Simulation of plasma sheath with PIC codes parallelized with CUDA

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The problem of simulating the sheath which takes place in the contact of a plasma with a metallic surface is studied. We have chosen Particle-In-Cell (PIC) algorithms to model the dynamic of the sheath. The cases of planar and cylindrical geometry have been considered. The simulations have been developed under the framework of Compute Unified Device Architecture (CUDA) for the sake of performance. The use of GPGPU techniques and some algorithmic simplifications, have allowed us to perform simulations in a reasonable time without the need of complex and expensive hardware equipment.

1. Introduction

Theoretical knowledge of the processes that take place in the sheath between a neutral plasma and a metallic surface are of great importance nowadays, due to the different applications based on plasma technology. The number of particles that reach the surface and their impact energy are key parameters, not only on modern surface treatment techniques, but also on plasma diagnosis by using electrostatic Langmuir probes or mass spectrometry [1-2].

Simulations based on Particle-In-Cell (PIC) algorithms represent a powerful tool in the study of the system described above. Some of the advantages of particle models over fluid models are, the complete description of the system and the possibility to easily introduce complex interactions between particles in the system. These advantages come at a price, and particle models require huge amounts of computational resources.

Over the last decade, GPUs have evolved into massively parallel computational systems due to the improvements in multimedia content. This fact, and the development of the Nvidia GPGPU framework (CUDA), has motivated the use of GPU computing in many research areas due to the low cost and simplicity of these systems.

It is our aim to develop a particle simulation of the sheath surrounding an electrostatic probe. This simulation will allow us to study the formation and dynamics of the sheath in those cases that fall outside the approximations of fluid models. In order to obtain results in a reasonable time, algorithmic simplifications and hardware acceleration with CUDA have been implemented into the simulation.

2. Simulation description

We are interested in the study of the sheath between a low pressure plasma and an electrostatic Langmuir probe, which is negatively biased with respect to the plasma. The plasmas that we are considering are composed of electrons and ions. We have developed two separate codes to simulate planar and cylindrical geometries of the probe (see Figure 1). Due to the symmetry of the problem, simulations are either 1D1V (planar geometry) or 1D2V (cylindrical geometry).

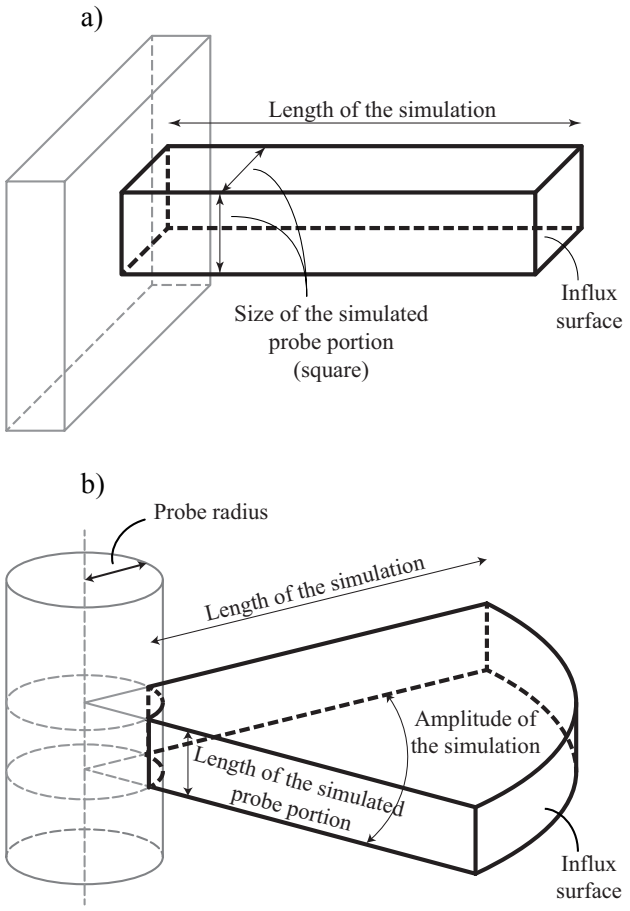

Figure 1. Simulation domain for both geometries: a) infinite planar probe and b) infinite cylindrical probe.

The dimensions of the simulation domain are adjusted in order to simulate a reasonable number of particles. As we have mentioned, due to symmetry considerations, simulations are monodimensional in

space. So, the simulation domain is gridded into an array of points where we assign macroscopic quantities, such as charge density, electric potential, electric field, etc. The spatial dimensions considered are: distance to the probe (planar probe), or radial distance to the probe's axis (cylindrical probe).

In addition, we are not taking account collisions in our simulations, since the smallest mean free path in the considered system is larger than the length of the sheath. However, collisions can be easily introduced in the code of the simulation.

3. Algorithms

Simulations are built on the basis of an electrostatic self-consistent PIC algorithm. These algorithms are well known [3-5], and a basic scheme of it can be seen in the flow chart shown in Figure 2.

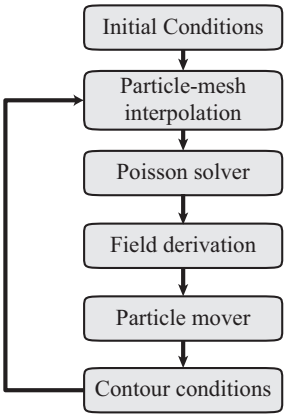

Figure 2. Flow chart of the code of the simulations

All the algorithms showed in Figure 2, have been parallelized with CUDA. One of the mayor drawbacks of working with CUDA is the limited amount of shared memory available. Over the last generations of CUDA enabled devices, shared memory has been greatly improved; nevertheless, it is still a problem.

Anyway, since our simulations are 1D, the spatial mesh is small enough to fit entirely into the shared memory space. This fact, allowed us to use sorting-free algorithms to weight particle-quantities into mesh macroscopic quantities. In this way, we don't need any sorting algorithm, as used in [6-8], in the contour condition module, which results in the speed up of the simulation.

The algorithm we use to weight particle-quantities into the grid points macroscopic quantities is the well known Cloud-In-Cell (CIC) algorithm. To solve Poisson's equation, we use a finite difference scheme and the Jacobi method for the resulting algebraic system. For the field differentiation we also use finite differences. And finally, we update particle positions and velocities with the leap-frog algorithm. All the methods listed above are easily parallelizable with CUDA.

3. Results

In order to ensure goodness of the results, when simulating conditions that fall outside the fluid models approximations, we have tested the codes comparing their results with the ones obtained from a fluid model under simple and similar conditions. Some of these comparisons can be seen in Figure 3.

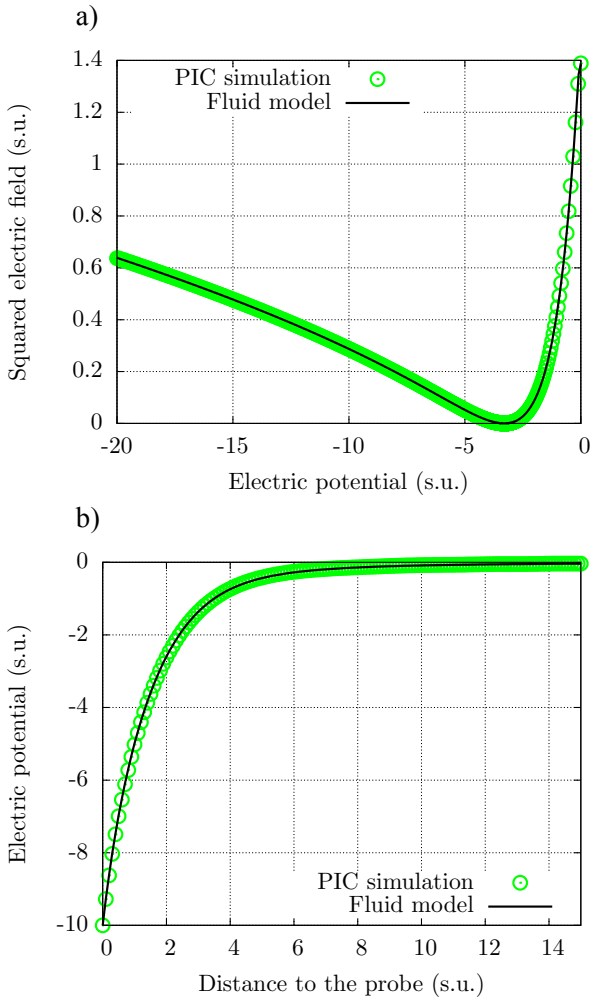

Figure 3. Comparison between results provided by the simulations and fluid models using the units of the simulation (s.u.): a) planar probe and b) cylindrical probe.

In the case of infinite planar probe, the fluid model allows us to obtain an analytic expression of the square of the electric field as a function of the electric potential. This is the expression we have used in Figure 3a) for the comparison between the simulation and the fluid model.

In the case of the infinite cylindrical probe, we have compared the results of the simulation with the

ones provided by the ABR model. In this case, contrary to the planar case, we cannot obtain an analytic expression from the fluid model. For this reason, we have integrated the equations of the fluid model in order to obtain the electric potential profile, with which we compare the results of the simulation in Figure 3b).

As can be seen in both graphs of Figure 3, the results provided by our simulations are in perfect agreement with fluid models.

Performance of the developed codes has also been analysed. The measured parameter has been the time the simulation needs per particle and per iteration. Some of the measurements can be seen in Table 1. There, it can be observed that the performance of the code is improved as we increase the number of particles simulated. This is explained because, when we do not have enough particles, not all the computational resources of the GPU are in use. For the same reason, if we increase the number of simulated particles more than a certain threshold, the GPU does not have enough resources to simulate all of the particles at the same time, so the performance drastically drops. This is the behaviour we can expect from a parallel code.

Table 1. Performance of the simulation of the cylindrical Langmuir probe, measured in time per particle and per iteration.

# particles (average number)	Cycle (ns/particle)
18.5 kpart	587
37.2 kpart	364
182 kpart	177
1.73 Mpart	113

In Table 1 we show the data corresponding to the simulation of the cylindrical probe, but similar data are obtained with the simulation of the planar one.

All the simulations have been run within a quite modest computer: Intel Core i3 530 with an Nvidia GeForce GTX 470. Therefore, the use of CUDA, allows us to obtain nearly supercomputer performance without the need of expensive and complex hardware.

4. Conclusions

We have developed a PIC code, that simulates the sheath between a negatively biased electrostatic Langmuir probe and a plasma. The code has been parallelized with CUDA, allowing us to perform simulations in reasonable time with a low cost computer. Two separate codes have been developed for the cases of planar and cylindrical geometries. The correct behaviour of the simulations has been tested, comparing their results with the ones obtained from fluid models in simple situations.

These simulations will allow us to study the behaviour of the sheath in those situations that are not covered by fluid models. For example, the transition from ABR to OML theories in the cylindrical case [9]. Also, the codes can be easily adapted to include more complex interactions such as collisions, ionizations, different ion species, etc.

Acknowledgements

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5. References

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