A Fully Kinetic and Self-Consistent Simulation of a µN-HEMP-Thruster Using Random Cell Scattering (RCS) for Solving the “Anomalous Electron Transport” Problem

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Abstract: The paper reports the authors progress simulating a newly designed µN to mN HEMP-thruster. The baseline code selected was XOOPIC, an open source 2d3v plasma simulation code written in C++ and developed by the Plasma Simulation Group around Charles K. Birdsall and John Verboncoeur at the Berkeley University of California. The modifications required for simulation of highly ionized and strongly magnetized plasma thrusters are reported.

Thruster simulation results, even on a PC, were obtained by a pronounced geometrical downscaling with the factor γ =1e-4. As scaling procedure, the Maxwell scaling laws were used and modified for plasma conditions. They provide self similarity for particle trajectories, collision probabilities, ion beams and space charge potentials, independent of the downscaling factor value.

A XOOPIC input file defines the new µN-HEMP-thruster geometry, its magnetic field, the operating anode voltage (1000V), the Xe anode gas supply (0,033 sccm), the neutralizer Xe gas source (0.003 sccm) and the neutralizer electron current (~6 mA). Magnet field configuration and channel geometry were selected to provide low ion beam divergence in accordance with a Thales patent. The main simulation results at a power consumption of ~ 3.2 W were: Thrust = 104 µN; total Isp = 3110 s; 95% divergence angle < 28°.

Though some of these results are meanwhile found to be essentially wrong for the given gas flow due to a number error in the input file, the ion beam characteristics and channel potentials, showing the physics of the µN HEMP-T, should remain valid for a higher gas supply leading to the simulated total ion current of 2.4 mA.

I. Introduction

Fully kinetic and self consistent simulations of highly magnetized thrusters like Hall effect thrusters (HETs) or HEMP thrusters[1)] (HEMPTs) using a modified XOOPIC plasma code[2)] on a PC or laptop have for long been considered to be impossible. In a recent paper[3)] of A.L. Fabris et al. on *Ion Velocimetry Measurements and Particle in Cell Simulation of a Cylindrical Cusped Field Plasma Accelerator* the simulations were performed using plasma sources instead of ionization for simplification. In this paper the author presents an innovative strategy allowing results after about 8 weeks of stable simulation time on a Linux Ubuntu 9.10 operating system mounted on a HP Pavilion laptop with an Intel Centrino dual core processor in single core mode. Approximately 12 million time steps with 5e-16 s were performed until quasi stationarity was obtained for the charged electron and ion currents of a newly designed µN HEMP-thruster fed with 0.033 sccm Xe gas supply to the anode and a voltage of Ua= 1000 V. The design was in accordance with a Thales patent[4] for low beam divergence. The simulation used an author modified XOOPIC source code[5,6] as described in the following chapters.

II. XOOPIC additional collision processes

The performed modifications had several goals:

- To treat the propellant background gas Xe as uncharged particles and to move those during each time step like the charged species. The gas supply can then be obtained in the code via area or volume emitters. This should allow continuous simulation of the thruster and eventually quasi stationary conditions. A similar work was performed by Sudhakar Mahalingam in his doctoral thesis[7] for gridded ion thrusters.
- The HEMP- thruster operates under highly magnetized and ionized conditions. Van Reijen[8] et al. reported that more than 60% of the ion current can be carried by multiply charged ions. Thus the collision processes leading to double and triple charged Xe ions had to be introduced in the code. This made it necessary to treat also the single charged Xe^{1+} as a background gas with own Monte Carlo Collision (MCC) module and electronic and ionic cross sections.
- Since Xe neutrals are treated as particles, also the fast Xe neutrals as result of a charge exchange process, could now be introduced in the simulation.

A list of all the added Xe collision processes is in table 1.

Table 1: Xe collision processes

collision process	particle reaction	Original XOOPIC	Author added
electron elastic	$e^- + Xe \rightarrow e^- + Xe$	x	-
electron excitation	$e^- + Xe \rightarrow e^- + Xe^*$	x	-
coulomb interaction	e^- and ions in cell	x	-
single ionization Xe	$e^- + Xe \rightarrow 2e^- + Xe^{1+}$	x	-
double ionization Xe	$e^- + Xe \rightarrow 3e^- + Xe^{2+}$	-	x
Single ionization Xe^{1+}	$e^- + Xe^{1+} \rightarrow 2e^- + Xe^{2+}$	-	x
double ionization Xe^{1+}	$e^- + Xe^{1+} \rightarrow 3e^- + Xe^{3+}$	-	x
charge exchange CEX	fast Xe^{1+} + Xe → slow Xe^{1+} + fast Xe	no fast Xe	also fast Xe
neutral elastic	Xe + Xe → Xe + Xe	-	x

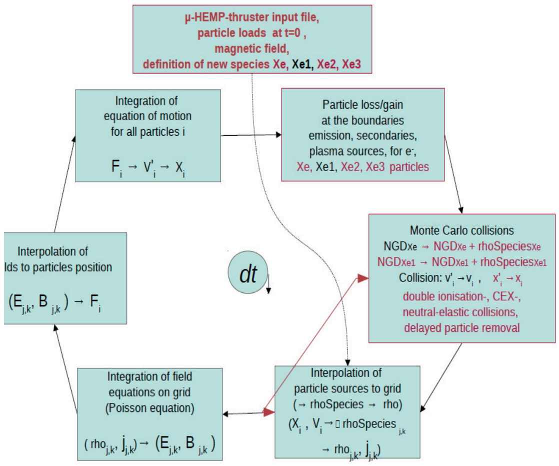

Fig. 1. Structure of the modified XOOPIC code.

The author implemented features are shown in red color.

Since in ionization or CEX processes the Xe or Xe1+ particles become new species, the original particles have to be removed. Within the existing C++ code, this could be done by saving the removal information in global variables for the next time step. The overall structure of the code and its modifications are shown in Fig.1. Trying to run the code under those conditions with a typical HEMP-thruster input file would lead to the severe problem that electrons are captured by the cusp mirror situation between the cusps. Their transport to the anode would be effectively suppressed by the strong radial magnetic fields at the cusps and the quasi-neutrality of the channel plasma would not be maintained, because the ions are leaving magnetically unhindered the channel downstream to the low plume potential. Under such conditions, the plot of the plasma potential is shown in Fig. 2. The negative space charge of the electrons has reduced the channel potential already a lot below the anode potential. This finally would lead to a thruster fade out in the simulation in contradiction to the experimental evidence. An extensive amount of literature described over the last decades the observed increased electron cross field transport as “anomalous” electron transport. Numerous approaches tried to explain this phenomenon in Hall thrusters with several physical phenomena but no generic success. An overview on this literature was recently presented e.g. in the paper of C. M. Lam et al.[9] and earlier by V. Latocha[10] et al. In this paper I use a completely different approach to solve the anomalous electron transport based on logical arguments within the Monte Carlo collision algorithms.

III. Random Cell Scattering (RCS), a solution to anomalous electron cross field transport.

The standard collision processes of the Monte Carlo PIC code do not provide sufficient cross field transport for the electrons. To understand that, I studied in detail the respective source code e.g. for ionization. Let us here consider just the basics, which are shown in Fig. 3. a and b before and after ionization, respectively. First consider a grid cell prior to ionization. We may have one computer particle electron and two computer particle Xe neutrals in this cell. Each of the computer particles represents the same number np2c real particles.

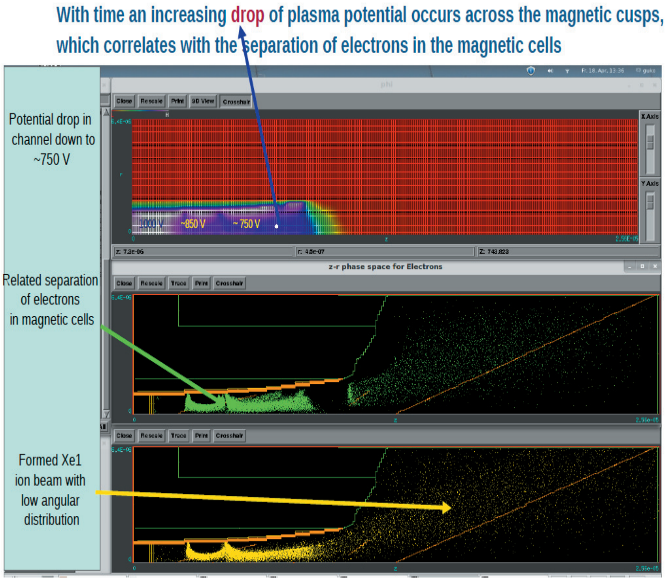

Fig. 2. Plasma potential (upper), electron- (middle) and ion distribution (lower) *as a simulation example with insufficient electron transport.*

The electron particle is bound in its motion to a magnetic flux line B shown in magenta. Now, the Monte Carlo code may have randomly selected just this electron particle for the chance to ionize. It will ionize, if the **Xe particle density in the cell** is sufficient to create an ion with the particle weight of the electron. Since there are 2 Xe particles available in the cell, this condition is fulfilled. But where should the Xe ion and the 2 leaving electrons localize? There are principally 3 options:

1) Standard, electron centered: The triple of one Xe ion and two electrons appears after ionization at the position of the impacting electron. This sounds on a first glimpse natural and is what the XOOPIC Monte Carlo collision module and probably most other codes are doing. But it is not really physically correct, because it would mean to "beam" a heavy Xe computer particle to the position of the electron computer particle. And it would also mean, that now 2 electron particles and thus 2*np2c real electrons are bound to the same flux line B, which essentially hinders their mobility as a result of the collision. Only the regular statistical scattering of their momenta, which is not especially discussed here, would contribute then partially to the electron cross field transport induced by the collision.

2) Xe neutral centered: The triple is produced at the position of one of the two Xe atoms. But which one of the two? Also, at the time step where electron collision occurs, the positions of the Xe atoms are not accessible in the object oriented code. And further, there should be procedural symmetry between electron- and Xe particles with respect to the location of the created particles. Therefore:

3) Cell centered, random cell scattering RCS: Methods 1) and 2) are **both logically wrong** because the ionization location is not the feature of a single computer particle, representing many real particles, but it is the statistical feature of the grid cell itself, in which the gas particle density is defined and the collision occurs. Therefore the location of the ionized triple **has to be randomly selected within the grid cell** as shown for instance in Fig. 3.b. **As a natural side effect of this algorithm correction we get the solution for the anomal electron transport by the additional scattering of electron locations in the collision process.** Physically this is clear because we statistically release two electron computer particles from their original magnetic flux line. The remaining statistical removal of one of the two Xe particles in the grid cell from the particles list is done in the next time step dt, when the locations of the Xe particles become available

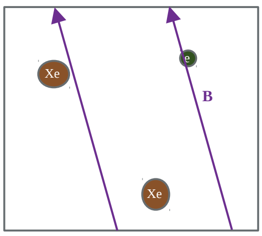

Fig. 3.a. Grid cell prior to

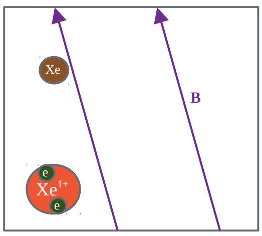

Fig.3.b. after ionization with RCS

again. RCS applies not only to ionization, but principally to all gas density related collisions e.g. to elastic and excitation collisions. Though not systematically investigated, insufficient electron cross field transport was so far never observed, even when testing for some grid mesh variations. Therefore it is assumed that RCS solves the problem generically and is applicable to all types of PIC codes suffering from the described logical error.

IV. PC friendly Maxwell Plasma Scaling

Geometrical scaling is an often used tool in plasma physics or astrophysics to bring a problem to a size which can be handled. A. A. Shagayda[11)] mentions in his recent paper several of those approaches. Trying to simulate a HEMP-thruster on a PC with a fully kinetic code for all particle types as neutrals, ions and electrons leads to the obvious problem of the many orders of difference in transit time and velocity of those particles and the pure number of particles to be treated in PIC codes. The PC power is not adequate to directly solve this numerical problem. Therefore a massive geometrical downscaling by the factor γ = 1/10000 (or 1e-4) was selected to reduce the size of the problem. From previous experience in vacuum electronics it was clear that the currents (source currents) **must** remain scaling invariant in order to leave the space charge potentials and the particle trajectories in the downscaled geometries invariant (self similar). In principle this requirement means, that the Maxwell Laws remain scaling invariant in the scaled system as described in the book "Space Charge Flow" of Kirstein, Kino, Waters, McGraw Hill, 1967). The following table 2 lists the Maxwell scaling properties of all relevant parameters with the extension to ionization. The requirements 1) to 7) are rather standard in plasma scalings. But often, e.g. in the paper of F. Taccogna[12)] et al., it is not recognized that the invariance or self similarity of the potential phi is **physically linked** to the invariance of the currents I and neutral mass flows M, because the potential phi includes the space charge potentials. Those are only correctly simulated, if the currents and thus mass flows for the neutrals are invariant in the scaled system. It is therefore **wrong** to interpret the plasma potential phi and velocity v as invariant, when the currents scale like I' = γ * I. The author proved that by tests of a simplified µN-HEMP-thruster model in which ionization was replaced by continuous plasma sources with source currents corresponding to the 0.033 sccm Xe-feed, later used in the full simulation. Simulated were the original, the unscaled plasma system and the system with "Taccogna scaling" at a factor γ =1/10 and the Maxwell scaling with a factor γ=1/10000. The "Taccogna scaling" leads already to substantial deviations from the original system as e.g. the comparison of the electron and ion particle distributions and the axial velocities uzz in Fig.4.a and Fig.4.b show. The plots were taken at corresponding times after achievement of steady state conditions for the electron and Xe^{1+} particle numbers.

Table 2: Scaling Factors for Maxwell Scaling

Scaling factor γ = 1e-4	scaled	comment
1) linear dimensions d	d' = γ * d	all geometrical dimensions
2) Simulation volume V	V' =γ^3 * V	massive reduction
3) Electric field E	E' = γ^{-1}E	calculated each time step
4) Magnetic induction B	B' = γ^{-1} B	static B calc. with Maxwell 2 D
5) Velocity v	v' = v	invariant
6) Time step dt	dt' = γ * dt	valid also for simulation time
7) Potential phi	phi' = phi	Invariant, only with 8)
8) Currents I	I' = I	invariant, **basic requirement**
9) Neutral mass flow M	M' = M	Invariant, analogues to current
10) Collision probability. p= n*σ*v*dt	p' =n'*σ'*v'*dt' p' = p	..along self similar trajectory: invariant, **basic requirement**
11) Density n	n' = γ^{-3} * n	At ignition not well defined
12) Cross section σ	σ' = γ^2 * σ	fictive parameter only
13) Product n*σ	n'*σ' =γ^{-1}*n*σ	provides interpretation room
14) Particle weight	np2c = 250	All particles e-,Xe0,Xe1,Xe2,Xe3

On the other hand, the proposed Maxwell scaling shows in Fig.4.c, even with the factor γ =1/10000, no deviations from the original at all. (Note: The geometrical scalings can be seen from the maximum r-, z- coordinates in the Figs.4.).

As important for the self similarity of the scaling as the invariance of the currents and mass flows is the invariance of the collision probability along a given trajectory during the time step dt. This is expressed in requirement 10) of table 2. We see, that this basic requirement is valid, in connection with the scalings of the time step dt, the density n and the cross section σ, items 6), 11) and 12), respectively. There are now two questions to be answered:

1. If we leave the source currents invariant and scale the grid dimensions with γ = 1e-4, the plasma density n' will increase by the factor 1e12 in the scaled system. If we estimate the Debeye length λ' in the scaled system according the approximation formula :

λ' = 7.4 SQR (T / n') [m] ~ 6.67e-10 m ; with n' ~ 1.25e-22 [cm- 3] and T ~ 10 [eV], we see from table 3, that the scaled cell dimension in z- direction is with d' = 5.8e-8m a factor ~100 larger than the Debeye length. Do we have to resize the grid meshing to become comparable with the Debeye length as usually

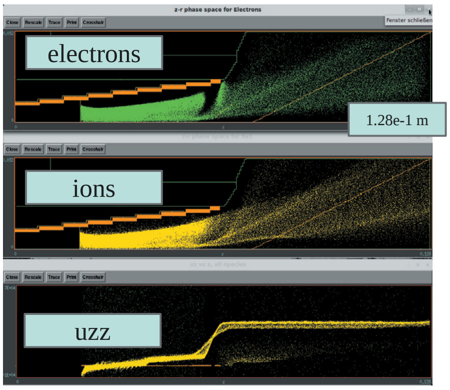

Fig.4.a: Original plasma test system
γ =1 at t=~3e-5 s, plasma source I. np2c=250e4; The electron gap d between channel and plume electrons corresponds to the main acceleration zone

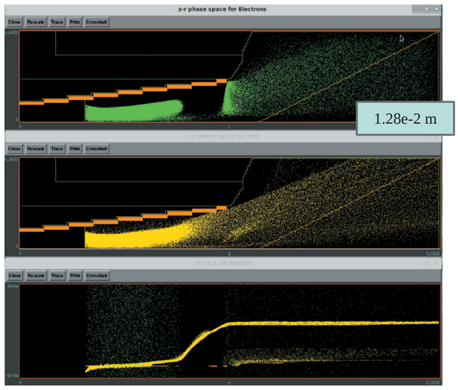

Fig.4.b: "Taccogna scaled" test system,
γ =1/10 at t'=~3e-6 s, I'=I/10.
np2c=250e2; the gap d~3 times larger than in the original, which agrees with Child-Langmuir law ($I=p*U^{3/2}$, and perveance p proportional to $1/d^2$).

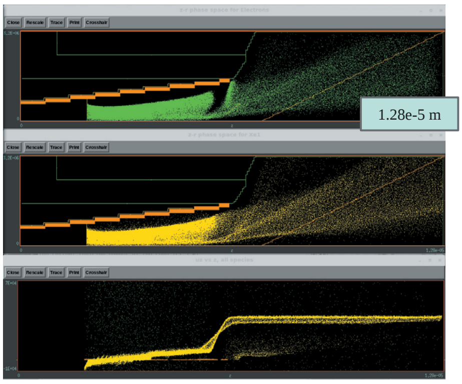

Fig.4.c: Maxwell scaled test system
γ =1/10000 at t'=~3e-9 s, I'=I. np2c=250; Except statistical - (not exactly same corresponding times), there are no differences to the original

requested for simulations and loose the numerical simulation advantage? The answer is: No!

The reasons are:

- The area of highest plasma density is deep inside the thruster channel, where the plasma potential is almost flat anyway. Exceptions are mesh sized, short term fluctuations of the plasma potential in the order of +- 15 eV, which do not lead to plasma self heating and numerical instability.
- In the important ion beam forming area, close to the thruster exit the plasma density is already several orders in magnitude lower, thus there we have agreement of the Debeye length with the grid mesh anyway and do not observe mesh sized short term fluctuations of the plasma potential.
- The Debeye length is no feature of the PIC- code at all. If the code works properly and the impacts of the violation of the Debeye requirement are understood, this might be justified in the interest of realistic thruster results obtained on a PC.

2. If we scale the particles density like $n' = \gamma^{-3} * n$, we leave the number of particles to be handled in the scaled system essentially constant. What did we gain then by the massive downscaling g = 1e-4 ? Here we remind ourself, that the number problem is mainly due to the high number of neutrals. This normally could easily be handled by selecting a much higher particle weight for the neutrals in the scaled system. In my case this treatment was forbidden, because my XOOPIC code modifications for neutral particle removal were not formulated sufficiently general to allow for partial removal of neutral particles after ionization with an individual particle weight. This would be a task for the future. To overcome this situation and maintain a unique particle weight np2c (here = 250) for all species, I use the interpretation room provided by item 13) in table 3 for the product n*s. In the scaled system we can write:

$$n'*\sigma' =(\gamma^{-3}*n)*(\gamma^{2}*\sigma) \quad \text{or:} \quad = (\gamma^{-1}*n) * \sigma.$$

That means, we scale the **neutral** starting density like $n'=(\gamma^{-1}*n)$ and leave their cross sections σ invariant as is done in the "Taccogna scaling". As long as the neutral collision probability item 10) remains within the long transit cycle time for the neutrals almost unchanged, this interpretation is allowed. In fact we reach quasi stationarity for the charged particles, electrons and ions, already after about 20 transit cycles for the ions in which the density of the neutrals does not change essentially. With this separation between neutrals and charged particles we are able to perform the simulation with the unique particle weight of 250 for all particles including the neutrals. Note: The mass flows for the neutrals are still considered as invariant to scaling.

V. Design and Simulation Results of a new µN to mN HEMP Thruster

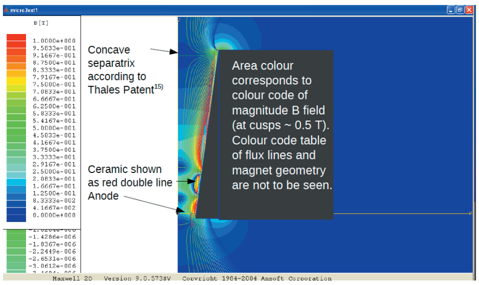

Fig.5. Geometry and magnet field of the newly proposed µN-HEMP thruster. The overall length between anode and exit separatrix is 6.3cm. The exit radius 1.4 cm. Magnet fields simulated with Maxwell 2D.

5.1 Design and simulation parameters

The attractive long life and operational simplicity of the standard 50 mN HEMP- thruster led early to experimental (see A. Keller et al.[13]) efforts to scale those thrusters down into the low mN and µN range. The principal problem there is the lack of much stronger magnet material compared to the already originally used SmCo permanent magnets. A downscaling in size by a factor 10, as was tried in[14] with a channel diameter of typically 3 mm, would require already permanent magnets with 10 times higher magnetic induction B on the thruster cusps at the inner channel diameter. Those magnets are not available today. If downscaling e.g. by a factor 10 is tried anyway, one looses the big advantage of a HEMP-thruster namely its plasma confinement off from the walls. Impingement of plasma electrons and ions with the wall leads to low gas utilization and low specific impulse there. The new µN to mN HEMP-thruster design proposed here (see Fig.5. and Table 3), tries to reduce the channel diameter only to the amount, which is in agreement with the available magnitude of induction B from todays magnets to maintain the contact free plasma confinement. Iterations with respect to geometry and magnet system were simulated.

At the same time the magnetic separatrix at the thruster exit was carefully, concavely designed in agreement with the Thales patent[3] in order to reduce the ion beam divergence angle and ease sufficiently the penetration of electrons from the plume torus, which deliver ionization energy, to support ionization under low gas pressure in the thruster channel. To save simulation time for the charging processes, the BN channel ceramics (DC = 3.5) are closed on the outer diameter by an electrode on anode potential. Only the last 2 downstream segments are left free to allow self consistent charging up of the segments by ion bombardment, which is required for the correct ion optics. Note: Surface conductivity is so far not included in the code. All parameters selected to simulate the new µN HEMP-thruster with the proposed code are listed in table 3:

Table 3: Simulation Parameters (scaled system)

Parameter	**Value**	**Comment**
Anode Voltage Ua	1000 V	invariant
Anode Xe gas flow	3.3e-2sccm	invariant, equiv. to 2.25 mA
Neutralizer gas flow	3.3e-3sccm	invariant, equiv. to 0.225 mA
Neutralizer e- source	~ 6 mA	Invariant, excessively supplied for self consistent adjustment
Plasma potential	Self consistent	Invariant, includes space charge & boundary potentials
Time step	5e-16 s	meets Courant condition
Particle weight	250	All species, for convenience
z-grid cell spacing	5e-8 m	256 equidistant meshes
r-grid cell spacing	2.5e-8 m	128 equidistant meshes
Channel length	6.3e-6 m	Anode to exit
Channel radius	0.55e-6 m /1.4e-6 m	At anode / at exit, respectively

5.2 Simulation results after 12 million time steps

Table 4
Evaluated µN HEMP thruster performance results

Parameter	Value	Comment
Thrust T	104 µN	dM/dt * v_z for Xe^{1+}, Xe^{2+}
Specific impulse	(3110 s)	includes neutralizer gas flow
95% divergence angle	< 28°	95% of ion particles within angle
Xe^{1+} current	1.88 mA	On boundaries
Xe^{2+} current	0.49 mA	21% of total ion current
Xe^{3+} current	0.9 µA	negligible
Total ion current	2.37 mA	<2.475mA, all gas singly ionized
Ionization efficiency	(85.9%)	calculated from ion currents
Power consumption	~ 3.5 W	estimated, because anode currents were initially not monitored

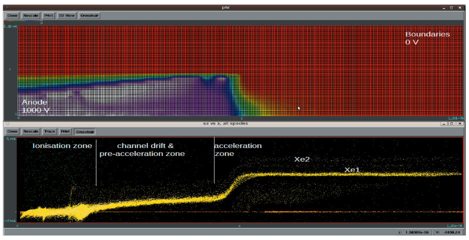

Fig.6. Potential phi and axial velocity.

Fig.7. Spatial distribution of electrons (green), Xe1+ ions (yellow) and Xe2+ ions (beige).

The ionization dependent data, in brackets in Table 4, are too high for the given gas flow due to an error in the input file for the neutral gas background gas density. The error was detected due to first test results of Franz Hey[15)] leading to a review of the input file. Meanwhile a simulation with corrected neutral gas density data has been started.
On the other hand the data provide the beam and power characteristics for a today unknown higher gas flow leading to the same total ion beam current of 2.4 mA. Their characteristics are shown in the Fig. 6. and Fig.7.

Fig.6. shows the plasma potential and axial velocity of all species. We note, that the plasma potential is not strictly following the magnetic separatrix. Positive velocity values are downstream, negative upstream to the anode. The electron velocities are strongly exceeding the shown velocity scale for ions from -1e4 m/s to +7e4 m/s. We note an axial separation of the area in 4 zones: The ionization zone near the anode and the 2 inner cusps, followed downstream by a channel drift and pre acceleration zone in which the plasma density becomes strongly reduced. At the exit we have a short main acceleration zone followed by the beam drift zone at plume potential and almost constant velocity.
Fig.7. shows the spatial distribution of electrons, single and double charged ions. The average ion beam angle is approximately 23° from axis. In the near plume region the electron density distribution is governed by the magnetic separatrix. In the far plume region, electrons are following the ion beam density keeping quasi neutrality.

VI. Conclusions

6.1 The XOOPIC code was modified to allow fully kinetic and self consistent simulations of all species in a Xe operated µN HEMP-thruster.
6.2. The new random cell scattering (RCS) approach for collision impacted particles was explained and used to solve the anomalous electron transport problem.
6.3 A massive downscaling according to Maxwell's scaling laws with factor $\gamma = 10^{-4}$ could be applied to simulate a µN-HEMP-T on a PC.
6.4. Possible scaling interpretations along difference in transition times between neutrals and charged particles were used to allow unique np2c =250 ratio for all species.
6.5. Essential features of HEMP-thrusters were simulated and are physically understood and explained by the simulation.

VII. Acknowledgment

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Tim Brandt from DLR in Bremen, I thank for his critical questions, which helped to improve my arguments around the modified Maxwell scaling.

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