Applications of hybrid computer models in plasma sheath physics

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Introduction

An increase in performance of computers over several past decades allowed computer modelling to be included among other plasma research tools as a valuable source of information. Problems that are adressed in plasma physics are often difficult to be treated analytically due to various reasons (nonlinear effects, nonequilibrium plasma states, complex 3D geometries, etc.) and thus, it becomes an area where computer models are able to provide deeper insight into the studied phenomena.

Plasma is known as an environment where phenomena over multiple length and time scales are coupled. However, particle computer models that are able to capture microscopic effects precisely enough demand huge computational resources. As a result, they are often limited to 2D configurations of limited size. On the other hand, macroscopic fluid models that are not so computationally demanding give results with only limited accuracy caused by the lack of microscopic information. Hybrid models (e. g. [1], [2]) that take advantage of both modelling techniques mentioned above seem to be a promissing concept to overcome these difficulties.

Findings of plasma sheath physics are of great importance in applications where plasma interacts with surfaces of solids (e.g. industrial plasma-based surface processing of materials, plasma facing components in fusion devices, etc.). Our contribution compares three computer modelling approaches to a simple 3D problem of plasma sheath creation near a biased metal wall which is in contact with electropositive argon plasma.

Problem statement and modelling approach

The first modelling approach used in our study was 3D fluid model based on drift-diffusion approximation. The following set of equations was considered:

$$\nabla \cdot \boldsymbol{\Gamma}_{\boldsymbol{e},\boldsymbol{i}} = 0, \tag{1}$$

$$\boldsymbol{\Gamma}_{\boldsymbol{e},\boldsymbol{i}} = \pm \mu_{e,i} n_{e,i} \boldsymbol{E} - D_{e,i} \nabla n_{e,i}, \tag{2}$$

$$\Delta \phi = -\frac{e}{\varepsilon_0} (n_i - n_e), \tag{3}$$

where n marks number density, $\boldsymbol{\Gamma}$ particle flux, $\mu = \frac{q}{m\nu_m}$ mobility coefficient, $D = \frac{k_B T}{m\nu_m}$ diffusion coefficient, ν_m collision frequency given by collision cross section and ϕ is the potential of

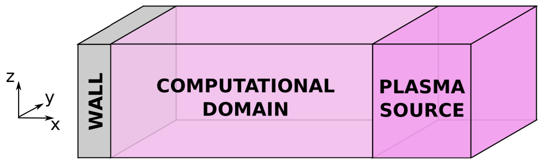


Figure 1: *Geometry of the modelled configuration. Periodic boundaries in Y and Z direction.*

electric field $\boldsymbol{E}$. The model was implemented by means of FENICS project [3]. Finite element method with Lagrange elements of the first order defined on a tetrahedral mesh was used to solve the set of equations. Dirichlet boundary conditions were imposed on the outer boundaries of the computational domain where plasma reaches metal wall and where computational domain joins plasma source.

3D Particle-In-Cell (PIC) algorithm with Monte Carlo null collision method for scattering processes treatment was the second modelling approach. CIC algorithm for collection of charge density and velocity Verlet algorithm for charged particle movement were employed. Fast Poisson Solver Routines of Intel MKL library were made use of to solve Poisson equation in every time step.

Simple 3D hybrid model was also implemented. This model started with one run of 3D fluid model described above to obtain electric field which was consequently used in non-selfconsistent particle model. It is a simpler version of iterative hybrid model which was discussed in [1] and [2].

The geometry of the modelled configuration depicted in the figure 1 was chosen as relatively simple since we wanted to keep the demands on computer resources sufficiently low, especially with regard to 3D PIC simulation. Physical dimensions of the computational domain were: $(2 \cdot 10^{-2}) \times (2 \cdot 10^{-4}) \times (2 \cdot 10^{-4})$ m. The investigated plasma was composed of electrons ($T_e = 2.36 \cdot 10^4\,\mathrm{K}$) and Ar^+ ions ($T_i = 3.0 \cdot 10^2\,\mathrm{K}$). Neutral argon gas in background was also taken into account. Only elastic collisions of charged particles with neutrals were taken into account: $\sigma_e = 6.0 \cdot 10^{-20}\,\mathrm{m}^2$ (electrons) and $\sigma_i = 4.0 \cdot 10^{-19}\,\mathrm{m}^2$ (Ar^+ ions). Table 1 contains values of plasma density for different neutral gas pressures that were investigated in our study. The bias of the metal wall was $U_p = +5\,\mathrm{V}$ with respect to plasma potential. PIC and hybrid models were run for $1.0 \cdot 10^5$ time iterations with total $1.2 \cdot 10^6$ of charged particles at 133 Pa pressure and $3.7 \cdot 10^5$ of charged particles at 13.3 Pa pressure.

Results

Figure 2 proves that 3D fluid model is able to predict widely known enlargement of the sheath with decreasing pressure.

Table 1: *Plasma density for different values of neutral gas pressure.*

Neutral gas pressure [Pa]	1.33e0	1.33e1	1.33e2
Plasma density [m^{-3}]	1.59e14	5.03e14	1.59e15

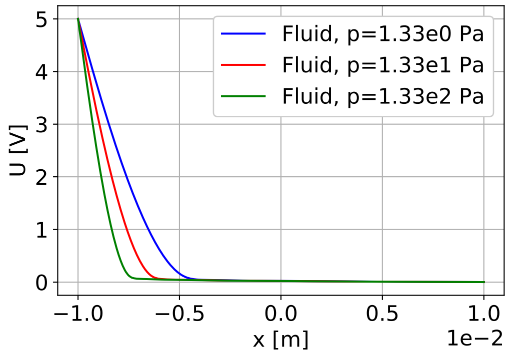


Figure 2: *Potential distribution near the metal wall biased at $U_p = 5$ V for different pressures.*

Figure 3a demonstrates that 3D fluid and 3D PIC model results for electrons are in a good agreement at higher pressure whereas differences are observed at lower pressures where PIC model results are considered to be more precise. The same can be stated for Ar^+ ions (figure 3b).

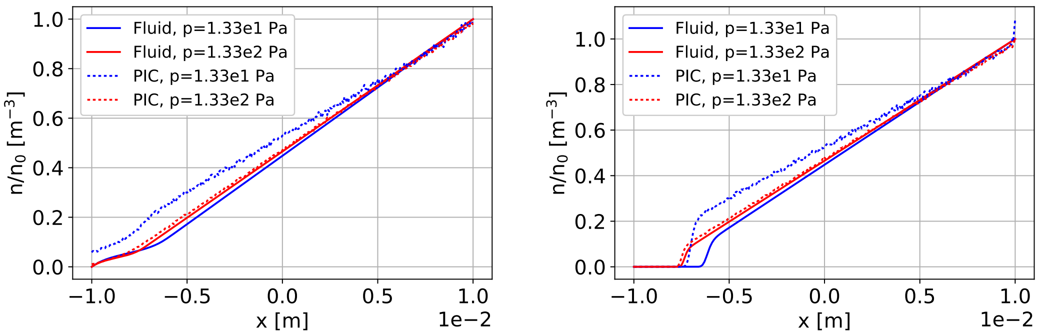
Figure 4a proves that even the simple hybrid model used in our study is able to reproduce PIC model results in the specified plasma conditions even at low pressure and at least for electrons while being faster than PIC model (about 30%).

On the other hand, figure 4b shows that the simple hybrid modelling approach does not provide satisfyingly precise results for Ar^+ ions. We attribute it to the failure of drift-diffusion approximation for Ar^+ ions in plasma sheath since it neglects Ar^+ ions inertia which becomes important in the sheath.

We also provide comparison of simulation times for particular modelling techniques in table 2.

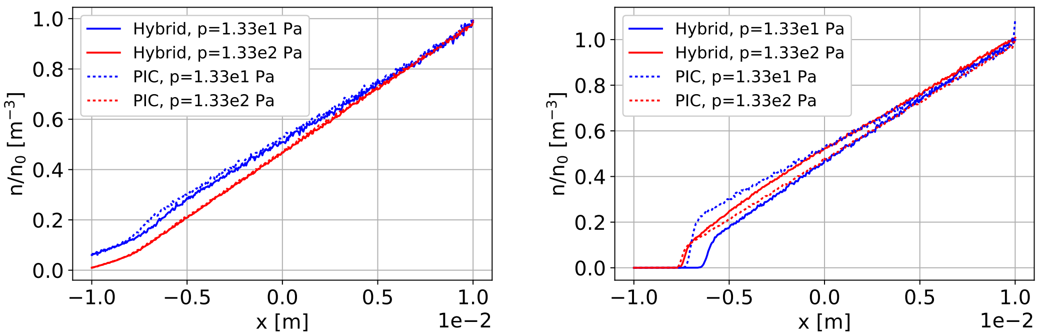
Table 2: *Comparison of simulation times for particular modelling techniques.*

Pressure	Fluid	PIC	Hybrid
13.3 Pa	5 min	2.52 h	1.65 h
133 Pa	5 min	11.5 h	8.7 h



a. *Electrons* b. *Ar^+ ions*

Figure 3: *Electron and Ar^+ ion density near the biased wall calculated by 3D fluid and 3D PIC model.*



a. *Electrons* b. *Ar^+ ions*

Figure 4: *Electron and Ar^+ ions density near the biased wall calculated by 3D fluid and 3D simple hybrid model.*

Conclusion

Our study confirms that even the simple hybrid models are beneficial for plasma sheath research. However, the fluid part has to be modified in order to be able to capture plasma conditions in which drift-diffusion approximation fails. There are several steps identified to achieve this goal: 1. Include inertial terms in the fluid description of plasma (at least for heavy ions) by moving to the full-momentum equation. 2. Employ methods of kinetic theory (e. g. Chapman-Enskog method) to improve fluid model in cases when distribution function is more general.

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