BOLOS Handbook

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1 Two-term approximation

This section is a summary of chapter 2 from Raimbault [2018]. Starting from Boltzmann's equation:

$$\frac{\partial f}{\partial t} + \mathrm{v} \cdot \frac{\partial f}{\partial \mathrm{r}} + \mathrm{a} \cdot \frac{\partial f}{\partial \mathrm{v}} = \left(\frac{\delta f}{\delta t}\right)_c \tag{1}$$

Assuming a two-term expansion (isotropic and anisotropic part):

$$f(\mathrm{r}, \mathrm{v}, t) = f_0(\mathrm{r}, v, t) + \frac{\mathrm{v}}{v} \cdot \mathrm{f}_1(\mathrm{r}, v, t) \tag{2}$$

Reinjecting and integrating over the solid angle the first and second moments of Boltzmann's equation yields:

$$\frac{\partial f_0}{\partial t} + \nabla_r \cdot \left(\frac{v}{3}\mathrm{f}_1\right) - \frac{1}{v^2}\frac{\partial}{\partial v}\left(v^2 \frac{e\mathrm{E}}{3m}\mathrm{f}_1\right) = \left(\frac{\delta f_0}{\delta t}\right)_c \tag{3}$$

$$\frac{\partial \mathbf{f}_1}{\partial t} + \nabla_{\mathbf{r}}\left(v f_0\right) - \frac{\partial}{\partial v}\left(\frac{e\mathbf{E}}{m} f_0\right) = \left(\frac{\delta \mathbf{f}_1}{\delta t}\right)_c \tag{4}$$

Assuming Boltzmann's form of the collision term:

$$\left(\frac{\delta \mathrm{f}_1}{\delta t}\right)_c^{\mathrm{cl}} = -\nu_m\left(v_e\right)\mathrm{f}_1\left(\mathrm{r}, v_e, t\right) \tag{5}$$

$$\left(\frac{\delta f_0}{\delta t}\right)_c^{\mathrm{cl}} = \frac{m}{M}\frac{1}{v_c^2}\frac{\partial}{\partial v_e}\left[v_e^2 \nu_m\left(v_e\right)\left(v_e f_0 + \frac{kT_n}{m}\frac{\partial f_0}{\partial v_c}\right)\right] \tag{6}$$

$$\left(\frac{\delta f_0}{\delta t}\right)_c^{\mathrm{exc}} = \frac{v_e'}{v_e}\nu_{exc}\left(v_e'\right) f_0\left(\mathrm{r}, v_e', t\right) - \nu_{\mathrm{exc}}\left(v_e\right) f_0\left(\mathrm{r}, v_e, t\right) \tag{7}$$

$$\left(\frac{\delta f_0}{\delta t}\right)_c^{\mathrm{ion}} = 4\frac{v_e'}{v_e}\nu_{\mathrm{ion}}\left(v_e'\right) f_0\left(\mathrm{r}, v_e', t\right) - \nu_{\mathrm{ion}}\left(v_e\right) f_0\left(\mathbf{r}, v_e, t\right) \tag{8}$$

2 BOLSIG+

The approximations made to solve the electron distribution function in the form of the electron energy distribution function (EEDF) in Hagelaar and Pitchford [2005] are presented in this part.

2.1 Two-term approximation

The electric field and the collision terms are uniform, the anisotropic part of the distribution function is directed along the electric field. Performing a change of variable to go to electron volt energy space:

$$\begin{aligned}
&\mathbf{E} = E\mathbf{e}_z, \quad \mathbf{f}_1 = f_1\mathbf{e}_z \\
&\epsilon = \frac{1}{2}mv^2/e = \left(\frac{v}{\gamma}\right)^2 \quad \text{with} \quad \gamma = \frac{2e}{m_e} \\
&f(v, \cos\theta, z, t) = f_0(v, z, t) + f_1(v, z, t)\cos\theta
\end{aligned}$$

Equations for f_0 and f_1 are:

$$\frac{\partial f_0}{\partial t} + \frac{\gamma}{3}\varepsilon^{1/2}\frac{\partial f_1}{\partial z} - \frac{\gamma}{3}\varepsilon^{-1/2}\frac{\partial}{\partial \varepsilon}\left(\varepsilon E f_1\right) = C_0 \tag{9}$$

$$\frac{\partial f_1}{\partial t} + \gamma\varepsilon^{1/2}\frac{\partial f_0}{\partial z} - E\gamma\varepsilon^{1/2}\frac{\partial f_0}{\partial \varepsilon} = -N\sigma_{\mathrm{m}}\gamma\varepsilon^{1/2}f_1 \tag{10}$$

Decoupling energy and time/space dependances:

$$f_{0,1}(\varepsilon, z, t) = \frac{1}{2\pi\gamma^3}F_{0,1}(\varepsilon)n(z, t) \tag{11}$$

where the energy distribution F_0 is normalized as:

$$\int_0^\infty \varepsilon^{1/2}F_0 \mathrm{d}\varepsilon = 1 \tag{12}$$

2.2 Growth of the electron density

Three different assumptions can be made regarding the dependence of the electron density. In all cases the Eq.9 reduces to:

$$-\frac{\gamma}{3}\frac{\partial}{\partial \varepsilon}\left(\left(\frac{E}{N}\right)^2\frac{\varepsilon}{\tilde{\sigma}_{\mathrm{m}}}\frac{\partial F_0}{\partial \varepsilon}\right) = \tilde{C}_0 + \tilde{R} \tag{13}$$

$\tilde{R}$ is the growth-renormalization term, it ensures that F_0 remain normalized in the case of net electron production.

2.2.1 No growth model

The electron density is supposed to be independent of time and space.

$$\tilde{\sigma}_{\mathrm{m}} = \sigma_{\mathrm{m}} \quad \text{and} \quad \tilde{R} = 0 \tag{14}$$

2.2.2 Temporal growth

The electron density is supposed to be independent of space.

$$\tilde{\sigma}_{\mathrm{m}} = \sigma_{\mathrm{m}} + \frac{\bar{\nu}_i}{N\gamma\varepsilon^{1/2}} \quad \text{with} \quad \frac{1}{n_{\mathrm{e}}}\frac{\partial n_{\mathrm{e}}}{\partial t} = \bar{\nu}_i \tag{15}$$

$$\tilde{R} = -\frac{\bar{\nu}_i}{N}\varepsilon^{1/2}F_0 \tag{16}$$

2.2.3 Spatial growth

The electron density is supposed to be independent of time.

$$\tilde{R} = \frac{\alpha}{N}\frac{\gamma}{3}\left[\frac{\varepsilon}{\sigma_{\mathrm{m}}}\left(2\frac{E}{N}\frac{\partial F_0}{\partial\varepsilon} + \frac{\alpha}{N}F_0\right) + \frac{E}{N}F_0\frac{\partial}{\partial\varepsilon}\left(\frac{\varepsilon}{\sigma_{\mathrm{m}}}\right)\right] \quad \text{with} \quad \alpha \equiv -\frac{1}{n}\frac{\partial n}{\partial z} = -\frac{\bar{\nu}_i}{w} \tag{17}$$

$$\tilde{\sigma}_{\mathrm{m}} = \sigma_{\mathrm{m}} \tag{18}$$

2.3 Collision terms

The collisions are seperated between between neutral-electron and coulomb collisions:

$$\tilde{C}_0 = \sum_k \tilde{C}_{0,k} + \tilde{C}_{0,e} \tag{19}$$

2.3.1 Elastic collisions

$$\tilde{C}_{0,k=\text{ elastic}} = \gamma x_k \frac{2m}{M_k}\frac{\partial}{\partial\varepsilon}\left[\varepsilon^2\sigma_k\left(F_0 + \frac{k_{\mathrm{B}}T}{e}\frac{\partial F_0}{\partial\varepsilon}\right)\right] \tag{20}$$

2.3.2 Inelastic collisions

$$\begin{aligned}\tilde{C}_{0,k=\text{ inelastic}} &= -\gamma x_k\left[\varepsilon\sigma_k(\varepsilon)F_0(\varepsilon)\right. \\ &\quad \left. -\left(\varepsilon+u_k\right)\sigma_k\left(\varepsilon+u_k\right)F_0\left(\varepsilon+u_k\right)\right]\end{aligned} \tag{21}$$

$$\begin{aligned}\tilde{C}_{0,k=\text{ ionization}} &= -\gamma x_k\left[\varepsilon\sigma_k(\varepsilon)F_0(\varepsilon)\right. \\ &\quad \left. -2\left(2\varepsilon+u_k\right)\sigma_k\left(2\varepsilon+u_k\right)F_0\left(2\varepsilon+u_k\right)\right]\end{aligned} \tag{22}$$

$$\tilde{C}_{0,k=\text{ attachment}} = -\gamma x_k\varepsilon\sigma_k(\varepsilon)F_0(\varepsilon) \tag{23}$$

2.3.3 Electron-electron collisions

$$\tilde{C}_{0,e} = a\frac{n}{N}\frac{\partial}{\partial\varepsilon}\left[3A_1F_0 + 2\left(A_2 + \varepsilon^{3/2}A_3\right)\frac{\partial F_0}{\partial\varepsilon}\right] \tag{24}$$

2.4 Equation for the EEDF

$$\frac{\partial}{\partial\varepsilon}\left(\tilde{W}F_0 - \tilde{D}\frac{\partial F_0}{\partial\varepsilon}\right) = \tilde{S} + \tilde{R} \tag{25}$$

where

$$\begin{aligned}
\tilde{W} &= -\gamma\varepsilon^2\sigma_\varepsilon - 3a\frac{n}{N}A_1 \\
\tilde{D} &= \frac{\gamma}{3}\left(\frac{E}{N}\right)^2\frac{\varepsilon}{\tilde{\sigma}_\mathrm{m}} + \frac{\gamma k_\mathrm{B}T}{e}\varepsilon^2\sigma_\varepsilon + 2a\frac{n}{N}\left(A_2 + \varepsilon^{3/2}A_3\right) \\
\sigma_\varepsilon &= \sum_{k=\text{elastic}}\frac{2m}{M_k}x_k\sigma_k \\
\tilde{S} &= \sum_{k=\text{inelastic}}\tilde{C}_{0,k}
\end{aligned}$$

3 Resolution

3.1 Discretization

The energy space is discretized on a grid in energy space, consisting of n cells of energy ϵ_i with boundaries $\epsilon_{i-1/2}$ and $\epsilon_{i+1/2}$. Integrating the equation for the EEDF yields:

$$\left[\tilde{W}F_0 - \tilde{D}\frac{\partial F_0}{\partial\varepsilon}\right]_{i+1/2} - \left[\tilde{W}F_0 - \tilde{D}\frac{\partial F_0}{\partial\varepsilon}\right]_{i-1/2} = \int_{\epsilon_{i-1/2}}^{\epsilon_{i+1/2}}\tilde{S}d\epsilon + \int_{\epsilon_{i-1/2}}^{\epsilon_{i+1/2}}\tilde{R}d\epsilon \tag{26}$$

3.1.1 Convective-diffusive flux

A Scharfetter-Gummel scheme is used to calculate the convective-diffusive flux:

$$\left[\tilde{W}F_0 - \tilde{D}\frac{\partial F_0}{\partial\varepsilon}\right]_{i+1/2} = \frac{\tilde{W}_{i+1/2}F_{0,i}}{1-\exp\left[-z_{i+1/2}\right]} + \frac{\tilde{W}_{i+1/2}F_{0,i+1}}{1-\exp\left[z_{i+1/2}\right]} \tag{27}$$

Defining the coefficients b_i and c_i:

$$b_i = \frac{\tilde{W}_{i+1/2}}{1-\exp\left[-z_{i+1/2}\right]} \tag{28}$$

$$c_i = \frac{\tilde{W}_{i+1/2}}{1-\exp\left[z_{i+1/2}\right]} \tag{29}$$

the left hand side of Eq. 26 yields:

$$\left[\tilde{W}F_0 - \tilde{D}\frac{\partial F_0}{\partial\varepsilon}\right]_{i-1/2}^{i+1/2} = -b_{i-1}F_{0,i-1} + (b_i - c_{i-1})F_{0,i} + c_iF_{0,i+1} \quad \text{for } i \in [\![2, n-1]\!] \tag{30}$$

We suppose that there is no flux in energy space at zero energy. A zero flux, equal flux or mean flux condition can be applied at the other boundary.

The matrix $SG(F_0)$ representing this flux is tri-diagonal:

$$\begin{pmatrix} b_1 & c_1 & & & \\ -b_1 & b_2 - c_1 & c_1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & c_{n-1} \\ & & & a_{n-1} & a_n \end{pmatrix} \tag{31}$$

3.1.2 Inelastic collisions

The inelastic collision terms are non-local in energy but linear in F_0. We discretize as follows:

$$\int_{\varepsilon_{i-1/2}}^{\varepsilon_{i+1/2}} \tilde{S} \mathrm{d}\varepsilon \equiv -P_i F_{0,i} + \sum_j Q_{i,j} F_{0,j} \tag{32}$$

where the two terms represent scattering-in and scattering-out terms:

$$P_i = \sum_{\text{inelastic}} \gamma x_k \int_{\varepsilon_{i-1/2}}^{\varepsilon_{i+1/2}} \varepsilon \sigma_k \exp\left[\left(\varepsilon_i - \varepsilon\right) g_i\right] \mathrm{d}\varepsilon \tag{33}$$

$$Q_{i,j} = \sum_{\text{inelastic}} \gamma x_k \int_{\varepsilon_1}^{\varepsilon_2} \varepsilon \sigma_k \exp\left[\left(\varepsilon_i - \varepsilon\right) g_i\right] \mathrm{d}\varepsilon \tag{34}$$

where the interval $[\epsilon_1, \epsilon_2]$ is the overlap of cell j and cell i shifted by the threshold energy u_k:

$$\varepsilon_1 = \min\left(\max\left(\varepsilon_{i-1/2} + u_k, \varepsilon_{j-1/2}\right), \varepsilon_{j+1/2}\right) \tag{35}$$

$$\varepsilon_2 = \min\left(\max\left(\varepsilon_{i+1/2} + u_k, \varepsilon_{j-1/2}\right), \varepsilon_{j+1/2}\right) \tag{36}$$

Finally we assume the distribution F_0 to be piecewise exponential (as is the case with the Gaussian distribution) so that

$$g_i = \frac{1}{\varepsilon_{i+1} - \varepsilon_{i-1}} \ln\left(\frac{F_{0,i+1}}{F_{0,i-1}}\right) \tag{37}$$

The matrix associated with this term is denoted $Q(F_0)$.

3.1.3 Incorporation of the growth term

The EEDF satisfies the following linear system:

$$A(F_0)F_0 = Q(F_0)F_0 \tag{38}$$

There is nothing more to be done in the case of no growth model and $A(F_0) = SG(F_0)$. For the temporal growth model:

$$\tilde{R} = -\frac{\bar{\nu}_i}{N} \varepsilon^{1/2} F_0 \tag{39}$$

Assuming a constant value of the EEDF within the cell:

$$\int_{\epsilon_{i-1/2}}^{\epsilon_{i+1/2}} \tilde{R} d\epsilon = -\frac{\bar{\nu}_i}{N} \left[\frac{2}{3} \epsilon^{3/2} \right]_{i-1/2}^{i+1/2} F_{0,i} = G_i F_{0,i} \tag{40}$$

For the spatial growth model we rewrite the growth renormalization term:

$$\begin{aligned} \tilde{R} &= \frac{\alpha}{N} \frac{\gamma}{3} \left[\frac{\varepsilon}{\sigma_\mathrm{m}} \left(2 \frac{E}{N} \frac{\partial F_0}{\partial \varepsilon} + \frac{\alpha}{N} F_0 \right) + \frac{E}{N} F_0 \frac{\partial}{\partial \varepsilon} \left(\frac{\varepsilon}{\sigma_\mathrm{m}} \right) \right] \\ \implies \tilde{R} &= \frac{\alpha}{N} \frac{\gamma}{3} \left[2 \frac{E}{N} \frac{\partial}{\partial \varepsilon} \left(\frac{\varepsilon}{\sigma_\mathrm{m}} F_0 \right) + \frac{\varepsilon}{\sigma_\mathrm{m}} \frac{\alpha}{N} F_0 - \frac{E}{N} F_0 \frac{\partial}{\partial \varepsilon} \left(\frac{\varepsilon}{\sigma_\mathrm{m}} \right) \right] \qquad (41) \\ \implies \tilde{R} &= \frac{\gamma}{3} \left[\frac{\partial}{\partial \varepsilon} \left(2 \frac{\alpha}{N} \frac{E}{N} \frac{\varepsilon}{\sigma_\mathrm{m}} F_0 \right) \right] + \frac{\alpha}{N} \frac{\gamma}{3} \left[\frac{\varepsilon}{\sigma_\mathrm{m}} \frac{\alpha}{N} F_0 - \frac{E}{N} F_0 \frac{\partial}{\partial \varepsilon} \left(\frac{\varepsilon}{\sigma_\mathrm{m}} \right) \right] \qquad (42) \end{aligned}$$

The first term in the right hand side of $\tilde{R}$ is added to the convective part of the Scharfetter-Gummel flux. The second part which we will name $\tilde{R}_2$ is integrated as follows:

$$\int_{i-1/2}^{i+1/2} \tilde{R}_2 d\epsilon = \frac{\alpha}{N} \frac{\gamma}{3} \left(\left[\frac{\varepsilon}{2} \right]_{i-1/2}^{i+1/2} \frac{\alpha}{\sigma_\mathrm{m} N} - \frac{E}{N} \left[\frac{\varepsilon}{\sigma_\mathrm{m}} \right]_{i-1/2}^{i+1/2} \right) F_{0,i} = G_i F_{0,i} \tag{43}$$

In both cases this term is added to the left hand side of the equation so that the left hand side matrix is:

$$A(F_0) = SG(F_0) - G_i I_n \tag{44}$$

where I_n is the identity matrix.

3.2 Iteration procedure

We start from a Maxwell distribution at a certain mean energy :

$$F_0^0 = \frac{2}{\sqrt{\pi}} \frac{1}{(kT)^{3/2}} \exp\left(-\frac{\epsilon}{kT} \right) \tag{45}$$

Convergence is done adding a time derivative:

$$\frac{\partial F_0}{\partial t} + A(F_0) F_0 = Q(F_0) F_0 \tag{46}$$

Iteration is performed the following way:

$$\begin{aligned} F_0^{n+1} - F_0^n + A(F_0^n) F_0^{n+1} \Delta &= Q(F_0^n) F_0^{n+1} \Delta \\ \implies F_0^{n+1} (I + A(F_0^n) \Delta - Q(F_0^n) \Delta) &= F_0^n \end{aligned} \tag{47}$$

Convergence is achieved when the L_1 norm of the error goes below a certain threshold:

$$L_1(|F_0^{n+1} - F_0^n|) = \int |F_0^{n+1} - F_0^n| \epsilon^{1/2} d\epsilon \tag{48}$$

In practice we start with an initial grid and the expand to a quadratic one after adjusting it to the mean energy of the first iteration.

4 Results and comparison with BOLSIG+

Argon has been used to test the solver because of the simplicity of its chemistry. Three cross sections are taken into account:

$$\begin{aligned} \mathrm{Ar} + \mathrm{e} &\longrightarrow \mathrm{Ar} + \mathrm{e} \\ \mathrm{Ar} + \mathrm{e} &\longrightarrow \mathrm{Ar}^{*} + \mathrm{e} \\ \mathrm{Ar} + \mathrm{e} &\longrightarrow \mathrm{Ar}^{+} + 2\,\mathrm{e} \end{aligned}$$

4.1 Iterations

Below is plotted the iteration procedure from a Maxwellian to the desired EEDF.

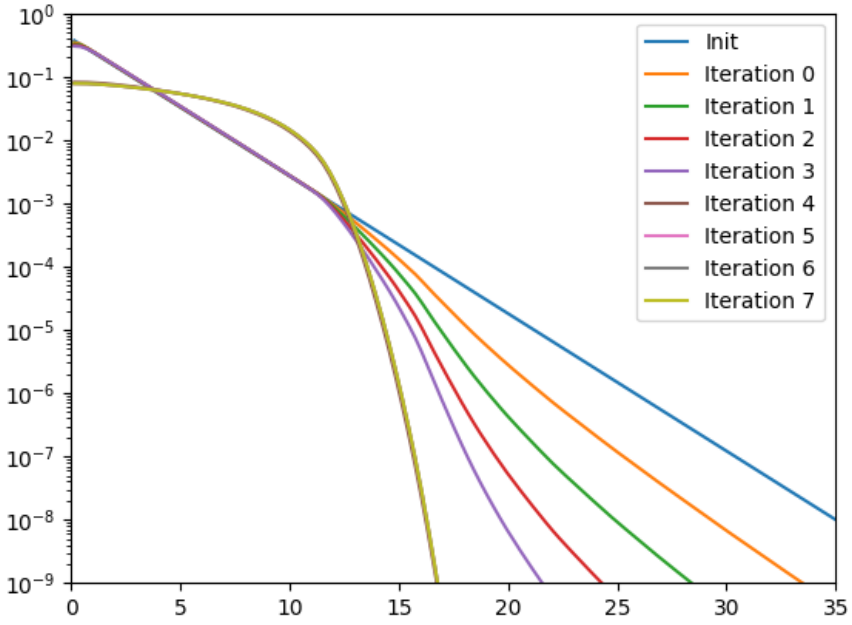

Figure 1: BOLOS - Iteration for the 10 Td EEDF starting from a maxwellian

4.2 Influence of the growth model

The temporal growth model corresponds to Pulsed Townsend experiments whereas the spatial growth model corresponds to Steady State Townsend experiments. In BOLOS convergence from a Maxwellian is achieved faster when using the spatial growth model. However careful initialization of the temperature of the Maxwellian is required in the spatial growth model due to the importance of a square root calculation in the computation of the spatial growth model.

The temporal and spatial growth models yield similar results in BOLOS and BOLSIG+. The no growth model in BOLOS deviates substantially from the no growth model in BOLSIG+.

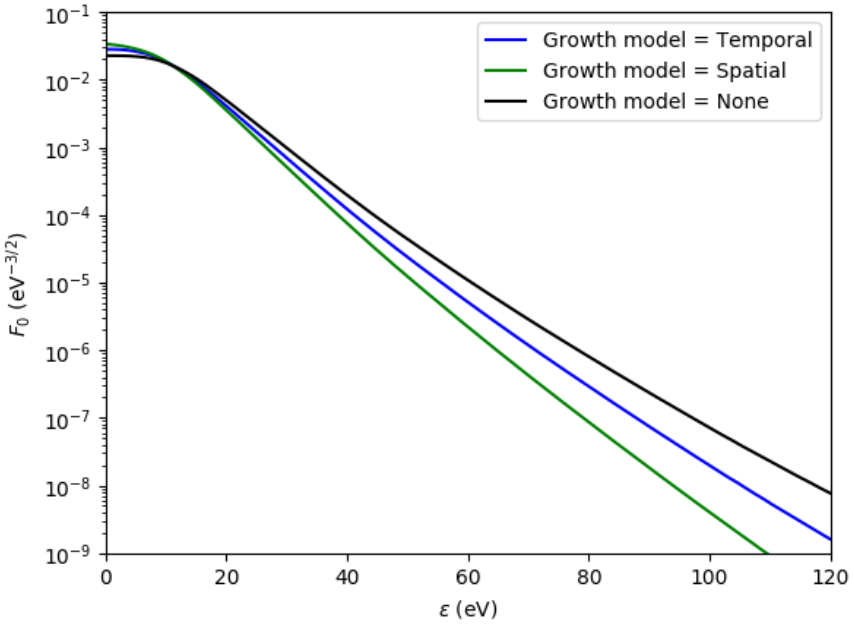

Figure 2: BOLSIG+ - EEDF for 600 Td in argon for different growth models

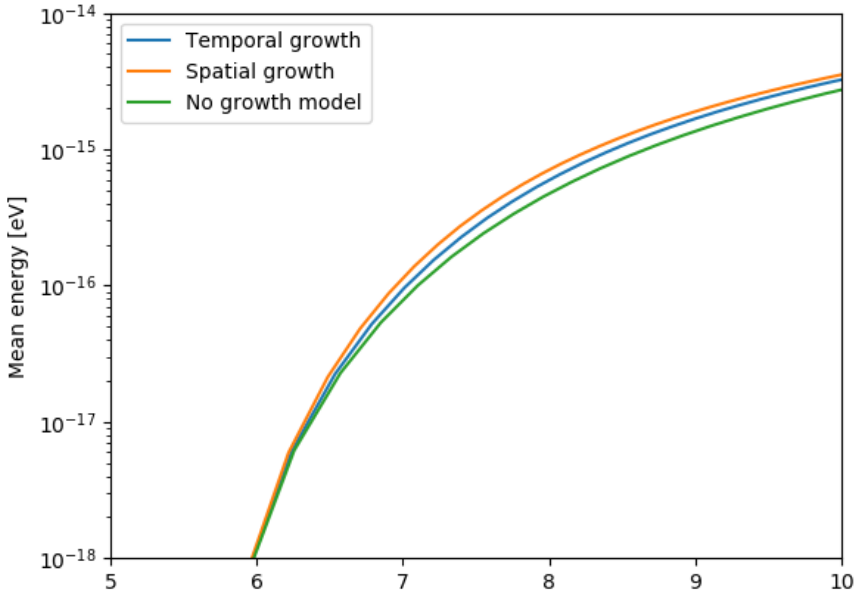

Figure 3: BOLSIG+ - Ionization rate in argon for different growth models

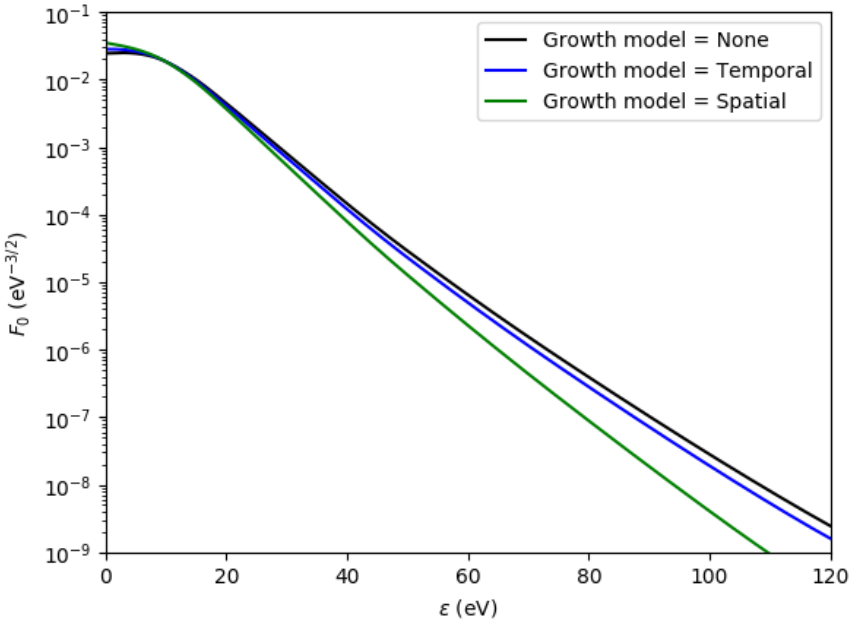

Figure 4: BOLOS - EEDF for 600 Td in argon for different growth models

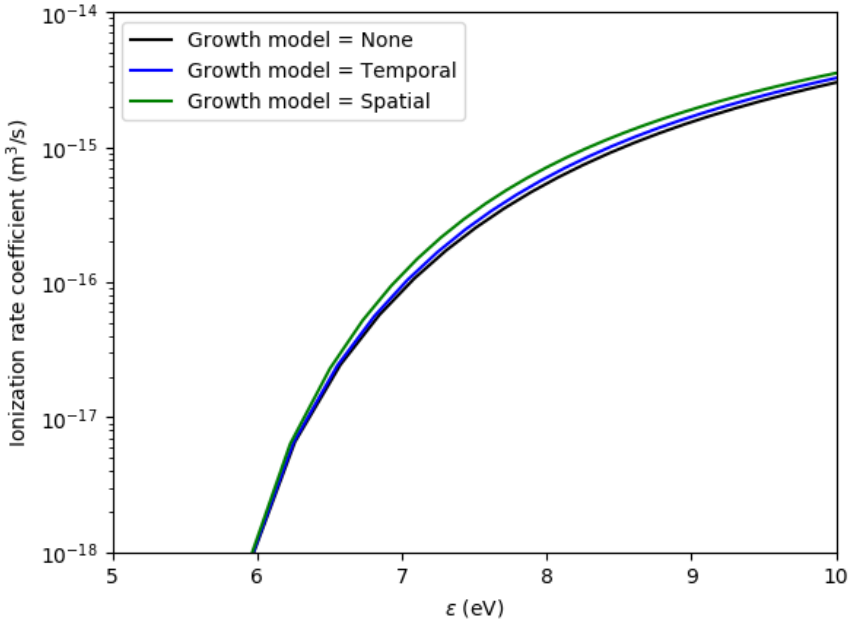

Figure 5: BOLOS - Ionization rate in argon for different growth models

4.3 Influence of the ionization degree

Due to the non-linearity introduced by the coulomb collisions in the system of F_0, convergence is much slower when coulomb collisions are turned on. Moreover the calculation of these non-linear terms, which involve integrals is rather costly.

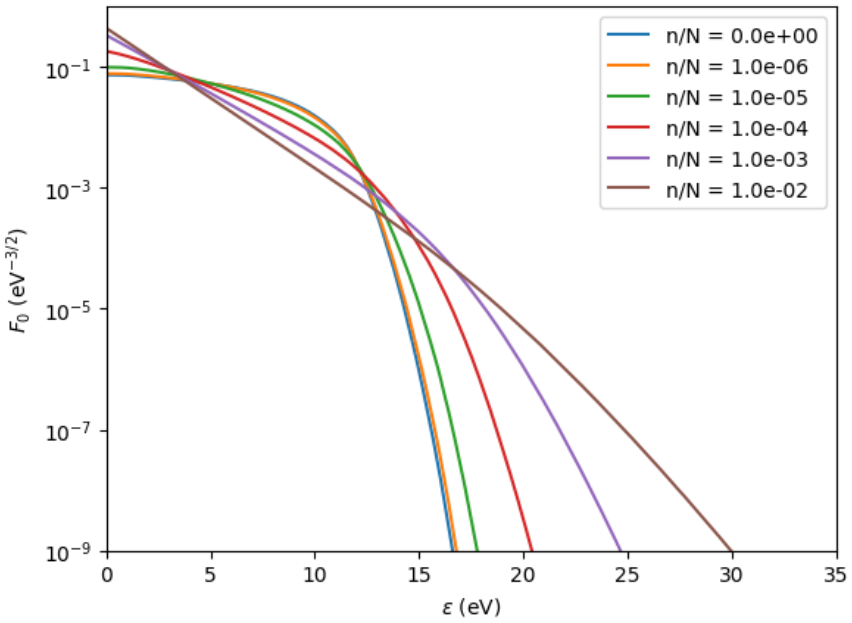

Figure 6: BOLSIG+ - EEDF for 10 Td in argon for different ionization degrees

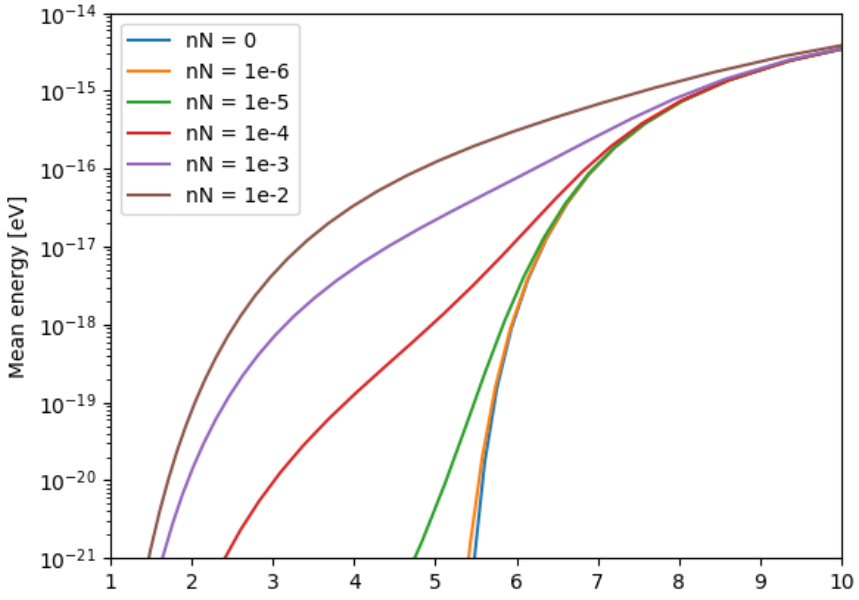

Figure 7: BOLSIG+ - Ionization rate in argon for different ionization degrees

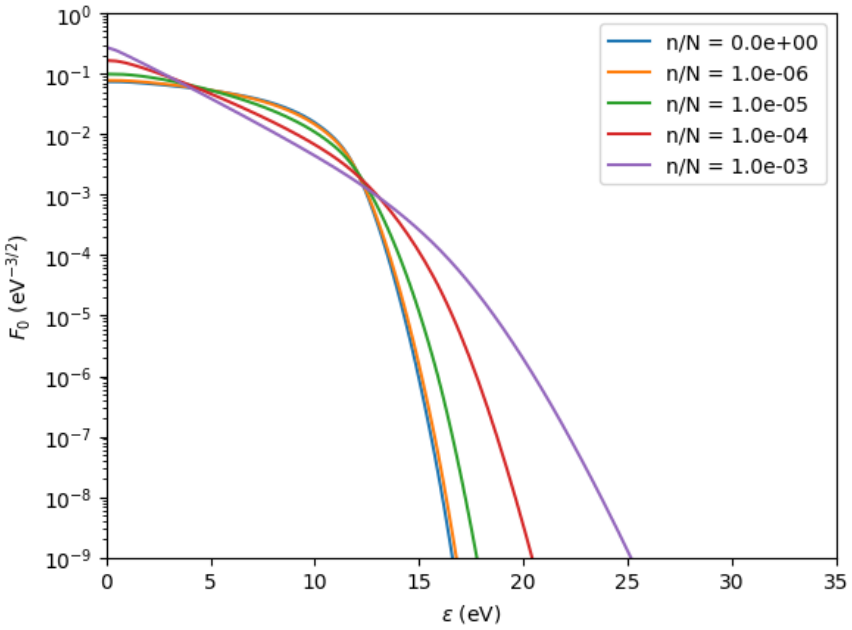

Figure 8: BOLOS - EEDF for 10 Td in argon for different ionization degrees

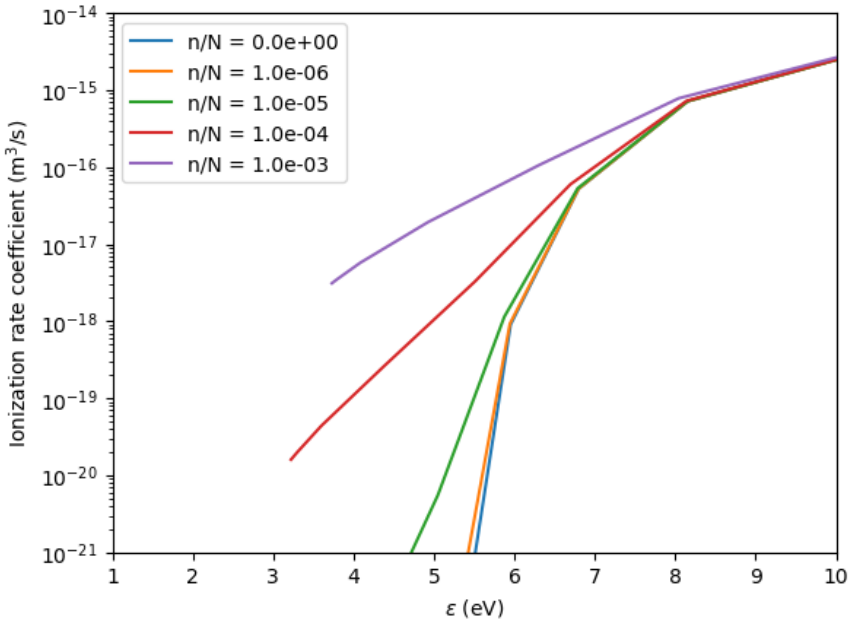

Figure 9: BOLOS - Ionization rate in argon for different ionization degrees

References

J-L. Raimbault. *Introduction to the kinetic theory of weakly ionized plasma*. Laboratoire de Physique des Plasmas, 2018.

G Hagelaar and L. Pitchford. Solving the boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models. *Plasma Sources Science and Technology*, 14, 2005. doi: 10.1088/0963-0252/14/4/011.