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Multi-dimensional particle codes for modelling in low-temperature and high-temperature plasmas in the presence of magnetic field

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Abstract

The understanding of physical and chemical processes in the boundary layer between plasma and immersed solids is important both in probe diagnostics and in modern plasma technologies. Especially there exists a considerable scientific and technological interest in processes taking part during the movement of charged particles in external magnetic fields, both in low-temperature and high-temperature plasma. This contribution deals with analysis of time requirements of multi-dimensional self-consistent particles codes studying plasma sheath in these conditions. Some physical results are also presented.

Introduction

As the detailed analysis of experimental data obtained in low-temperature and high-temperature plasmas is sometimes rather difficult, computer modelling is now being widely used. From various techniques of computational physics the particle simulation approach can bring the most detailed information, however, this approach is very time-consuming and its effectiveness decreases with increasing dimensionality of problems studied. In high-temperature plasma physics there exist problems for which standard computer codes are not well suited, e.g. probe diagnostics in the tokamak edge plasma using modern sophisticated techniques as Katsumata probe or tunnel probe, where due to complicated forms of probes the application of high-dimensional codes is unavoidable. Similar situation can emerge in low-temperature plasma physics and plasma chemistry during plasma treatment of materials.

For this purpose we prepared our own two- and three-dimensional particle codes. However, to apply these models correctly, it is first necessary to obtain detailed information about the sheath and presheath in the presence of magnetic field. Special attention will be also given to detailed analysis of time requirements of principal parts of programs in order to increase the efficiency of resulting computer codes, and to the difference in performance of individual codes in low-temperature and high-temperature plasmas.

Computer model

Our models are based on the combination of deterministic and stochastic techniques. For the description of movement of charged particles in both local and external electric and magnetic fields the molecular dynamics is used – the Verlet algorithm with combination of half acceleration - rotation - half acceleration algorithm (HARHA, e.g. [1]) for the description of movement of charged particles in the presence of magnetic field. Scattering events are treated by Monte Carlo method. Due to energy dependence of cross-sections of scattering events considered [2], the null-collision method is employed. The electric field is determined by the self-consistent PIC-CIC simulation technique and the magnetic field is treated non self-consistently. The Poisson equation is solved by iterative methods, so one can choose the suitable method and preciseness of potential computation.

The problem studied is the formation of plasma sheath in the vicinity of metal probe immersed into plasma. The dimensionalities of our codes are *2d3v* or *3d3v*, respectively. Unfortunately, the fully three-dimensional code is too time-consuming, solving the Poisson equation being the crucial part. Without using more sophisticated algorithm or even development of completely new code based on different approach, this code is practically inapplicable. Therefore, next text is devoted to two-dimensional code.

Results and discussion

The main part of this contribution is the detailed time analysis of the computer codes for different plasma types and condition. For this purpose the codes were divided into several parts – *Flux* concerning new particles coming from undisturbed plasma outside studied region and particles leaving this region, *Poisson* containing charge summation, calculation of electric potential and forces, *Mov*e incorporating time integration algorithm (Verlet and HARHA) together with force interpolation, *Scatter* treating scattering events of charged particles with neutral background, *Probe* dealing with particles impinging the metal probe.

From Fig. 1 it can be seen the differences in time demands for mentioned crucial parts for different plasma or computer model parameters. The presence of magnetic field in low-temperature plasma causes the change in subroutine *Move* time demands due to HARHA algorithm incorporation. The increase of magnetic field value induces additional increase of part *Move* time because of charged particles' pendulum motion with smaller Larmour radius and consequent increase of number of particles in the region and hence the number of differential equations to be solved. Different time steps for electrons and ions used in these codes can be used for steady state problems only. Otherwise the same (smaller) time step must be used. The difference in *Scatter* (less collisions for ions) can be seen. For high-temperature plasma, the particles are much more energetic (especially ions) causing bigger fluctuations in the system and hence the increase of *Poisson* time demands, and more noticeable change in *Scatter* time requirements due to much higher probability of scattering event in one time step. Using same time steps for both types of particles again lowers this probability. *Poisson* time demands are lower too, the reason being smaller fluctuations in the system.

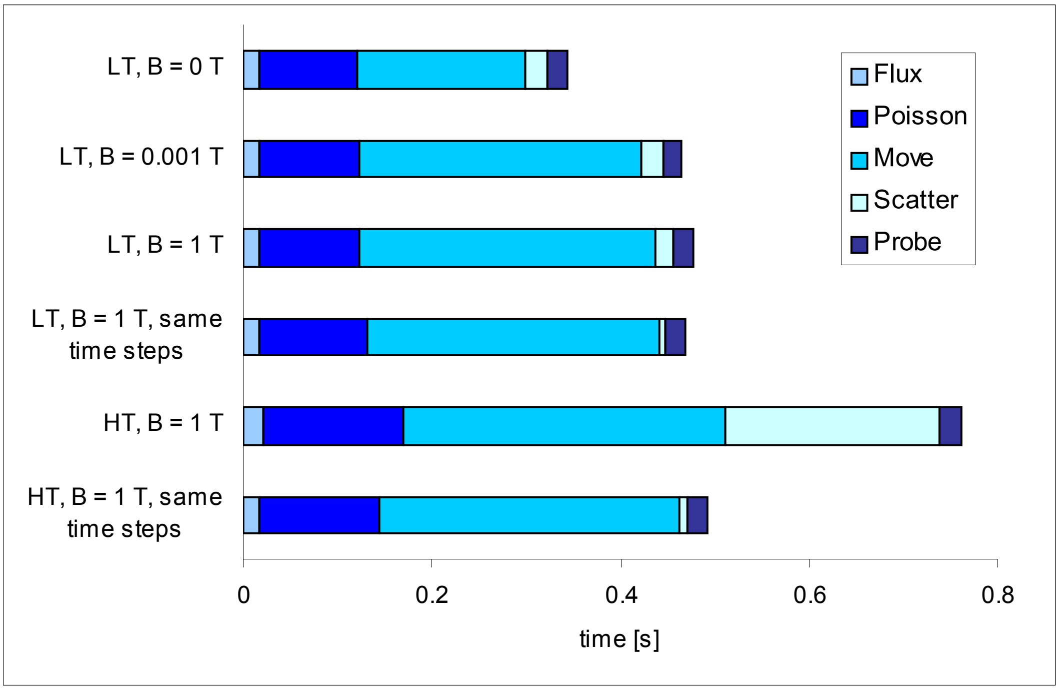

Fig. 1 – Time analyses for different plasma and computer model parameters – real times of crucial parts execution during one time step. LT – low-temperature plasma (T_e = 2 eV, T_i = 0.026 eV), HT – high-temperature plasma ($T_e = T_i$ = 20 eV), $\Delta t_e = 10^{-12}$ s, $\Delta t_i = 10^{-9}$ s. Intel Fortran compiler 8.1, CPU – Intel P4 3.2 GHz.

The physical results of these simulations are potential distribution, concentrations of charged particles, probe current, angular and velocity distributions, etc. In Fig. 2 it can be seen how the shape of the sheath is affected by the presence of magnetic field in one direction (x-axis, parallel to working area). As another examples there are spatial distributions of electric potential and concentrations of both types of charged particles depicted in Fig. 3.

We can conclude that the presence of magnetic field affects both physical quantities of plasma systems studied and time demands of the codes. The change of physical parameters of the model (e.g. energy of particles) also affects the time demands.

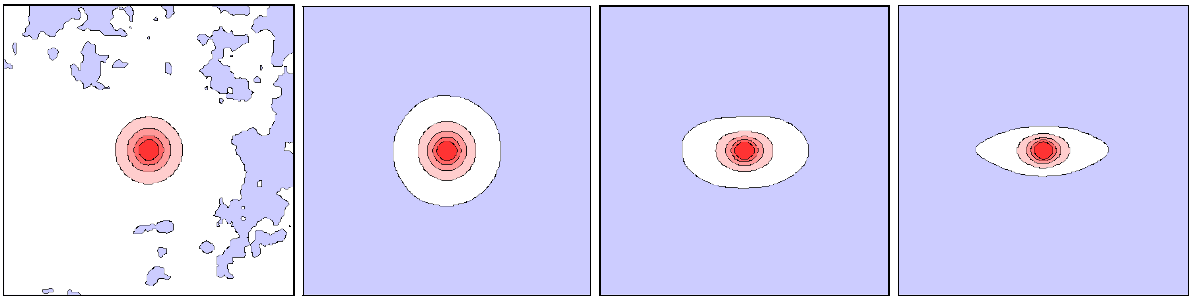

Fig. 2 – Plasma sheath in the vicinity of cylindrical probe in different magnetic field (from the left: LT, $B_x = 0$ T; LT, $B_x = 0.001$ T; LT, $B_x = 1$ T; HT, $B_x = 1$ T).

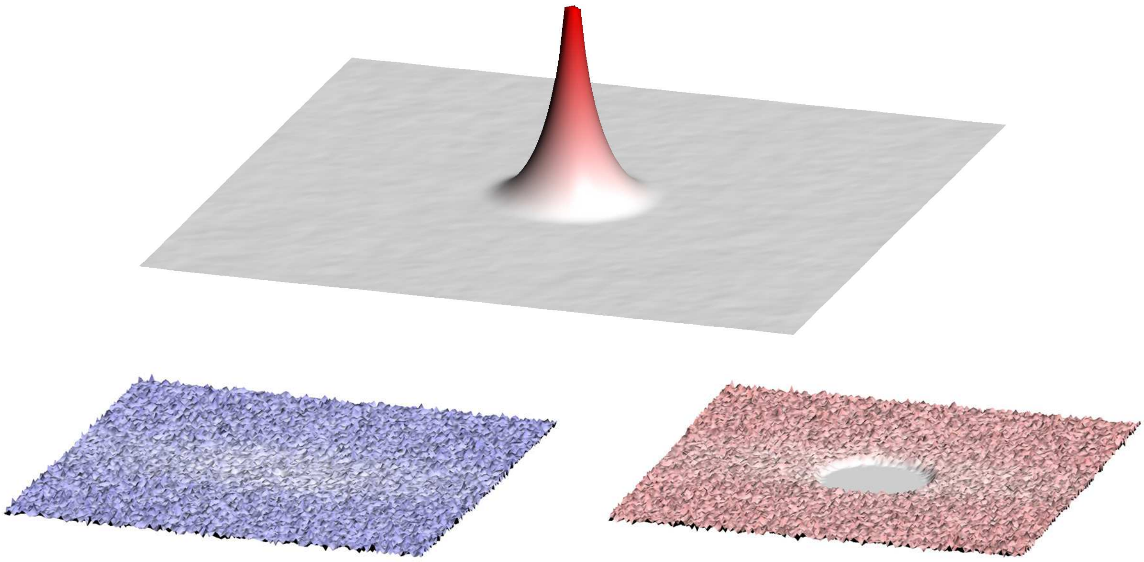

Fig. 3 – Potential distribution (top), concentration of electrons (left) and positive ions (right) for positive bias and $B_x = 0.01$ T.

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[2] Brown S. C.: Basic Data of Plasma Physics, AIP Press, New York 1994.