Three Dimensional Simulation of Micro Newton RITs

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Abstract: A 3D plasma simulation tool is very important for the understanding and optimization of μ N-RIT's. We have developed a full 3D PIC code including electrodynamics. Our code supports arbitrary geometries, which can be imported from a CAD format. We have successfully implemented the Message Parsing Interface for all parts of our simulation to handle the enormous computational effort. We will demonstrate that even a massive parallelization with more than 300 cores can be carried out. Therefore, simulation runs can be decreased to several hours. Furthermore, we will show a first simulation of a μ N-RIT 1.0.

Nomenclature

| $\vec{E}(\vec{r},t)$ | = time dependent electric field |
|--|---|
| $\vec{J}(\vec{r},t)$ | = time dependent total current density |
| $\vec{\tilde{A}}(\vec{r})$ | = complex amplitude of the vector potential |
| $\vec{\tilde{E}}(\vec{r})$ | = complex amplitude of the electric field |
| $\tilde{\tilde{J}}(\vec{r})_{coil}$ | = complex amplitude of the coil current density |
| $\vec{\tilde{J}}(\vec{r})_{electrons}$ | = complex amplitude of the electron current density |
| ω | = angular frequency |
| μ_0 | = vacuum permeability |
| ϵ_0 | = dielectric constant |
| P | = power deposition to plasma |
| V | = volume occupied by plasma |
| Т | = period of oscillation |
| μ N-RIT | = micro newton Radio frequency Ion Thruster |
| PIC | = Particle in Cell |
| DSMC | = Direct Simulation Monte Carlo |
| sccm | = standard cubic centimeter per minute |
| \mathbf{RF} | = radio frequency |

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I. Introduction

U ^P to date challenging scientific space experiments have high demands, especially in terms of energy consumption, thrust control and stability of the thruster employed. One of the most promising thruster designs is the μ N-RIT (micro newton Radio frequency Ion Thruster)¹ (figure 1) developed at the University of Giessen. This type uses an inductive plasma discharge, which is the key to an extreme long life time. Featured with an extraction grid system for accelerating the ions enables a high specific impulse for good efficiency. As a matter of fact the μ N-RIT fulfills the requirements of a wide range of controllable thrust with high precision.

Nevertheless, the understanding and optimization of such thruster is an ongoing process. Besides experiments the plasma modeling is an essential tool for this task. The typical neutral gas pressure in our thruster is in the order of 0.1 Pa. As a consequence validity of fluid dynamics is not guaranteed and standard commercial tools cannot be used.

Therefore, we designed our own tools for describing the μ N-RIT. The neutral density distribution inside the thruster can be calculated with our 3D simulation tool "FlowSim"², which is based on Direct Simulation Monte Carlo (DSMC)³ methods. The neutral density distribution is one of the main input parameter for the plasma simulation. To model the typical plasma densities of about 1×10^{17} per cubic meter Particle in Cell (PIC)⁴ methods are required.

Due to the geometry of the thruster, especially the coil and the extraction grid, the thruster symmetries cannot be exploited for the modeling. For this reason we wrote a full 3D PIC code to describe the inductive coupled plasma discharge. However, PIC requires large computational power and thus it is time consuming. Hence, we massively parallelized our code for all parts of the simulation. Moreover, both codes can handle arbitrary geometries. These geometries can be created with standard CAD tools and can then be imported into our codes.



Figure 1: μ N-RIT 2.5 (the number indicates the discharge chamber diameter in cm)

II. Modeling of a μ N-RIT

The modeling of an inductive coupled plasma discharge as for our thruster requires an electrodynamic treatment. Due to the necessity of resolving the speed of light such a fully electrodynamic treatment is computational too expensive. Assuming that the electromagnetic field and current densities are varying harmonic in time the PIC code can be split into an electrostatic part⁵ and an electromagnetic part^{6–8}. Within the electrostatic part the Poisson equation has to be solved in every time step. This is done by the finite difference method Successive over Relaxation (SOR).

For the electrodynamic part the Telegrapher's equation has to be solved

$$\mu_0 \frac{\partial}{\partial t} \vec{E} \left(\vec{r}, t \right) = \left(\Delta - \mu_0 \epsilon_0 \frac{\partial^2}{\partial t^2} \right) \vec{E} \left(\vec{r}, t \right). \tag{1}$$

By expressing the time varying electric field $\vec{E}(\vec{r},t)$ by the complex amplitude $\vec{E}(\vec{r})$ and the applied frequency ω of the coil current \tilde{J}_{coil} the time dependent part can be separated

$$\vec{E}\left(\vec{r},t\right) = \tilde{\vec{E}}\left(\vec{r}\right)e^{i\omega t} \tag{2}$$

$$\left(\Delta + \mu_0 \epsilon_0 w^2\right) \vec{\tilde{E}}(\vec{r}) = i\omega \left(\vec{\tilde{J}}(\vec{r})_{coil} + \vec{\tilde{J}}(\vec{r})_{electrons}\right).$$
(3)

That separation is very important in the way that now this equation has not to be solved every time step to obtain the electric field. It is sufficient to calculate the electric field every RF cycle. As a consequence the computational effort is dramatically reduced. Another speed-up is achieved due to the high mass of the ions, because only the current of the electrons has to be taken into account. Furthermore, both real and imaginary parts of the complex amplitudes as well as all three space components are independent from each other. Consequently, these six elliptic differential equations can be solved by the same field solver for the Poisson equation. The boundary conditions for the complex electric field amplitude are given by the definition of the vector potential \vec{A} and the Biot-Savarts law

$$\vec{\tilde{E}}(\vec{r},t) = -\frac{\partial}{\partial t}\vec{\tilde{A}}(\vec{r},t)$$
(4)

$$\vec{\tilde{E}}(\vec{r}) = -i\omega\vec{\tilde{A}}(\vec{r}) = -i\omega\frac{\mu_0}{4\pi} \int d^3r' \frac{\left(\vec{\tilde{J}}(\vec{r})_{coil} + \vec{\tilde{J}}(\vec{r})_{electrons}\right)}{\left|\vec{r} - \vec{r'}\right|}.$$
(5)

In the simulation the power deposition is a predefined target value. The actual achieved power deposition P is averaged over time T of one RF cycle and calculated by

$$P = \frac{1}{T} \int_{T} \int_{V} \vec{J}(\vec{r},t) \cdot \vec{E}(\vec{r},t) \mathrm{d}^{3}r \mathrm{d}t.$$
(6)

The coil current will be readjusted every RF cycle until the actual achieved power deposition matches the predefined target value.

III. Neutral Density Calculation

Besides the magnitude of power the neutral density inside the discharge chamber is a more decisive input parameter. This value primarily influences the electron energy and the efficiency of the power coupling. The neutral density can be calculated with our 3D DSMC tool "FlowSim"². Because the density profile variation is smaller than 20% (figure 2 and 3) we used for simplification a homogeneous average density. However, the



Figure 2: 2D density profile: bottom gas inlet, 37 apertures, 0.21 sccm mass flow.⁹ Figure 3: 2D density profile: top gas inlet, 13 apertures, 0.08 sccm mass flow.⁹

density profile calculation does not consider the influence of the plasma and the ion extraction. However, we have shown $earlier^9$ the change of density profile is a constant scaling only but the distribution is almost

unaffected. In particular, with ion extraction the density distribution will scale down by a factor of about two assuming a 50% mass efficiency. Indeed our μ N-RIT has a high mass efficiency between 40% and 60%. That can be explained as follows.

Due to the low pressure in the discharge chamber there is no gradient pushing neutral particles out of the discharge chamber. Therefore, particles only have a statistical probability to pass through the extraction system. Because the molecular gas flow dominates in the extraction system the probability is approximately proportional to the density inside the discharge chamber. Additionally, the probability depends on the geometry but this is fixed. Furthermore, in the steady state the number of exiting particles is conserved and is equal to the number of entering particles from the gas inlet into the discharge chamber. Turning on the plasma and the ion extraction 50% of the exiting particles will be ions. Consequently, the number of neutral exiting particles has to drop by a factor of two. Therefore, also the neutral density is reduced within the chamber by a factor of two. Keeping in mind that the number of exiting particles is approximately proportional to the average neutral gas density within the discharge chamber.

IV. Massive Parallelization of the PIC Simulation

Performing a 3D PIC plasma simulation demands a huge amount of computational power. For example the Poisson equation has to be solved for vast meshes of the size $100 \times 100 \times 100$ and larger. Million of particles have to be accelerated for a couple of million of time steps. To do such simulations in reasonable run time a massive parallelization is essential. For that reason, we have incorporated the Message Parsing Interface (MPI) into our 3D PIC code by applying the domain decomposition method. Thereby, the total simulation space is dived in sub spaces and each sub space is assigned to a single thread. These threads only have to communicate boundary information of their sub spaces with their six neighbors.

We payed tremendous attention for the design of the field solver because this is the part with the highest communication. Hiding communication was achieved by transferring the boundary information during the calculation of the inner part of the sub space. Since there is not always a homogenous distribution of particles over the sub spaces we added to our code some kind of balancing to avoid wasting of computational power. This balancing is accomplished by skillful overloading the available cores. In particular, more sub spaces and accordingly more threads than available cores are created. The threads are in this manner distributed over the cores to even up the number of particles per core.



Figure 4: Speed-up of the plasma simulation for a mesh size of $100 \times 100 \times 100 \times 100$ cells and 3×10^6 particles.

Figure 4 demonstrates the excellent speed-up of our 3D PIC code. The speed-up is split into particle operations and field solver operations. It is suspicious that speed-up of the particle mover is larger than the expected maximum speed-up. But this is only contradictory at the first sight. It is caused by the hardware

architecture of the CPU and the algorithm design. In a PIC code particle operations have a high demand of memory transactions. For that reason, the limiting factor for the speed-up is the bandwidth to the memory and not the computational power. By increasing the number of sub spaces the size of a sub space will shrink. As a consequence more sub space information will reside at the CPU cache, which has a larger memory bandwidth. Consequently, a better performance of the particle operations can be facilitated compared to the non-parallelized version. Of course this can be carried out by optimizing the serial version. However, this is not required because it is carried out automatically by the parallelization without any further programming overhead.

The speed-up of the field solver is not as good as the particle mover. It is limited to a maximum speed up of 100. This is related to the increasing number of cells located on sub space boundaries compared to the cells inside a sub space. As a result the communication between the threads increases while the calculation time for inner cells decreases. Nonetheless, it is very remarkable that the speed-up of the field solver does not decrease.

Since the computational effort of the field solver and the particle mover are comparable an excellent speed-up of the total simulation is obtained.

V. Preliminary Simulations of a μ N-RIT 1.0

For first tests of our 3D PIC code we simulated a μ N-RIT 1.0. We chose the small diameter of 1 cm for testing purposes and to keep the computational effort reasonable. For a μ N-RIT 2.5 the system size will increase by a factor of 2.5 in every direction. Assuming the same plasma density and electron temperature for a μ N-RIT 2.5 the cell size can be kept constant. Accordingly, the number of required cells in every direction for this simulation will also increase by a factor of 2.5. Consequently, the total number of cells will increase by a factor of about 15 as well as the number of particles. For that reason the total simulation time will increase at least by a factor of 15.

The imported geometry was designed with a CAD program and is shown in figure 5.



Figure 5: μ N-RIT 1.0 with initial homogeneous ion density distribution; variations due to statistical cause; for scale see figure 7(a)

Figure 6: selected ion density area of interest

It shows the coil (red) surrounding the discharge chamber (light gray). The initial ion density (blue) is confined by the discharge chamber and the two extraction grids (dark gray). Figure 6 clarifies, which area of the ion density is shown for the transient of the plasma discharge of a μ N-RIT 1.0 in figure 7. The used input parameters are a neutral density of 7×10^{19} m⁻³ and a power deposition of 0.08 watt. The coil operates at a frequency of 5 MHz. The used mesh size for this simulation is $75 \times 75 \times 75$ and the amount of particles totals up to 3 million. The simulation was done by 96 cores in 48 hours. After 1.2 million time steps the simulation has reached the steady state. This corresponds to a simulation time of 3.3 μ s



Figure 7: Reaching steady-state of a plasma discharge simulation in a μ N-RIT 1.0

VI. Conclusion

We are now able to perform 3D plasma simulations for μ N-RIT's using the PIC method. Our self developed simulation code supports arbitrary geometries, which can be easily designed by standard CAD tools. All parts of the plasma simulation are parallelized. We have shown that our simulation code consists of a very impressive speed-up which enables a massive parallelization. Therefore, the calculation time reduces to only a few days or hours depending on the amount of available cores. Our next steps will be the increase of the system size and thus enter the verification phase. We are now on the verge to predict performance parameters for new designs of our thrusters on a microscopic level.

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