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# Improvements on particle accuracy in a Hall thruster hybrid code

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**Time-centering algorithms to increment the temporal accuracy of the state of macroparticles in the hybrid code HPHall-2 are presented. As a result, one order-of-magnitude increment in temporal precision is achieved. Errors in the conservation of mass flow along the chamber are reduced by one order-of-magnitude too. In a second part, the algorithm controlling the population of particles per cell is improved with the aim of reducing both the statistical oscillations and the computational cost.**

## I. Introduction

HPHall[1] has become one of the most widely used hybrid codes for simulation of Hall thrusters. It provides reasonable results for different thruster configurations with a relatively low computational cost. Recently it has undergone a careful and necessary upgrade into HPHall-2.[2] However, performance prediction is not fully satisfactory yet and thus we have started a program to develop an advanced hybrid simulation code.[3–5] Part of this work is presented in this article.

HPHall-2 is a quasineutral hybrid PIC-fluid model. Ions and neutrals are modelled as macroparticles with a Particle-In-Cell plus Monte-Carlo Collisions (PIC-MCC) method while electrons are considered a continuum and their behavior is described by fluid equations. Forces acting on macroparticles are the magnetic and the electric fields. On the one hand, the magnetic field is considered stationary and determined by the magnetic circuit configuration. On the other hand, the electric field is computed each time step by solving the electron macroscopic equations. The electron submodel needs as inputs from the PIC method the electron density, $n_e$, and the ion current flux, $\vec{j}_i$. Because of this strong connection between both submodels, they must be consistent in terms of accuracy in order to obtain meaningful results.

This paper describes some improvements with respect to HPHall-2, mainly referred to the PIC-MCC submodel. First, plasma magnitudes weighting algorithms are improved in order to achieve the required accuracy. These changes also affect macroparticle loading into the computational domain (e.g. injection, ionization) and macroparticle-wall collisions modelling. Second, novel ionization algorithms are used to control the macroparticle population since PIC-MCC methods require to have a minimum number of macroparticles per cell (e.g. 30) in order to avoid statistical oscillations.

The rest of the paper is organized as follows. Section II is devoted to improvements in the weighting algorithms, the macroparticle loading and the wall collisions. In section III improved algorithms for ion creation are presented. Conclusions are summarized in last section.

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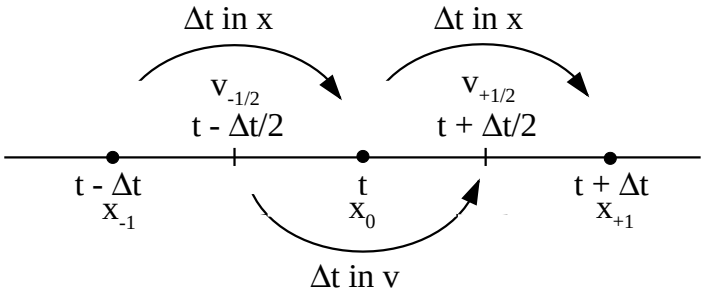


**Figure 1. 'Leapfrog' integration scheme for macroparticle motion.**

## II. Time-centering of plasma magnitudes

This work intends to correct certain inconsistencies found in both HPHall and its upgraded version HPHall-2 that mainly affect the PIC submodel. The problems are related to the 'leapfrog' integration scheme[6] and its connection with the weighting algorithms employed to transform macroparticle information into macroscopic variables such as densities, particle fluxes, energy fluxes, etcetera.

Macroparticle equations of motion are deduced from Newton´s law:

$$M_p \frac{d^2\vec{x}_p}{dt^2} = \vec{F}(\vec{x}_p, \vec{v}_p, t) \equiv q_p\Big(\vec{E}(\vec{x}_p, t) + \vec{v}_p \times \vec{B}(\vec{x}_p)\Big) \tag{1}$$

where $q_p$, $M_p$, $\vec{x}_p$ and $\vec{v}_p$ are respectively macroparticle charge, mass, position and velocity and $\vec{E}$ and $\vec{B}$ are the electric and the magnetic fields respectively. Besides, another force term can be added accounting for both ion-neutral and charge-exchange collisions. The 'leapfrog' scheme permits to integrate numerically the equations of motion of all the macroparticles using the following algorithm:

$$\vec{v}_{p,t+\Delta t/2} = \vec{v}_{p,t-\Delta t/2} + \Delta t \cdot \vec{F}(\vec{x}_{p,t}, t) \tag{2}$$

$$\vec{x}_{p,t+\Delta t} = \vec{x}_{p,t} + \Delta t \cdot \vec{v}_{p,t+\Delta t/2} \tag{3}$$

where $\Delta t$ is the PIC integration time step, $\vec{F}$ is the force on the macroparticle, and subindexes stand for the time step in which variables are computed. Notice that position and velocity are computed at instants that differ $\Delta t/2$, figure 1.

The numerical error associated to the 'leapfrog' scheme is $O(\Delta t^2)$ in velocity and $O(\Delta t^4)$ in position, *provided that* forces acting on macroparticles are known with $O(\Delta t^2)$ accuracy. Therefore, the electric field, which is computed by the electron subcode, must have $O(\Delta t^2)$ accuracy. In turn the electron sub-code needs, from the PIC sub-code, the electron density, $n_e$, and the ion current flux, $\vec{j}_i$. Thus, for the electric field to be known with $O(\Delta t^2)$ accuracy, $n_e$ and $\vec{j}_i$ must be computed with the same precision. Both HPHall and HPHall-2 fail to keep this level of accuracy. We explain next the corrections made to the different macroparticle algorithms in order to solve this precision problem.

### A. Time-centered weighting of macroscopic variables

The ion density, $n_i$, and the ion current flux, $\vec{j}_i$, at a generic node $(j,k)$, are obtained by the PIC sub-code from the weighting formulas[2]

$$(n_i)_{jk} = \frac{1}{m_i \Delta V_{\text{weight},\,jk}} \sum_p M_p S_{jk}(\vec{x}_p), \tag{4}$$

$$(\vec{j}_i)_{jk} = \frac{e}{m_i \Delta V_{\text{weight},\,jk}} \sum_p M_p \vec{v}_p S_{jk}(\vec{x}_p), \tag{5}$$

where $S_{jk}(\vec{x})$ is the (bi-linear) weighting function, $\Delta V_{\text{weight},\,jk}$ is the volume of influence of the node,[7] the summation extends to all macroions in the vicinity of the node (where $S_{jk} \neq 0$), $M_p$ is the macroparticle mass (which varies as a result of ionization), and $e$ and $m_i$ are the charge and mass of the ion species. Similar weighting formulas apply for the pressure and higher-order variables.

In HPHall-2 the ionization process is modelled differently for the macroneutrals than for the much lighter (singly-charged) macroions: in each timestep, ionization leads to the loading of new macroions in the domain, but to a weak reduction of the mass of each macroneutral.[1] A similar process regulates the creation of doubly-charged macroions from macroneutrals or singly-charged macroions. Here, for simplicity, we consider that only one species of (singly-charged) ions is present, so that mass variation affects to macroneutrals only.

In HPHall-2, the macroscopic magnitudes are computed using position and mass at time $t$ and velocity at time $t - \Delta t/2$, so their precision is only $\mathrm{O}(\Delta t)$. In order to obtain all weighted variables at instant $t - \Delta t/2$ with precision $\mathrm{O}(\Delta t^2)$, the position and mass of macroparticles at time $t - \Delta t/2$ must be used. The simple interpolation rules

$$\vec{x}_{p,\,t-\Delta t/2} = \frac{\vec{x}_{p,\,t} + \vec{x}_{p,\,t-\Delta t}}{2}, \tag{6}$$

$$M_{p,\,t-\Delta t/2} = \frac{M_{p,\,t} + M_{p,\,t-\Delta t}}{2}, \tag{7}$$

provide precision $\mathrm{O}(\Delta t^2)$. Besides, the velocity obtained with the 'leapfrog' scheme has a numerical error of the same order. Therefore, the weighting process has the required $\mathrm{O}(\Delta t^2)$ accuracy.

### B. Time-centered loading of particles

At each timestep, HPHall-2 loads macroparticles into the simulation domain in order to account for different processes, such as neutral gas injection and ionization, particle wall recombination, etcetera. Care must be taken regarding the instant of loading. The MCC method of HPHall-2 provides an statistical distribution of the location and velocity of the loaded particles, but not on the instant of loading. Thus, the location and velocity are implicitly assigned to instants $t$ and $t - \Delta t/2$, respectively. The enhancement proposed here is to determine randomly the instant of loading, that is $t - f\Delta t$, with $f \in [0,1]$. Thus, the location and velocity provided by the MCC method correspond to that instant. It is then necessary to center the position and velocity of the loaded particles at times $t$ and $t - \Delta t/2$, with errors $\mathrm{O}(\Delta t^4)$ and $\mathrm{O}(\Delta t^2)$, respectively, in order to be consistent with the leapfrog scheme. The algorithm of Cartwright *et al.*[8] is adapted to HPHall in Ref.[9] Particle centering is achieved using the force $F$ on the particle at time $t - \Delta t$.

Finally, the mass of macroneutrals that are loaded at the domain boundaries, is known at $t - f\Delta t$. The mass centering at time $t$ yields

$$M_{p,\,t} = M_{p,\,t-f\Delta t}\,[1 - \nu_i(\vec{x}_{p,t-f\Delta t}, t - \Delta t) f \Delta t] \tag{8}$$

where $\nu_i(\vec{x}_{p,\,t-f\Delta t},\, t - \Delta t)$ is the ionization frequency at the time $t - \Delta t$ and the position of the macroparticle at time $t - f\Delta t$.

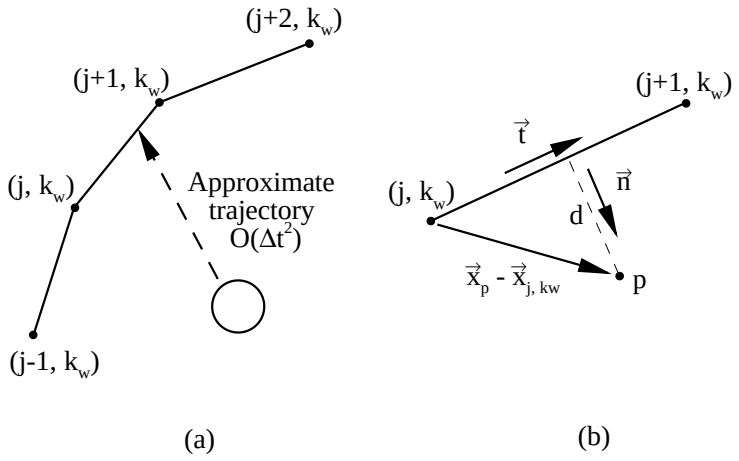


**Figure 2. (a) Sketch of the impact of a macroparticle with the boundary. (b) Distance to the boundary.**

### C. Time-centered collisions with walls

Energy losses and wall erosion rates determine respectively thruster efficiency and lifetime. A correct evaluation of these performances will benefit from an accurate computation of macroscopic magnitudes at the time of impact, $t - f\Delta t$ with the walls.

Both the parameter $f$ defining the time of impact and the macroparticle state at that instant must be determined from an iteration scheme. In this scheme, given a value for $f^{(i)}$, the macroparticle position at instant $t - f^{(i)}\Delta t$ is obtained by inverting the algorithm of Cartwright *et al.*. Then, the distance $d$ between $\vec{x}_p(t - f^{(i)}\Delta t)$ and the wall is obtained in the following manner. For the boundary panel whose limiting nodes are $(j,\, k_w)$ to $(j+1,\, k_w)$ in figure 2, the distance is given by:

$$d = \begin{cases} \|\vec{x}_p - \vec{x}_{j,\,k_w}\| & \text{if } \vec{t}\cdot(\vec{x}_p - \vec{x}_{j,\,k_w}) \in ]-\infty,\, 0] \\ |\vec{n}\cdot(\vec{x}_p - \vec{x}_{j,\,k_w})| & \text{if } \vec{t}\cdot(\vec{x}_p - \vec{x}_{j,\,k_w}) \in ]0,\, s[ \\ \|\vec{x}_p - \vec{x}_{j,\,k_w} - \vec{t}s\| & \text{if } \vec{t}\cdot(\vec{x}_p - \vec{x}_{j,\,k_w}) \in [s,\, \infty[ \end{cases} \tag{9}$$

where $s = \|\vec{x}_{j+1,\,k_w} - \vec{x}_{j,\,k_w}\|$ is the distance between the two nodes of the boundary panel, and $\vec{t}$ and $\vec{n}$ are unit vectors parallel and normal to the panel. The distance is computed only for the panels close to the macroparticle and the smallest panel-particle distance is chosen. If this distance is below the tolerance, $f^{(i)}$ is considered as the correct impact instant and the iteration stops. Otherwise, the new value

$$f^{(i+1)} = f^{(i)} + \frac{\vec{n}\cdot(\vec{x}_{p,\,t-f\Delta t} - \vec{x}_{j,\,k_w})}{\vec{n}\cdot\vec{v}_{p,\,t-f\Delta t/2}\Delta t} \tag{10}$$

is proposed and iteration continues. The initial value for $f^{(i)}$ is obtained from a linear interpolation between the positions at $t - \Delta t$ and $t$, and corresponds to a straight trajectory in figure 2. Once $f$ is known with enough accuracy, the velocity is computed with precision $\mathrm{O}(\Delta t^3)$ by the inverted Cartwright algorithm too.

The complete inverted Cartwright algorithm yields macroparticle position and velocity at time $t - f\Delta t$ with accuracy $\mathrm{O}(\Delta t^4)$ and $\mathrm{O}(\Delta t^3)$, respectively, from the position and velocity at instants $t$ and $t - \Delta t/2$, respectively, obtained from the leapfrog scheme. For simplicity only the case with electric field and no magnetic field is presented here; the complete expressions where the magnetic field is accounted for are available in reference 9 although its influence on macroparticles is negligible.

Let $\vec{e} = q_p\vec{E}/M_p$ be the acceleration produced by the electric field on a particle and let use the notation $\vec{e}_{-h} \equiv \vec{e}(\vec{x}_{p,\,t},\, t - h\Delta t)$ and a similar one for $\nabla\vec{e}$. The position at instant $t - f\Delta t$ is given by

$$\vec{x}_{p,\,t-f\Delta t} = \vec{x}_{p,\,t} - f\Delta t\ \vec{v}_{p,\,t-f\Delta t/2}, \tag{11}$$

with

$$\vec{v}_{p,\,t-f\Delta t/2} = \vec{v}_{p,\,t-\Delta t/2} + \frac{1-f}{2}\Delta t\ \vec{e}_I, \tag{12}$$

$$\vec{e}_I = \left(\frac{5}{3} - \frac{f}{3}\right)\vec{e}_{-1} + \left(\frac{f}{3} - \frac{2}{3}\right)\vec{e}_{-2} + \left(\frac{1}{6} - \frac{f}{3}\right)\Delta t\ \vec{v}_{p,\,t-\Delta t/2}\cdot\nabla\vec{e}_{-1}. \tag{13}$$

The velocity at instant $t - f\Delta t$ is given by

$$\vec{v}_{p,\,t-f\Delta t} = \vec{v}_p' + \left(\frac{1}{2} - f\right)\Delta t\ \vec{e}_{II} \tag{14}$$

with

$$\vec{v}_p' = \vec{v}_{p,\,t-\Delta t/2} - \frac{\Delta t}{24}(\vec{e}_{-1} - \vec{e}_{-2}) - \frac{\Delta t^2}{24}\vec{v}_{p,\,t-\Delta t/2}\cdot\nabla\vec{e}_{-1} \tag{15}$$

$$\vec{e}_{II} = \left(\frac{7}{4} - \frac{f}{2}\right)\vec{e}_{-1} + \left(\frac{f}{2} - \frac{3}{4}\right)\vec{e}_{-2} + \left(\frac{1}{4} - \frac{f}{2}\right)\Delta t\ \vec{v}_{p,\,t-\Delta t/2}\cdot\nabla\vec{e}_{-1}. \tag{16}$$

Finally, the particle mass at the time of impact is calculated with error $\mathrm{O}(\Delta t^2)$ by the linear interpolation

$$M_{p,\,t-f\Delta t} = (1-f)M_{p,\,t} + fM_{p,\,t-\Delta t}. \tag{17}$$

### D. Results

The increase in time-accuracy of the code has some relevant effects on the simulation results regarding the mass conservation and the numerical error.

In first place, the mass flow along the channel is conserved more accurately. Figure 3 depicts ion, neutral and total mass flow for an SPT-70 like simulated thruster computed using both HPHall and the modified algorithms. HPHall presents a mass flow loss of 5% between the anode and the channel exit, while the error is below 0.3% with the new method. Note that the most important change takes place in the neutral flow. This is likely due to the centering of the macroneutral mass to properly account for the macroparticle mass variation.

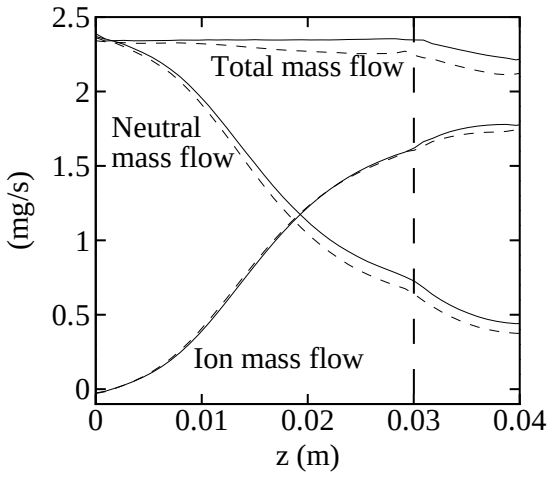


**Figure 3. Mass flows in a SPT-70 like simulated Hall thruster computed by HPHall (dashed lines) and the new algorithms (solid lines).**

In second place, the numerical error of the simulation was evaluated using a Richardson extrapolation. Values of the discharge current through the thruster computed for one time-step size and for half the same time step size are compared. The resulting numerical error estimation is plotted as a function of the time step size $\Delta t$ in Figure 4 for the old and new algorithms. It illustrates clearly that HPHall has an error $O(\Delta t)$, which is inconsistent with the 'leapfrog' scheme, whereas the new algorithms reduce the error below the noise level of the PIC-MCC scheme.

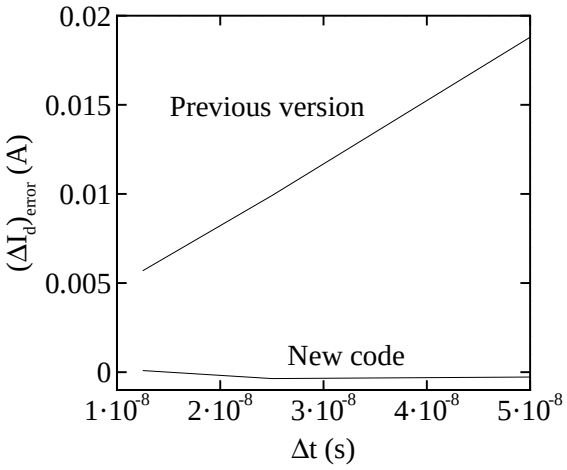


**Figure 4. Comparison of the error in the current through the Hall thruster between a previous version and the new code.**

Finally, we have analyzed the role of time-centering inaccuracies on the lack of fulfillment of the Bohm condition by HPHall at the contour of the quasineutral domain.[10] Figure 5 shows a weak improvement on the ion velocity with the new algorithm but results are far from fulfilling $v_i \simeq c_s$. This confirms the numerical problem with the Bohm condition was not on temporal accuracy but on spatial accuracy of the weighting algorithm at contour nodes.[11,12]

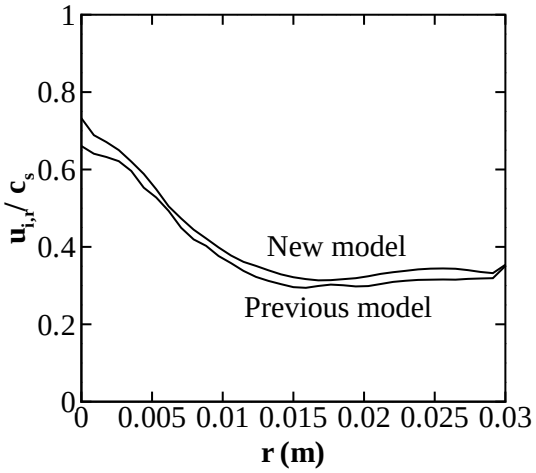


**Figure 5. Velocity perpendicular to the outer wall divided by the Bohm velocity ($c_s = \sqrt{T_e/m_i}$) in different axial positions of an SPT-70 type Hall thruster.**

## III. Control of the particle population

### A. Modified ionization algorithm

PIC methods are based on simulating the behavior of a given species by integrating the motion of a high enough number of macroparticles, each one of them representing many particles. Macroscopic variables (e.g. densities, particle fluxes) are obtained by weighting macropaticle magnitudes to the nodes of the computational domain. However, in order to avoid statistical oscillations, the number of macroparticles per cell must be high enough. A good trade-off between accuracy and computational cost is around 20 to 30 macroparticles per cell.

HPHall fails to maintain an acceptable minimum number of macroparticles per cell, mainly near the anode where ionization is not strong enough and plasma density is small. This fact has important consequences since thruster efficiency depends on energy losses to walls that in turn depend on ion macroscopic variables, mainly density and particle flux to the walls. Thus, we decided to modify the ionization algorithm in order to better control the ion population. This algorithm is still of the MCC type and ensures a minimum number of particles.

The singly charged ion mass to be introduced into cell $(j,k)$ at a given time step is computed from the PIC sub-code from[2]

$$(\Delta m_i)_{jk} \cong m_i \langle \dot{n}_i \rangle_{jk,t-\Delta t} \Delta V_{jk} \Delta t \tag{18}$$

where $\Delta V_{jk}$ is the cell volume and

$$\langle \dot{n}_i \rangle_{jk} = \frac{(\dot{n}_i)_{jk} + (\dot{n}_i)_{j+1,\,k} + (\dot{n}_i)_{j,\,k+1} + (\dot{n}_i)_{j+1,\,k+1}}{4} \tag{19}$$

is the average ionization rate for cell $(j,k)$.

MCC methods are based on performing a number $N_{prob,jk}$ of probability tests to determine the real number of macroions to be created, $N_{jk}$, in a particular cell and time step. The relationship between $N_{prob,jk}$ and $(\Delta m_i)_{jk}$ is given by:

$$M_{i,jk} N_{prob,jk} P_{jk} = (\Delta m_i)_{jk}, \tag{20}$$

where $M_{i,jk}$ is the mass of the created macroions and $P_{jk}$ is a probability. Once $N_{prob,jk}$ is known the real number of macroions to be created in cell $(j,k)$, $N_{jk}$, is determined comparing $N_{prob,jk}$ random numbers with $P_{jk}$. Notice that $N_{prob,jk}$ represents the maximum number of macroions that could be created in the cell in the time step considered.

Two of the three magnitudes of the left-hand-side of equation (20) can be chosen arbitrarily. HPHall and HPHall-2 take $P_{jk} = 0.30 - 0.85$ (depending on the ionization rate) and fix either the value of $M_{i,jk}$ or $N_{prob,jk}$ equal to one. In both cases, few particles are generated in low density regions. In order to control better the number of particles per cell, the ionization algorithm has been improved in the following way. First, a law for the probability $P_{jk}$ is chosen; it can be constant (e.g., 0.5) or a function of the ionization rate as in the existing codes. Second, lower and upper limits of macroions per cell are defined, $N_{min}$ and $N_{max}$. Then, three situations are considered, depending on the numbers of existing macroions in the cell $N_{i,jk}$:

1. If $N_{i,jk} < N_{min}$ then $N_{prob,jk} P_{jk} = N_{min} - N_{i,jk}$ (what ensures that the minimum of macroions is respected) and $M_{i,jk}$ is obtained from equation (20).

2. If $N_{min} < N_{i,jk} < N_{max}$ then $M_{i,jk}$ is chosen close to the average value of the mass of the macroions in the cell and the *integer* $N_{prob,jk}$ is computed from equation (20).

3. If $N_{i,jk} > N_{max}$ then $N_{prob,jk} = 1$ (what reduces the computational cost and ensures that there are no cells with too many particles) and $M_{i,jk}$ is obtained from equation (20).

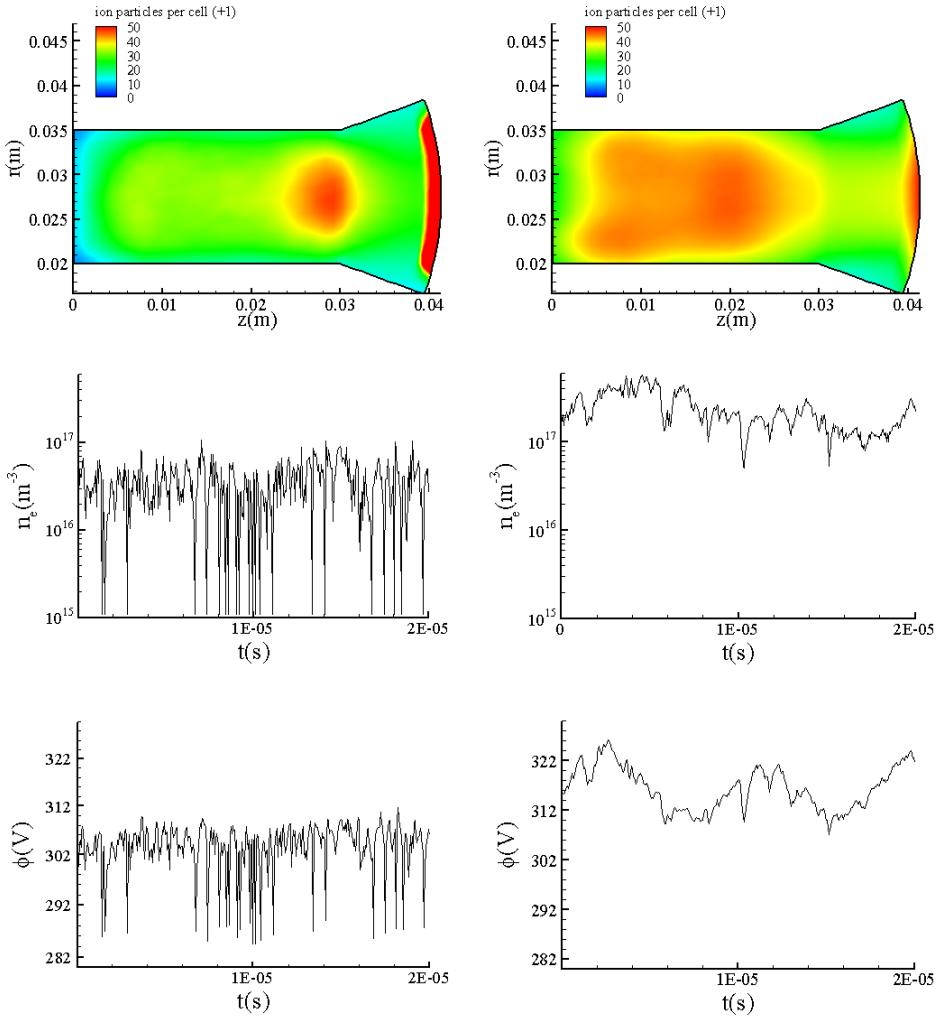


**Figure 6. Comparison between HPHall-2 (left column) and the new hybrid simulation code (right column): Contour Number of macroions per cell, temporal evolution of plasma density and potential in a node of the anode sheath edge.**

## B. Results

The main advantages of the new algorithm with respect to the previous one are:

1. it avoids statistical oscillations by ensuring a minimun number of particles in every cell.
2. computational cost is reduced by controlling the maximum number of macroions per cell.
3. macroscopic variables are weighted properly near the walls since an acceptable number of macroions exists.

Figure (6) shows the differences between HPHall algorithms results and the results obtained with the algorithms proposed in this article. Clearly, the advantages aforementioned are achieved. The new algorithm is capable of limiting the ion population per cell between 20 and 50, approximately. In comparison, HPHall generated too many particles at the exit of the channel ($\sim 130$), what increased computational cost without improving simulation accuracy, whereas it worked with few particles ($< 10$) near the anode, what caused large temporal oscillations, in the scale $\Delta t$ and of

statistical character. Indeed, HPHall had to add an artificial background density of $10^{15}$ part/m$^3$) to $n_e$ to avoid 'near-singular' values. These minima are clearly observable in the plots of $n_e(t)$ for HPHall. The new population controal algorithm solves excellently that issue. The statistical oscillations of $\phi(t)$ follow those of $n_e(t)$. Differences on the temporal evolution, in scales much larger than $\Delta t$ are due to other improvements between HPHall-2 and the new code.[3,5]

## IV. Conclusions

Two types of improvements have been implemented into a PIC-MCC method for simulation of Hall effect thrusters. In the one hand, the improvement of the time-accuracy in the PIC submodel has had a non-negligible effect on results. It seems that the time-centered weighting is the dominant effect in the observed changes. We have not been able to observe a noticeable effect derived from the time-centered macroparticle loading and the time-centered macroparticle-wall collision, even though they may be important in other type of problems (the problem described by Cartwright,[8] for example). On the other hand, the new ionization algorithm has allowed us to better control the macroion population, mainly near the anode and in the plume.

## Acknowledgments

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