Particle in Cell (PIC) Simulations on Plasma-Sheath Boundary In Collision-Free Plasmas With Warm Ion Sources

Janez Krek\textsuperscript{1}, Nikola Jeli\v{c}\textsuperscript{2}, Jože Duhovnik\textsuperscript{1}

\textsuperscript{1}LECAD Laboratory, Faculty of Mechanical Engineering
Aškerčeva 6, SI-1000 Ljubljana, Slovenia
Janez.krek@lecad.fs.uni-lj.si, joze.duhovnik@lecad.fs.uni-lj.si

\textsuperscript{2}Association EURATOM-ÖAW,
Institute for Theoretical Physics, University of Innsbruck,
Technikerstraße 25, A-6020 Innsbruck, Austria
nikola.jelic@uibk.ac.at

\textbf{ABSTRACT}

In this work we investigate how fluid plasma parameters are related to the kinetic plasma properties for plasmas with warm ion sources and finite Debye lengths. This is an important issue in applying fluid codes to experimental, laboratory, technological and fusion plasmas. Namely, fluid codes for scrape-off layer (SOL) region in fusion devices are applicable only up to the plasma-sheath boundary (also called plasma edge or sheath entrance) and cannot be extended to the material boundaries themselves, because the sheath region is far from thermodynamic equilibrium and hence near the wall plasma can be correctly described only in terms of some kinetic model. Since, accordingly, the boundary conditions for plasma modeled in the fluid description should be defined at the plasma-sheath boundary (rather than at the physical surfaces), this boundary needs to be appropriately identified. However, identifying such a boundary and calculating the hydrodynamic parameters there is a demanding task which up to now has been solved only approximately and for a limited number of plasma discharges (i.e., only for some particular particle and energy production and loss balance scenarios).

In available PIC codes the ion source strength profile is usually hard-coded into program and does not change during the simulation (see e.g., Berkeley codes or BIT1). On the contrary, we have built very flexible PIC procedure enabling one to use different source strength profiles in each simulation step. In the present work we present the results obtained with the ion source strength profiles proportional to potential - $S_i(x) \approx e^{a \Phi(x)}$. We run simulation for cases with $\alpha = 1$ and compare results of simulation with results recently reported theoretical results of Kos et al. [Phys. Plasmas 26(9), (2009)] and found excellent agreement.
1 INTRODUCTION

Defining and finding the plasma-sheath boundary (also called “plasma edge”, “sheath edge” or “sheath entrance”) is a problem of ubiquitous relevance and importance in plasma physics, and particularly so in the context of laboratory, space and fusion plasmas. In a customary approach this problem starts from Poisson’s equation the assumptions that (i) the electron density distribution is a known function of the local potential, (ii) the ion source velocity distribution is known, and (iii) the potential profile is monotonic. The basic unknowns of the problem to be determined are the spatial potential profile $\Phi(x)$ (or, equivalently, the electric-field profile) and the final ion velocity distribution function (ion VDF) $f_i(\Phi, v)$ at any location of the discharge (or, equivalently, for any potential), where $x$ (position) and $v$ (velocity) are the usual phase-space coordinate. Mathematically, this problem is defined by a coupled set consisting of the Boltzmann and Poisson equations, which in plane-parallel geometry (i.e., for the considerations of the present work) read:

$$\frac{\partial f_i}{\partial x} - \frac{e}{m_i} \frac{d\Phi}{dx} \frac{\partial f_i}{\partial v} = S_i(x, v)$$  \hspace{1cm} (1)

and

$$\int_{-\infty}^{\infty} f_i(\Phi, v) dv = n_e(\Phi) - \frac{\epsilon_0}{e} \frac{d^2 \Phi}{dx^2}$$ \hspace{1cm} (2)

with $e$ the positive elementary charge, $m_i$ the ion mass, $\epsilon_0$ the vacuum dielectric constant, and $S_i(x, v)$ the ion source term. The problem is closed provided that the boundary conditions are well defined.

A formal solution of Eq. (1) is

$$f_i(\Phi(x), v) = \int_{\Phi}^{\Phi'} \kappa(\Phi, \Phi', v) d\Phi'$$ \hspace{1cm} (3)

where

$$\kappa(\Phi, \Phi', v) = \frac{S_i \left( \Phi', v^2 - \frac{2e}{m_i} (\Phi' - \Phi) \right)}{\sqrt{v^2 - \frac{2e}{m_i} (\Phi' - \Phi)}}$$ \hspace{1cm} (4)

so Eq. (2) takes the form of an integro-differential equation

$$\int_{\Phi}^{\Psi} \kappa(\Phi, \Phi') d\Phi' = n_e(\Phi) + \frac{\epsilon_0}{e} \frac{dx/d\Phi}{|\Psi|^3}$$ \hspace{1cm} (5)

where

$$\kappa(\Phi, \Phi') = \int_v \kappa(\Phi, \Phi', v) dv$$ \hspace{1cm} (6)

is the known kernel of the integro-differential equation provided $S_i$ is prescribed. The unknown function to be found from Eq. (5) is the negative value of the inverse electric field $\Psi \equiv dx/d\Phi \equiv -1/E$. Once this quantity has been found the ion velocity distribution can be obtained from Eq. (3).

Solving the above problem is very demanding, even with present day numerical methods and computational resources. The first difficulty arises when choosing a particular source function, which has to be physically meaningful and at the same time amenable to analytic or numerical integration for obtaining the kernel. For the “regular” case of “warm” ion sources
(when ions are generated with a distribution of finite initial velocities), the kinetic problem formulated above is of such complexity that it was never solved in the whole discharge region. In 1929, Tonks and Langmuir [1] triggered this kinetic problem, however assuming a “singular” or “cold” ion source distribution (i.e., all ions are born with zero initial velocity). 

Mathematically speaking, the ion source distribution in their model is defined as $S_i(x, v) = s_i(\Phi)\delta(v)$, where $\delta$ is the well-known Dirac $\delta$ function being infinite at a single point and zero elsewhere. However, at that time the problem still appeared too difficult for dealing with the complete “plasma and sheath equation”, as Tonks and Langmuir termed the model. In our terminology, they felt able to deal with $\varepsilon \to 0$ plasmas only but not with finite-$\varepsilon$ ones, where the smallness parameter $\varepsilon$ is defined as $\varepsilon \equiv \lambda_D^2 / L^2$, with $L$ the presheath (plasma) characteristic length and $\lambda_D \equiv \sqrt{\frac{e^2 kT}{ne^2}}$, the electron Debye length, a fundamental quantity on which a plasma can be defined at all.

It is well known that the plasma state is defined for $\varepsilon \ll 1$, otherwise the ionized system is not a plasma but just an ionized gas unable to establish quasi-neutrality. Tonks and Langmuir employed condition $\varepsilon \to 0$ (“asymptotic two-scale limit”), i.e., neglected the term originating from the second derivative of the potential. In this way they obtained the nowadays famous “plasma equation”, which holds in the case of strict plasma quasi-neutrality. They solved the plasma equation using an analytic expansion method. Harris on and Thompson, however, found an exact analytic solution of that in 1959 [2]. Furthermore, a rigorous mathematical formulation of the asymptotic two-scale plasma and sheath problem was given in 1962 by Caruso and Cavaliere on the basis of boundary-layer theory. Self in 1963 [3], on the other hand solved, the one-dimensional “plasma and sheath equation” numerically without splitting the discharge into the plasma and the sheath region. One important consequence emerging from his work is that, for finite-$\varepsilon$, the plasma-sheath boundary is a rather arbitrary concept from the academic point of view but that, anyway, it is important to define it for practical purposes. The only situation for which the plasma-sheath boundary is unambiguous is the asymptotic two-scale limit ($\varepsilon \to 0$), in which case it is defined by the famous Bohm criterion, which was originally obtained in 1949 by using a rather simple fluid model [4]. This criterion was upgraded to another famous formulation [2] known as the Harrison-Thompson plasma-sheath criterion (frequently also named generalized Bohm criterion) which is valid for arbitrary electron and ion velocity distributions. The Harrison-Thompson criterion for the case of Maxwellian distributed ion sources with non-negligible temperatures was confirmed explicitly by Bissel and Johnson [5] and Scheuer and Emmert [6]. Physical interpretations of this criterion were given in both fluid [7] and kinetic treatments [8]. There the plasma-sheath transition was interpreted as a surface where slow perturbations ($\omega / k \to 0$) originating from that the sheath region are incapable to penetrate into the plasma.

In particular, it would be of great importance to unify the plasma and sheath descriptions for various discharge scenarios with finite $\varepsilon$. One way to do this is to find some universal rules which hold in the whole discharge region, i.e., some kind of “similarity variables” which reduce the dimensionality of the problem. This task has already been partially performed for plasmas modelled in the fluid [9] and kinetic approaches [10] by using solutions which hold in the intermediate plasma region to match together plasma and sheath solutions obtained in the asymptotic two-scale approach. While these scalings are well confirmed in both fluid and kinetic models with cold ion sources, scaling in kinetic models with warm ion sources were just predicted (see e.g., [11][12]) on the basis of rather general kinetic considerations, but never confirmed explicitly due to lack of appropriate analytic and/or numerical solutions for of the intermediate region.

From the practical point of view, unifying the plasma and sheath descriptions is frequently...
not of primary importance, but on the contrary distinguishing the plasma and the sheath regions is the issue at hand. In particular, for simulations of the SOL regions in tokamak devices with fluid codes (like, e.g., SOLPS and EDGE2D [13]) it is necessary to define the boundary conditions at the quasi-neutral plasma edge and not at the wall. Investigations of Kuhn et al. [14] and Jelic et al. [15] indicate that the plasma-sheath boundary can be identified using the concept of the “local polytropic coefficient” $\gamma(x)$, which exhibits a characteristic kink-like behaviour at the transition between the quasi-neutral presheath plasma and the non-neutral sheath. The knowledge of $\gamma$ enables reliable calculation of the ion sound velocity $c_s(x) = \sqrt{(kT_e + \gamma kT_i)/m_i}$. It will be shown here that the place where the ion sound velocity with such calculated ion polytropic coefficient equals the ion fluid velocity is an excellent candidate for defining the plasma-sheath boundary for finite-$\varepsilon$ plasmas.

2 NUMERICAL (PIC) SIMULATION

For PIC (Particle-In-Cell) simulation, we choose to use PIC simulation program BIT1, that has a special feature: in the region of quasi-neutral plasma, it is capable to maintain the electron velocity according to Maxwellian distribution even in the absence of collisions - just like in real experiments.

The initial, i.e., the source velocity distribution of both electrons and ions is Maxwellian. Electrons are born with fixed temperature $T_{e,src} = 1 \text{eV}$, (index “src” means “source temperature”) while the ion initial temperature $T_{i,src}$ is changed in simulations. In our simulations electrons and ions are injected in the simulation domain in pairs randomly distributed over the simulation volume. After a steady state is established electron velocity distribution remains Maxwellian with a cutoff in the tail of velocity distribution. The place of cutoff of electron VDF depends on the local plasma potential. However, this cutoff of the tail does not have serious consequence to the electron temperature which is in the steady state also very close to $1 \text{eV}$. On the contrary, (as will be seen bellow) the final velocity distribution is far from Maxwellian-like in spite of the fact that the ion source distribution is also Maxwellian. In any case, the cutoff is an inherent result of simulation and, unlike the theoretical models where it is usually ignored, it would be even hardly possible to avoid this effect (e.g., for for the purposes of fitting some theoretical models).

Currently available version of BIT1 did not offer the possibility to change ion source profile during simulation - one could define it at the beginning in the form of the input file, but not during simulation. We updated BIT1 and added this possibility in the following manner.

When new electrons are born, their position is selected randomly in source area (which was in our case whole system, from $x = -L/2$ to $x = L/2$). To be able to take into account the shape of the ion source strength profile (which we define as $S_i(x) = e^{\alpha \Phi(x)}$) we calculated sum of all values $L_i$ and we got $L_{total}$ (Eq. [7]). In geometry sense, we calculated area between ion strength profile and line $\Phi(x) = 0$.

$$L_i = e^{\alpha \Phi(i)} \quad \quad \quad \quad L_k = e^{\alpha \Phi(k)} \quad \quad \quad \quad L_{total} = \sum_{i=0}^{N} L_i = \sum_{i=0}^{N} e^{\alpha \Phi(i)}$$

For calculating positions of new particles, we are interested in calculated total length $L_{total}$. We use this value as a domain upper limit from which we selected random positions of new (inserted) electrons. New positions for electron are selected from 0 to $L_{total}$ and that position is used to calculate the cell in which we put new electron in. With this we still use random generator to insert particles and use ion source strength profile to define new position of particles.
The system of our consideration is one-dimensional, plan-parallel spaced between plane electrodes which are perfect particle absorbers (Fig. 1). The distance between electrodes is \( L = 0.03m \) and distance is divided into 8192 cells. Simulations are performed with enhanced and updated BIT1 (Berkeley-Innsbruck-Tbilisy) one dimensional code [16]. The plates at \( x \pm L \) are assumed to be perfectly absorbing and electrically floating. The electrostatic potential \( \Phi(x) \) is assumed to be monotonic decreasing (for \( x > 0 \)) and is defined to be zero at \( x = 0 (\Phi(0) = 0) \).

![Figure 1: The geometry of our system.](image)

3 RESULTS

We performed various simulations with updated version of BIT1 and compare the results with theory, presented in Kos et al. [17] and with current BIT1 version (with \( S_i = \text{const} \)).

First we compare simulation results with theory, developed in Kos et al. [17]. Theoretical potential profile utilize the limit value for \( \varepsilon \): \( \varepsilon = 0 \). With this in mind, theoretical results are valid for plasmas with small values of \( \lambda_D \) and very high densities. Because in PIC simulation \( \varepsilon \) is small, but not 0, density is always limited and can never be as high as in theory.

From Fig. 2 one can observe, that in simulations with higher densities, potential profile is approaching theoretical potential profile. If one would run a simulation with very high density, we can expect that both potential profiles, from theory and from simulation, would coincide. For this, huge computer resources are necessary, or at least some kind of multiprocessor (OpenMP or MPI) version BIT1 that is capable to use multiple threads/processors in clusters. OpenMP version would be used for running simulation on “smaller” crunching machines (machines with multiple processors and multiple cores per processor), MPI version would be used on “big” computing clusters with large number of nodes.

Potential profiles in simulations are not directly “ready” to be displayed and compared in graphs, because on microscopic scale, values can differ a lot and resulting graphs are very “saw”-like (like graph of times on Fig. 3). To get more representative results and to remove those “saw-tooth” structures, we run simulations till they reach steady state. After that we made several simulation steps (\( M \) steps), average results from last \( M \) steps, and display them in the graph to compare them against theoretical results.

Because PIC simulation with \( S_i \approx e^\Phi \) is more demanding regarding computer power/time than \( S_i = \text{const} \), we also compared the simulation times for both versions of ion source strength profile. We measured times required to perform two simulation that were the same in all parameters (initial conditions, temperatures, system geometry and dimensions, etc.) and they differ.

Figure 2: Comparison of potential between PIC simulation and theoretical result for $S_i \approx e^\Phi$

only in ion source strength profiles: one being constant and the others with profile proportional to $\Phi$. Figure 3 shows difference in simulation times. Time stamps were taken every 4096 simulation steps - which is the frequency of writing dump and data files in BIT1.

Although computation of ion source strength values takes some additional time in every time step, we can observe from Fig. 3 that ion source strength profile does not influence much the overall simulation time.

Figure 3: Comparison of simulation times for set of 4096 steps for $S_i = \text{const}$ and $S_i = e^{\Phi(x)}$. 
4 DISCUSSION AND CONCLUSION

Theory and PIC simulation potential profiles shown in this paper show fair agreement. Since the existing theories assume zero $\varepsilon$, it is surprising that our results which inherently are based on finite $\varepsilon$ fit better than expected. Anyway, for higher reliability (despite modern computers and clusters), current and forthcoming PIC simulations are and will still remain very demanding. To be able to compare theory with PIC simulations with high (fusion relevant) plasma densities the speed of PIC simulations should be considerably increased. PIC codes that utilize more that one processor (thread and/or computer) should be used. One of our future tasks would be to enable available PIC codes for such demanding tasks.

The particular result of present manuscript is a comparison of PIC results obtained either for flat ion-source profile or for an arbitrary one, e.g., proportional to the local plasma potential as measured with respect to the plane of symmetry of the physical (and computational) region. In available PIC codes the ion source strength profile is usually hard-coded into program. Namely, it does not change during the simulation (see e.g., Berkeley codes or BIT1) but the ionization profile is fixed in advance. On the contrary, we have build very demanding PIC procedure enabling one to use a temporary ion-source strength profile in each simulation step. Our approach is a rather universal one. However, in the present work we present only some particular results obtained with the ion source strength profiles proportional to potential - $S_i(x) \approx e^{\alpha \Phi(x)}$. Simulations for $\alpha = 1$ are presented and interpreted in the light of recently reported theoretical results of Kos et al. An excellent agreement between results obtained via these two approaches (theoretical and PIC) is well demonstrated in present manuscript.

ACKNOWLEDGMENTS

This work was supported by the European Commission under (i) the Contract of Association between EURATOM and the Austrian Academy of Sciences and (ii) the Contract of Association between The European Atomic Energy Community (EURATOM) and the Ministry of Higher Education, Science and Technology of the Republic of Slovenia No. FU06-CT-2007-00065, and by (iii) the Austrian Science Fund (FWF) under project P19333-N16. It was carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission. Numerical calculations associated with this work were supported by the Austrian Ministry of Science and research (BMWF) as part of the UniInfrastrukturprogramm of the Forschungsplattform Scientific Computing at the Leopold-Franzens Universität (LFU) Innsbruck.

The authors are indebted to Prof. K.-U Riemann and S. Kuhn for their perpetual advising us on various aspects regarding the theoretical issues and D. Tskhakaya jr. for his kind advice regarding optimization of the BIT1 code.

REFERENCES


