energy Flux and Heat Flux Digest

The flow status of the energy is given concern since the analysis of the energy flux and heat flux is crucial in the expansion process. The energy flux is digested directly from the distribution function as shown below:

$$\tilde{E} = \langle \frac{1}{2} \tilde{n} \tilde{m} \tilde{v}^3 \rangle \quad (17)$$

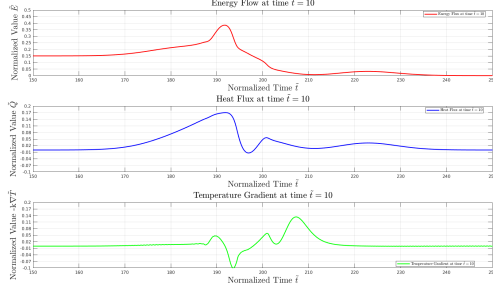
The heat flux from kinetic view can be seen as the third moment of the relative velocity. Thus the heat flux can gained from kinetic view as:

$$\tilde{Q} = \langle \frac{1}{2} \tilde{n} \tilde{m} (\tilde{v} - \langle \tilde{v} \rangle)^3 \rangle \quad (18)$$

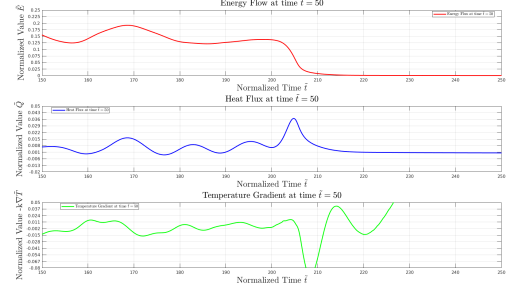
If the electrons can be viewed as a ideal fluid then the Fourier Law can be used to gain the heat flux from the fluid view.

$$\tilde{Q} = k \nabla \tilde{T} \quad (19)$$

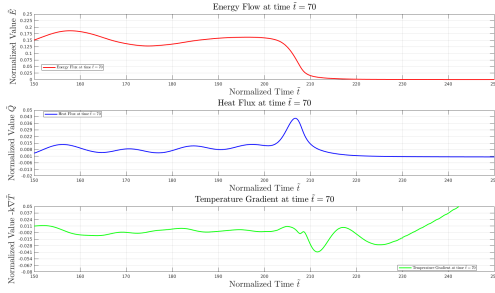
We thus digest all of the three above variables and then plot the results versus the spatial domain. The results shown are digested at the same time moment with the results above. It is shown that the heat flux get a peak near the expansion



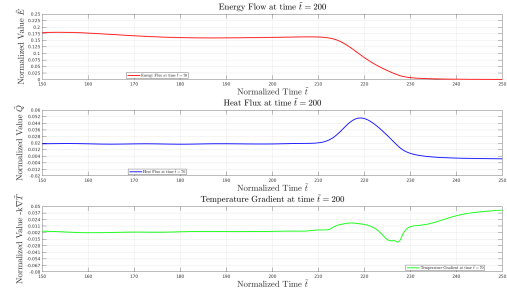
(a) Energy Flux and Heat Flux at $\tilde{t} = 10$



(b) Energy Flux and Heat Flux at $\tilde{t} = 50$



(c) Energy Flux and Heat Flux at $\tilde{t} = 70$



(d) Energy Flux and Heat Flux at $\tilde{t} = 200$

Fig. 10 Energy Flux and Heat Flux at Different Time Moment

front, this may because of the electrons are cooled down by the expansion process and then the heat flux is established from the deep back to supply the energy for electrons. The fluid view of heat flux are shown to be noisy as expected. The fluid view and kinetic view of heat flux can not meet with each other at the expansion front since the electrons are proven to be not identically Maxwellian distributed around this point. Thus it is not a good choice to treat the electrons as fluid in the simulation of expansion process if the electrons kinetic effects are expected to play a role inside.

IV. Conclusion

The ion thruster plume expansion on axial direction can be analogous to a 1D semi-infinite plasma expansion and a 1D semi-finite plasma expansion on the transverse direction. A direct grid-based Vlasov method model is developed and verified. A one-dimensional semi-infinite model is studied as an abstract model for the ion thruster axial plume expansion. The electrons kinetic properties are shown to be non-equilibrium at the start of the expansion process and be back to the near-equilibrium status after the expansion is well-established. Both fluid view and kinetic view of the heat flux is calculated from simulation results and they are shown to be not identical to each other and thus it is not a good choice to treat the electrons as fluid in the simulation of expansion process if the electrons kinetic effects are expected to play a role inside. Further study will need to be performed on a semi-finite model to simulate the transverse expansion of the plume and finally a 2D model for the planar expansion.

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