Grid-free tree-code simulations of the plasma-material interaction region

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Abstract. A fully kinetic grid-free model based on a Barnes-Hut tree code is used to self-consistently simulate a collisionless plasma bounded by two floating walls. The workhorse for simulating such plasma wall transition layers is currently the PIC method. However, the present grid-free formulation provides a powerful independent tool to test it \cite{Ref1} and to possibly extend particle simulations towards collisional regimes in a more internally consistent way. Here, we use the grid-free massively parallel Barnes-Hut tree-code PEPC - a well established tool for simulations of Laser-plasmas and astrophysical applications - to develop a 3D ab initio plasma target interaction model. With our approach an electrostatic sheath naturally builds up within the first couple of Debye lengths close to the wall rather than being imposed as a prescribed boundary condition.

We verified the code using analytic results \cite{Ref2} as well as 1D PIC simulations \cite{Ref3}. The model was then used to investigate the influence of inclined magnetic fields on the plasma material interface. We used the code to study the correlation between the magnetic field angle and the angular distribution of incident particles.

1. Introduction
A magnetically confined plasma in a fusion device interacts with the surrounding material at the first wall as well as in the divertor region. The degradation of the plasma facing components is significantly influenced by the properties of the plasma particles close to the walls. Erosion rates, for example, depend non-linearly on the energy of bombarding particles so that a detailed knowledge of particle properties is essential.

If a plasma is in contact with a surface, the plasma particles impinge upon this surface and charge it up electrically. Due to the higher mobility, electrons hit the surface first and charge it negatively. Thus, the potential at the wall $\Phi_w$ is negative relative to the plasma potential in the center $\Phi_0 = \Phi(x = 0)$. The potential drop and the associated electric field slow down electrons and decrease the electron flux out of the plasma on the one hand and accelerate ions on the other. If the surface is floating, the electron and ion flux is balanced, resulting in zero net current in equilibrium. Due to Debye shielding, the largest part of the potential drop occurs over the first couple of Debye lengths $\lambda_D$ close to the wall. This area is called electrostatic sheath, collector sheath or sometimes just sheath. The large electrical fields in the sheath have a strong influence on the properties of particles hitting the adjacent wall.
The codes mainly used in plasma-edge-modeling – large scale fluid models – lack the kinetic physics and the resolution necessary to handle the sheath area. Therefore, macroscopic boundary conditions at the walls, or more specifically at the sheath entrance, have to be prescribed for these codes. However, for many realistic configurations, commonly used simple 1D Bohm sheath conditions are not valid. By contrast, a kinetic model of the plasma wall interaction region can describe the sheath region in microscopic detail and with the necessary spatial and temporal resolution. A fully kinetic simulation can possibly provide correct boundary conditions for fluid or gyro-kinetic codes operating on larger spatio-temporal scales.

In kinetic particle simulations, an ensemble of simulation particles is investigated. The particle trajectories are advanced according to the self consistent electric (or more generally electromagnetic) field. In order to compute the electric field for one particle, the contribution to this field from all other particles is needed. Thus, the computation of the self-consistent field requires $O(n^2)$ operations. There are several grid-free as well as grid-based methods used for particle simulations whose common purpose is the reduction of the complexity of the force computation to $O(n \log(n))$ or even further. The Barnes-Hut tree code [4] is one well-established grid-free scheme, the Fast Multipole Method (FMM) [5] is another. On the grid-based side, Particle-In-Cell (PIC) is the most widely used.

The simulation model for the plasma-wall transition area presented here is based on the grid-free Barnes-Hut tree-code PEPC (Pretty Efficient Parallel Coulomb solver)[6]. PEPC has been successfully used for simulations of a variety of systems such as laser-plasma-interactions or gravitational problems [7, 8, 9] and can efficiently make use of modern many processor super computers [7, 10].

The paper is organized as follows. In section 2, the code and the simulated system are described. In section 3 results of simulations with and without an oblique magnetic field are presented. For latter configuration, analytic [2] and numerical [3] results are known and we use those to verify our model. Results for systems with a constant external magnetic field with varied field inclination are also shown. Finally, conclusions are presented in section 4.

2. Model of the plasma-wall transition region
The sketch of the simulated plasma-wall transition region and a typical plasma potential without an external magnetic field is given in Fig. 1. The system is filled with a plasma over the range $-L \leq x \leq L$. A volumetric source emits particles in the source region ($-L_s \leq x \leq -L_c$ and $L_c \leq x \leq L_s$). In between the two parts of the source region ($-L_c < x < L_c$), there is a collisional, source-free plasma where particles may undergo collisions. The region $x > L_s$ and $x < -L_s$ is also source-free. According to Emmert et al [2] the plasma potential is constant for $L_s < x < L_{sc}$ and $-L_{sc} < x < -L_s$. At $x \geq L_{sc}$ and $x \leq -L_{sc}$, we find the electrostatic sheath. It has a width of several Debye lengths. Within the sheath, the strongest electric fields are present. The main part of the total potential drop $\Phi_{sc}$ is localized here.

Most one-dimensional analytic models for the collisionless plasma-wall transition region are based on a kinetic description of the ions and assume that electrons follow a Boltzmann relation (see e.g. [2, 11, 12]). For the desired steady-state solutions the kinetic equation for ions reduces to

$$\frac{\partial}{\partial x} [f(x, E)v(x, E)] = S(x, E),$$  

(1)

with $x$ the position, $E = 1/2mv^2 + q\Phi(x)$ the total Energy, $v$ the ion velocity, $f(x, E)$ the ion distribution function and $S(x, E)$ the ion source function. The total ion Energy $E$ is taken to be a constant of motion. The density is obtained by integrating $S(x, E)/v(x, E)$ over the $(x, E)$ phase space. Inserting the particle densities in the Poisson-equation gives an integro-differential equation for the potential that, in general, has to be solved numerically.
The used source velocity distribution along the magnetic field is the same as used by Emmert et al. [2] and can be written as

\[
S(x, v_\parallel) = S_0 h(x) \left( \frac{m_\parallel v_\parallel}{kT_0} \right) \exp \left( \frac{-m_\parallel v_\parallel^2}{2kT_0} \right). \tag{2}
\]

\(S_0\) is the source strength, \(h(x)\) is a given spatial source profile, which is a constant inside the source region in our case and \(T_0\) is the ion source temperature. This type of source function is applicable, if the plasma has a non-drifting Maxwellian velocity distribution far from the wall[12].

The collisional, source-free region in the system center plays a major role in the present particle simulations. In a collisionless system there is no mechanism to refill the high energetic tail of the electron distribution function that is depopulated due to the loss of these electrons at the walls. A mechanism to achieve the necessary repopulation has to be added to the simulation model. In our model, the collisional region is condensed to a plane at \(x = 0\). Electrons that cross this plane are rethermalized. That is, their velocity in \(x\)-direction is resampled according to (2).

To simulate the described system, a specially adapted version of the PEPC code is used. Starting with an empty system, a constant number of electrons and ions per time-step is inserted. Particles hitting the walls are removed from the system and their charge is added to the total charge of the wall. When a steady-state is reached, the particle influx from the source is balanced by an equal particle outflux towards the walls.

For all simulations, the ion to electron mass ratio is set to \(\mu = m_i/m_e = 100\) and temperature ratio is \(\tau = T_i/T_e = 1\). The artificially low mass ratio reduces the ratio of the ion Lamor radius

\[
r_L = \frac{m_i v_{\perp}}{q_i B} \tag{3}
\]

to the Debye length \(\lambda_D\) as well as the ion traversal time

\[
t_{\text{trav},i} = \frac{L}{\sqrt{kT_i/m_i}}. \tag{4}
\]

t_{\text{trav},i} is proportional to the time that is needed until the system reaches steady state. Thus, a lower ion to electron mass ratio reduces the simulation time. It also influences the particle
Figure 2. Potential (a) and density (b) profiles along the x-axis for \( x \geq 0 \). The end of the source region is indicated by the dashed black lines.

fluxes as well as the potential drop and has to be considered when transferring the simulation results to experimental plasmas. The super-particle factor \( f_{sup} \), the factor that describes the ratio of simulation particle mass (charge) and the particle mass (charge) is set to \( f_{sup} = 400 \). The electron and ion source temperature is set to \( kT_{e0} = kT_{i0} = 10 \text{ eV} \), the magnetic field to \( B = 0.33 \text{ T} \). The system size is \( 2L_x \times 2L_y \times 2L_z = 12 \text{ mm} \times 1 \text{ mm} \times 1 \text{ mm} \). We use periodic boundary conditions in \( y \) and \( z \) direction. With the resulting densities and the electron source temperature we get \( \lambda_D = 4.7 \times 10^{-5} \text{ m} \) for the Debye length \( \lambda_D \) and thus \( L_x \approx 125\lambda_D \) for all simulations. The equilibrium particle numbers are approximately \( N_I \gtrsim N_e \approx 7 \times 10^6 \).

3. Modeling results

**Code verification.** To verify the developed code, we can relate to analytic [2] as well as numerical results [3]. Both are one dimensional and do not take a magnetic field into account. However, if the magnetic field is perpendicular to the wall, it does not alter the plasma properties because parallel transport is not influenced by the magnetic field.

The potential and density profile of a simulated plasma are shown in figure 2. Both profiles show a drop within the source region. The ions are accelerated due to the potential drop and satisfy the Bohm criterion at the end of the source region. Within the source-free section the profiles are almost flat. There is a small remaining potential drop. The chosen super-particle factor \( f_{sup} > 1 \) leads to an exaggerated collisionality within the simulated plasma and the collisions cause the slight slope of the potential profile in the source-free region. We need to further investigate the exact relations between this effect and the mentioned parameter. However, for the chosen configuration, the effect is very small. To take the potential drop in this region into account, we define the source potential drop between the center of the system (\( x = 0 \)) and the center of the source-free region (\( x = 0.0035 \text{ m} \)) instead of the source exit. For the source potential drop we find \( \Phi_I = (0.39 \pm 0.01) e/(kT_e) \). The larger part of the total potential \( \Phi_w \) drop is located in the sheath close to the wall. While the main plasma is quasi-neutral in the source region as well as in the source free region, ion and electron densities differ in the sheath region. On the scale of several Debye lengths a positive space charge shields the plasma from the negative wall. The total potential drop in our simulation, \( \Phi_w = (1.59 \pm 0.01) e/(kT_e) \), is...
Figure 3. Potential profile (a) along the x-axis for \( x \geq 0 \) for a plasma with a perpendicular magnetic field and with 30° inclination. The graph on the right (b) shows the space charge of the plasma for both cases.

in agreement with \( \Phi_w = (1.575 \pm 0.011) e/(kT_e) \), the value in table I from [3]. The grid-free model as well as the PIC model both yield a potential drop which is higher than the value from analytic theory [2] which is \( \Phi_w = 1.51 e/(kT_e) \). In the analytic solution leading to this value, the assumption that the electrons follow a Boltzmann relation is made. This requires high electron-electron collisionality and implies the assumption \( m_I \gg m_e \) which is not the case for both simulations, where \( m_I = 100 m_e \). In addition, rethermalization only takes place at \( x = 0 \) in the simulation, so that the electron velocity distribution is not Maxwellian for all \( x \). Thus, a small difference was to be expected.

**Oblique magnetic fields** Next, we study a case with a magnetic field with varying inclination angle \( \alpha \). We change the inclination angle from \( \alpha = 90^\circ \) to \( \alpha = 30^\circ \) in 15° steps. The basic structure of the potential of a plasma-wall transition area with an oblique magnetic field was first shown by Chodura in 1982 [14]. Adjacent to the electrostatic sheath region a potential drop on the length scale of the ion Larmor radius \( r_L \) develops. This area is the so-called magnetic pre-sheath. While the total potential drop only changes weakly with the angle \( \alpha \), the ratio of the sheath and pre-sheath potential drop changes more significantly.

Figure 3 a) shows the potential profiles of a case with a perpendicular magnetic field and a case with an inclination of 30°. The potential drop in the source region is slightly larger for the case with inclined magnetic field. Within the source free region the potential of the case with inclined magnetic field starts to decrease a few \( r_L \) from the wall, while the potential of the 90° case drops a few \( \lambda_D \) from the wall. Figure 3 b) shows the difference of the ion and electron density for both cases. For both cases, quasi-neutrality holds throughout the whole plasma except for the electrostatic sheath close to the wall. Thus, the potential of the plasma with inclined magnetic field starts to decrease within the quasi-neutral plasma. The total potential drop in the 30° case is a little larger, but similar. This agrees with the results in [14]. Chodura simulated the plasma from a plasma interface at one end of the simulation domain to the wall at the other end. To ensure a smooth transition at the plasma interface, he uses the boundary condition

\[
v_{ix0} \geq C_s \sin \alpha, \quad C_s = \sqrt{\frac{\gamma_i T_i + \gamma_e T_e}{m_i}},
\]
Figure 4. Ion velocity profiles along the x-axis for $x \geq 0$ for a plasma with perpendicular magnetic field (a) and $30^\circ$ inclination angle (b). For the computation of the ion sound speed $C_s$ the parameters $\gamma_i = 2$, $\gamma_e = 1$ are used.

where $v_{ix0}$ is the ion flow velocity of the instreaming ions in x direction and $C_s$ is the ion sound speed. This condition is equivalent to the condition $v_{ix0} \geq C_s$.

\begin{equation}
 v_{ix0} \geq C_s.
\end{equation}

In the present work, we simulate a plasma that has a stagnation point in the center, and the self-consistently computed electric field within the source region accelerates the plasma so that it meets Chodura’s boundary condition right outside of the source region as a result, rather than as a boundary condition. This can be seen in figure 4 for the $90^\circ$ case as well as for the $30^\circ$ case. Figure 4 b) also shows, that in addition to the aforementioned condition, the inequality $v_{ix0} \geq C_s$, the Bohm criterion, is fulfilled at the entrance of the electrostatic sheath. Figure 5 a) shows the plasma potential at different positions in the plasma. The position $x_1$ is localized in the center of the source free region. As expected, the potential $\Phi_1$ does only depend weakly on $\alpha$. The potential at the wall $\Phi_w$ changes slightly more with the magnetic field angle $\alpha$, but the variation is still small, as stated before. At the intermediate point $x_3$ though the changes of the potential $\Phi_3$ are stronger. $x_3$ is located directly at the entrance of the sheath region. The potential there is significantly influenced by $\alpha$ because of the magnetic pre-sheath adjacent to the electrostatic sheath.

The average energy of particles hitting the wall shown in figure 5 b) depends on the total potential drop $\Phi_w$. Thus, the variation of the energy is also small. The ion energy $E_i$ grows with decreasing $\alpha$ and increasing $\Phi_w$. The electron energy changes inversely and its variation is even smaller.

The variation of the average angle of incidence $\beta_{i/e}$ is also shown in figure 5 b). While the changes are small for $\alpha = 90^\circ, 75^\circ$ and $60^\circ$ they grow with shallower angles, especially for ions. For large magnetic field angels $\alpha$ the ion velocity in x-direction is larger than that in the yz-plane due to the acceleration by the electric field in the electrostatic sheath. This leads to larger angles of incidence ($\beta = 90^\circ$ is a perpendicular hit with $v_x \gg v_y, v_z$). With shallower angles, the velocity in the $y$-direction grows. Thus, the angle of incidence gets smaller. The angle of the electrons does not vary that strongly. It is also closer to $\beta = 45^\circ$ which indicates a more isotropic velocity distribution.
Figure 5. a) Potential relative to $\Phi_0$ at different distances $\Delta x = x - L$ from the surface. These are $\Delta x_1 = -62.8\lambda_D = -13.1r_L$, $\Delta x_2 = -16.6\lambda_D = -3.5r_L$, $\Delta x_3 = -5.25\lambda_D = -1.1r_L$, $\Delta x_4 = -1.47\lambda_D = -0.3r_L$. $\Phi_w$ is measured directly at the wall. b) Average particle energy and angle of incidence of particles hitting the surface.

4. Conclusions
We successfully established a grid-free simulation model based on the parallel Barnes-Hut tree-code PEPC. Using this tool, we simulated an almost collisionless plasma-wall transition region with and without an oblique magnetic field. The results of the cases with a perpendicular magnetic field are in agreement with an analytic solution as well as with PIC simulations, validating the applicability of the grid-free method for simulations of the plasma-wall interaction zone.

The results for plasmas with oblique magnetic field also confirm PIC results. We furthermore computed the ‘boundary conditions’ at the pre-sheath entrance self-consistently and these turn out to be consistent with assumptions made in the original work on the magnetic pre-sheath.

The remaining slope of the potential profiles in the source free region indicates that collisions alter the simulated systems, which would not be expected due to the used plasma parameters. Further research on this effect and its connection to numerical parameters and particle resolution has to be conducted.

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