A coupled PIC-Poisson-solver code for the extraction of charged particles from a negative ion source

F. Sattin$^1$, A. Tanga$^2$, M. Cavenago$^3$, V. Antoni$^1$

$^1$Consorzio RFX, Associazione Euratom-ENEA per la fusione, Corso Stati Uniti 4, 35127 Padova, Italy;
$^2$Max-Planck-Institut für PlasmaPhysik, Boltzmannstrasse 2, 85748 Garching, Germany;
$^3$INFN-LNL, viale dell’Università, 35020 Legnaro (PD), Italy

Neutral beams from negative ion sources are expected to be one of the heating techniques chosen for ITER. The numerical simulation of the production and extraction mechanisms of negative hydrogen ions is necessary for the optimization of the source efficiency and as basis for the ion optics. Numerically, the problem is that of solving the equations of motion for a large set of charged particles moving within an electric field that is partially imposed by the outside (extraction potential) and partially generated by the charges themselves. All is supplemented by non-trivial boundary conditions. The extraction region is very often virtually identified with the sheath or pre-sheath region [1]. In sources designed to deliver high-intensity beams, however, the Debye length shrinks to such a small value that the sheath region is invisible to investigation. The dynamics of the extraction occurs over spatial lengths much larger than that, due both to high density and to large extraction potentials: in BATMAN source, the electron Debye length is $\lambda_D \approx 10^{-5}$ m. Length scales thought to be relevant for extraction (e.g., extraction holes’ diameters, distances between electrodes, …) are instead of several mm’s. The region of interest for this work is the one around the grids: there are three of them in cascade, namely Plasma Grid, Extraction Grid, Acceleration Grid. They are separated by a few mm’s, and among them extraction potentials of some kV may be applied. Particles are extracted through holes of about 1 cm of diameter.

FIG. 1. Basic cell for computations. The black rectangles stand for the Plasma Grid, with the Extraction Hole in between. Above them, there is the confined plasma, and below the Extraction Region. The bottom of the figure stands for the Extraction Grid; the top for the “plasma boundary” (whose precise meaning is to be better explained later). The geometric sizes $L_x$ (width of the cell), $L_G$ (diameter of the hole), $d$ (thickness of the Plasma Grid), $L_{y1}$ (distance between Plasma Grid and Extraction Grid) are all geometric parameters known in advance of the computation. $L_{y2}$, instead, will be determined later.

An enlarged view of the basic 2-dimensional unit cell composing the grid is considered in Fig. (1). Uniformity is assumed along the third direction: holes in the
grid, actually, do have circular shape. One must imagine a periodic array of these basic cells extending along x-axis.

A simplified model for plasma dynamics will be considered, neglecting particle-particle collisions (including ionization and recombination). Also, particle-surface collisions will just lead to absorption of the particle. A confining magnetic field (magnetic filter) is explicitly included. Actual magnetic filters have a complicated pattern, however, we just limit to a constant magnitude field, directed along z-axis.

Finally, three-components-plasmas will be considered: electrons, protons, and negative Hydrogen ions. The calculation performs iteratively, solving the Poisson equation at each iteration $k$

$$\nabla^2 \phi^{(k)} = - \frac{e}{\varepsilon_0} \delta n^{(k-1)}, \quad k > 0$$  \hspace{1cm} (1)

where $e \delta n = e (n_p - n_e - n_i)$ is the local charge density imbalance between electrons ($n_e$), protons ($n_p$) and negative ions ($n_i$), assumed known from the previous step $k-1$.

Particle orbits are determined by solving a set of $N$ equations of motion:

$$m_i \frac{d\mathbf{v}_i^{(k)}}{dt} = q_i (\mathbf{E}^{(k)} + \mathbf{v}_i^{(k)} \times \mathbf{B}) \quad , \quad i = 1, ..., N$$  \hspace{1cm} (2)

for each of the $N$ particles composing the plasma. The magnetic field $\mathbf{B}$ is generated by magnets located in the source. The electric field $\mathbf{E}^{(k)} = - \nabla \phi^{(k)}$ comes from equation (1). The charge density is proportional to the average time spent by the $N$ test particles into each cell of the numerical grid spanning the whole extraction region. The normalization constant, in physical units, is then obtained by imposing that, well inside the plasma, the density be equal to the pre-assigned plasma density $n_p$.

Equation (1) must be supplemented by boundary conditions for $\phi$, as well as by an initial guess for $\delta n^{(0)}$: $\delta n^{(0)} \equiv 0$ everywhere. Boundary conditions used are sketched in Fig. (1). Plasma Grid is chosen as the ground: $\phi_{PG} \equiv 0$. Extraction Grid is set to the value of the extraction potential: $\phi_{EG} \equiv \phi^{(ext)}$. Because of periodic conditions, the left- and right-hand boundary must fulfil $\nabla_n \phi = 0$, where $\nabla_n$ is the normal derivative to the boundary: $\nabla_n \equiv \partial_x$. The upper boundary is chosen deeply enough inside the plasma, that the externally applied electric field be completely shielded. In actual computations $\partial_y \phi = 0$ as the boundary condition was used. The $x$-derivative, of course, is not exactly zero because of the perturbing effect over the spatial uniformity exerted by the hole. However, by increasing the distance from the Plasma Grid (i.e., larger $L_y$), this lack of uniformity may be reduced as much as one wishes. The plasma potential is recovered from the solution of Eq. (1): $\phi_{Plasma} \equiv \phi(y = L_y1 + d + L_y2)$. Electrons and protons were placed uniformly along $x$ on top of the cell, $y = L_y1 + d + L_y2$, with velocity $U$ directed along the negative $y$ direction. Negative ions, instead, are generated very close to the grid.

A first test run is shown in Fig. (2). Parameters were: core plasma density $n_p = 10^{17}$ m$^{-3}$, extraction potential $\phi^{(ext)} = 10$ kV. Magnetic field is absent and no negative ions were considered. Geometric parameters are: $L_y1 = 4.5$ mm, $L_x = 21$ mm, $L_G = 14$ mm, $d = 2$ mm. The Grid-plasma distance $L_y2$ was set to $L_y2 = 40$ mm. The kinetic energy of the particles was taken equal to the plasma potential at the plasma boundary. $L_y2$ may be given the meaning of extraction depth: the typical scale length over which the plasma goes from its core value ($n_p$) to edge value (about zero). This value may be estimated by direct measurements in actual sources. The extraction depth, for high applied potentials (i.e., some kV) is, actually, a few centimeters [2], providing a (qualitative) confirmation to our model.
One finds that the solution of Eq. (1) depends upon the adimensional parameter 
\[ \frac{e}{\varepsilon_0}(L^2 n_p / \phi^{\text{ext}}) , \]
where \( L \) is a typical size of the system; hence only upon the ratio \( r = n_p / \phi^{\text{ext}} \), if the geometry of the source is left untouched. In Fig. (2) one is exploring the case \( r \approx 0 \): the starting guess is expected to be the closer to the true solution, the smaller the ratio \( r \).

The magnetic filter is now added: a constant field of magnitude \( |B| = 50 \) Gauss along the \( z \)-axis. The presence of the magnetic field introduces a new length scale: the Larmor radius \( \rho_L \). Fig. (3) displays electrons’ trajectories for this system. The initial kinetic energy of the electrons is chosen small, so that \( \rho_L / L < 1 \). Recall that particles are collisionless, hence there are not mechanisms available to shift them from their starting position more than one \( \rho_L \) along the \( y \) direction.

For each energy there is a threshold field \( B_0 \), above which electrons are perfectly confined. It is easy to relate this field with electron energy \( U \) and with initial electron location: the initial electron-grid distance \( L \) must be larger than Larmor radius \( \rho \): \[ L = \rho \to B_0 \propto U^{1/2} . \] This scaling was verified numerically. Even in the zero-magnetic-field situation, the fraction of escaping electrons decreases when increasing \( U \), albeit slightly. The reason is that, the greater its velocity, the lesser the electron remains stucked to electric field line. Hence, a fraction of the electrons collide with the grid even though no field line is actually intersecting it.

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**FIG. 2.** Top-left: starting potential \( \phi^{(1)} \); top-right: electron trajectories; bottom-left: proton trajectories; bottom-right: first-iterate potential \( \phi^{(2)} \). Geometric, plasma and external potential parameters are given in the main text. For this set of parameters, the contour plots for \( \phi^{(1)}, \phi^{(2)} \) do appear almost identical.

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**FIG. 3.** Top-left: starting potential \( \phi^{(1)} \); top-right: electron trajectories; bottom-left: proton trajectories; bottom-right: first-iterate potential \( \phi^{(2)} \). Geometric, plasma and external potential parameters are given in the main text. Magnetic field is added. Electrons are effectively shielded above \( y = 8 \) by magnetic filter.
Negative ions represent eventually the main subject of this work. Fig. (4) displays H trajectories under conditions that should be representative of different generation mechanisms. In all cases, negative ions were very small in number, hence they act as test particles and do not appreciably perturb the potential profile. (It is known not to be true in all experimental situations). In two cases, particles with zero kinetic energy are initialized on the surface of the Plasma Grid. This is a simplified scheme for pure surface production. In the other case, instead, particles are still initialized at a small distance from the Plasma Grid, but allowing them to be generated even in correspondence of the hole, in an attempt of simulating of volume production. The true dominating production mechanism is still a matter of debate, and is likely to be a mixture of the two, with relative weights that may change from one source to another. There is not, hence, evidence to favour one over the other. It is remarkable, however, that the present results hint that surface production should be very sensitive to geometric details of plasma grid, since only ions generated very close to the hole have some chance to escape.

It is remarkable that, within the limitations of this code, extraction from the plasma of negative ions generated on the grid’s inner surface is very effectively suppressed. The reason is that, just on the grid, the electric field is such to accelerate a negatively charged particle right into the plasma. A larger initial velocity or larger electric field corresponds just to accelerating faster the particle, without altering its direction. (This statement was checked against actual simulations).

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