

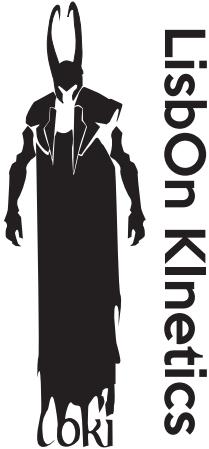
# The LisbOn KInetics Boltzmann solver - user manual

Current version: LoKI-B\_v2.2.0

Antonio Tejero-del-Caz and Luís Lemos Alves

email: [loki@tecnico.ulisboa.pt](mailto:loki@tecnico.ulisboa.pt)

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The following is the user manual of the LisbOn KInetics Boltzmann (LoKI-B) simulation tool [1, 2]. LoKI-B solves the space independent form of the two-term electron Boltzmann equation (EBE) for non-magnetised non-equilibrium low-temperature plasmas, excited by DC/HF electric fields or time-dependent (non-oscillatory) electric fields (a new feature introduced in version 2.0.0) [2] from different gases or gas mixtures. The tool uses a stationary description for DC fields, a Fourier time-expansion description for HF fields, and a time-dependent description for time-varying fields. LoKI-B was developed as a response to the need of having an electron Boltzmann solver easily addressing the simulation of the electron kinetics in any complex gas mixture (of atomic / molecular species), describing first and second-kind electron collisions with any target state (electronic, vibrational and rotational), characterized by any user-prescribed population. LoKI-B includes electron-electron collisions, it handles rotational collisions adopting either a discrete formulation or a more convenient continuous approximation, and it accounts for variations in the number of electrons due to non-conservative events (ionisation and attachment) by assuming either a space-homogeneous exponential temporal growth or a time-constant exponential spatial growth of the electron density. LoKI-B is developed with flexible and upgradable object-oriented programming under MATLAB® [3], to benefit from its matrix-based architecture, adopting an ontology that privileges the separation between tool and data.

On input, LoKI-B defines the operating work conditions (*e.g.* the applied reduced electric field and frequency, the gas pressure and temperature, the electron density, and the fractions of the different gases in the case of mixtures), the distribution of populations for the electronic, vibrational and rotational states of the atomic / molecular gases considered, and the relevant sets of electron-scattering cross sections obtained from the open-access website LXCat (<http://www.lxcat.net/>). On output, it yields the isotropic and the anisotropic parts of the electron distribution function (the former usually termed the *electron energy distribution function*, EEDF), the electron swarm parameters, and the electron power absorbed from the electric field and transferred to the different collisional channels. The latter parameters can be calculated using either the distribution function obtained from the solution to the EBE or some other form prescribed by the user, *e.g.* a generalized Maxwellian EEDF.

LoKI-B leverages on the scientific heritage in the field of non-equilibrium plasma kinetics of the Portuguese group N-Plasmas Reactive: Modeling and Engineering (N-PRiME) [4], and it was developed resorting to well-grounded scientific foundations established years ago [5, 6]. LoKI-B is an open-source tool, licensed under the *GNU general public license*. LoKI-B is freely available at <https://github.com/IST-Lisbon/LoKI>, for users to perform electron kinetics calculations, and for modellers who are invited to continue testing the tool and/or to contribute for its development and improvement.

**You are much welcome to report any problem or bug you may find using the code, or to send any feedback with suggestions for further developments.**

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# 1 Introduction

The simulation tool LoKI-B solves the space independent form of the two-term EBE, calculating the EEDF and the corresponding electron macroscopic parameters [1]. LoKI-B can also adopt a prescribed EEDF, such as a generalized Maxwellian. The current version of the tool is for non-magnetised LTPs. The initial capabilities of LoKI-B have been extended to the solution of the EBE for electrons under the action of a time-dependent (non-oscillatory) electric field [2], as described in section 1.3.

The scientific foundations of LoKI-B were established years ago [5, 6], and are based on the early works of Lorentz, Holstein, Allis and Delcroix [7–10]. The topical review [11], integrated in the collection *Foundations of low-temperature plasmas and their applications* published by *Plasma Sources Science and Technology*, gives a summary of the essentials of the EBE, when written for an electron distribution function expanded in Legendre polynomials  $P_l(\cos(\theta))$  around the angle  $\theta$ , defining the spatial orientation of the velocity vector with respect to the polar direction of the total anisotropy (produced by electric fields and density gradients). The users are advised to carefully read the extensive literature on the two-term EBE [11], for obtaining details about its solution.

Also, the topical review [1] presents the basic features of LoKI-B (also included in this user manual), along with examples of results obtained for different model and real gases, verifying the tool against analytical results, benchmarking it against numerical calculations, and validating the output by comparison with available measurements of swarm parameters.

## 1.1 General description of the problem

LoKI-B describes the electron kinetics of a plasma with electron density  $n_e$ , excited from a general mixture of atomic / molecular gases, by applying an electric field along the  $z$ -axis with the form

$$\vec{E}(t) = -E_p \cos(\omega t) \vec{e}_z , \quad (1)$$

where the oscillation frequency  $\omega$  is either

- $\omega = 0$ , in the DC case;
- $\omega \gg \nu_c$  ( $\nu_c$  is the typical collision frequency), in the HF case.

LoKI-B can also describe plasmas excited by time-dependent (non-oscillatory,  $\omega = 0$ ) electric fields along the  $z$ -axis (see section 1.3).

LoKI-B handles simulations in a gas mixture, with user-defined distributions for the internal degrees of freedom (electronic, vibrational and rotational) of each gas, organized as a system of “Russian puppets”. Table 1 exemplifies the system of states for a N<sub>2</sub>-N-He gas mixture. Here,

- **System:** is the ensemble of all the gases present in the simulation (N<sub>2</sub>  $\cup$  N  $\cup$  He  $\cup$   $\dots$ ).
- **Gas:** refers to each type of atom or molecule present in the simulation (N<sub>2</sub>, N, He,  $\dots$ ). Each gas  $k$  has mass  $M_k$  and individual density  $N_k$ , being composed by several electronic / vibrational / rotational levels.
- **State:** specific configurations of electronic ( $i$ ), vibrational ( $v$ ) and/or rotational ( $J$ ) levels belonging to a given gas (e.g., N<sub>2</sub>(X), N<sub>2</sub>(X,v=0), N<sub>2</sub>(X,v=0,J=2), N(<sup>4</sup>S), He(<sup>2</sup>S),  $\dots$ ). Each gas  $k$  is composed by several electronic states  $k_i$  with absolute density  $N_{k_i}$ ; each  $k_i$ -state can include several vibrational states  $k_{i_v}$  with absolute density  $N_{k_{i_v}}$ , each one composed by several rotational states  $k_{i_v_J}$  with absolute density  $N_{k_{i_v_J}}$ .
- **Parent (state):** state of a certain gas comprising a set of child states. Parent states can be electronic or vibrational, but not rotational (e.g., N<sub>2</sub>(X) is the parent of N<sub>2</sub>(X,v=0,1,2, $\dots$ )). Each parent level comprises all of its children.
- **Child (states):** ensemble of states that share the same parent. Child states can be vibrational or rotational, but not electronic (e.g., N<sub>2</sub>(X,v=0,J=0,1,2, $\dots$ ) are the children of N<sub>2</sub>(X,v=0)).
- **Sibling (states):** relation between the states that share the same parent (e.g., N<sub>2</sub>(X,v=0,1,2, $\dots$ ) are siblings).

Table 1: Example of a gas mixture (childless states are displayed in red).

| Gases         |  | States   |   |
|---------------|--|--|---|
| <b>System</b> | <b>N<sub>2</sub></b>   | <b>N<sub>2</sub>(X)</b> <small>Parent of<br/>← Childs of →</small>     | <b>N<sub>2</sub>(X,v=0)</b> <small>Parent of<br/>← Childs of →</small>  |
|               |  |  | <b>N<sub>2</sub>(X,v=0,J=0)</b><br><b>N<sub>2</sub>(X,v=0,J=1)</b><br><b>N<sub>2</sub>(X,v=0,J=2)</b><br><small>⋮</small><br><b>N<sub>2</sub>(X,v=1)</b><br><b>N<sub>2</sub>(X,v=2)</b><br><small>⋮</small> |
|               |  | <b>N<sub>2</sub>(A)</b><br><b>N<sub>2</sub>(B)</b><br><small>⋮</small> |   |
| <b>N</b>      | <b>N(<sup>4</sup>S)</b><br><b>N(<sup>2</sup>D)</b><br><b>N(<sup>2</sup>P)</b><br><small>⋮</small>                |  |   |
| <b>He</b>     | <b>He(<sup>1</sup>S)</b><br><b>He(<sup>2</sup>S)</b><br><b>He(<sup>2</sup><sup>1</sup>S)</b><br><small>⋮</small> |  |   |
|               |  |  | <small>⋮</small>  |

- **Childless (states):** ensemble of the innermost states (without children) (e.g., N<sub>2</sub>(X,v=0,J=0) is childless).

The previous terminology, allows introducing several definitions and relations for the particle densities with the different species (gases / states) in the system.

- **Total gas density:** total particle density of the heavy species in the system, evaluated as:

$$N = \frac{p}{k_B T_g} , \quad (2)$$

where  $p$  is the total pressure,  $k_B$  is the Boltzmann constant and  $T_g$  is the gas temperature (assumed equal for all  $k$ -gases in the system).

In the code, this quantity is stored in variables labeled with `totalGasDensity`.

- **Individual gas density:** total particle density of a gas in the system. For gas  $k$  this is given by  $N_k$ , with  $\sum_k N_k = N$ .

In the code, this quantity is stored in variables labeled with `individualGasDensity`.

- **Gas fraction:** fraction of a gas in the system. For gas  $k$  this is given by  $\chi_k \equiv N_k/N$ .

- **Absolute density:** particle (absolute) density of a state. For a generic state  $i$  of gas  $k$  this is represented by  $N_{k_i}$ .

In the code, this quantity is stored in variables labeled with `abs`.

- **Population:** density of a state relative to its siblings. For a generic state  $i$  of gas  $k$  this is represented by  $\xi_{k_i} \equiv N_{k_i}/N_{\text{parent of } k_i} = N_{k_i}/(\sum_{i \in \text{siblings}} N_{k_i})$ .
- **Density:** particle density of a state relative to the total gas density. For a generic state  $i$  of gas  $k$  this is represented by  $\delta_{k_i} \equiv N_{k_i}/N$ .  
In LoKI-B, this quantity is stored in variable `density`.

From the previous definitions, it is straightforward to obtain the following normalisation conditions

$$\sum_{k \in \text{system}} \chi_k = 1 \quad (3a)$$

$$\sum_{i \in \text{siblings}} \xi_i = 1 \quad (3b)$$

$$\sum_{i \in \text{childless}} \delta_i = 1 , \quad (3c)$$

concluding also that the following relationships hold

$$\delta_i = \xi_i \delta_{i \text{'s parent}} \quad (4a)$$

$$\delta_{k_i} = \xi_{k_i} \chi_k . \quad (4b)$$

LoKI-B uses SI units for all physical quantities, except the energies that are expressed in eV (electron-volt) and the reduced fields that are expressed in Td (Townsend; 1 Td =  $10^{-21}$  V m<sup>2</sup>).

## 1.2 The electron Boltzmann equation

In the classical two-term approximation, the electron distribution function can be written assuming a separation between the Legendre expansion of the energy distribution and the space-time profile of the electron density  $n_e(z, t)$  as follows

$$\begin{aligned} F(z, u, t) &\simeq \left\{ f^0(u) + \left[ \vec{f}^1(u) \cdot \frac{\vec{v}}{v} \right] \cos(\omega t) \right\} n_e(z, t) \\ &= [f^0(u) + f^1(u) \cos(\theta) \cos(\omega t)] n_e(z, t) , \end{aligned} \quad (5)$$

where  $u = m_e v^2/(2e)$  is the electron kinetic energy in eV (with  $m_e$  and  $e$  the electron mass and charge, respectively);  $f^0(u) \equiv f(u)$  is the isotropic part of the electron distribution function, identified with the EEDF in the framework of the two-term approximation, and satisfying the normalisation condition  $\int_0^\infty f(u) \sqrt{u} du = 1$ ; and  $f^1(u)$  is the (real part of the) first-anisotropy of the electron distribution function.

Under the previous conditions, the EBE including a non-conservative collisional operator can be written as (with  $\gamma \equiv \sqrt{2e/m_e}$ )<sup>1</sup>

$$\frac{1}{\gamma \sqrt{u}} \frac{\langle \nu_{\text{eff}} \rangle}{N} u f(u) + \frac{1}{N} \frac{1}{\gamma} \frac{dG(u)}{du} = S(u) \quad (7a)$$

$$f^1(u) = -\frac{\zeta(E/N)}{\Omega_{\text{PT}}(u)} \frac{df(u)}{du} , \quad (7b)$$

or

$$\frac{1}{3} \frac{\alpha_{\text{eff}}}{N} u f^1(u) + \frac{1}{N} \frac{1}{\gamma} \frac{dG(u)}{du} = S(u) \quad (8a)$$

$$f^1(u) = -\frac{(\alpha_{\text{eff}}/N)}{\Omega_{\text{SST}}(u)} f(u) - \frac{(E/N)}{\Omega_{\text{SST}}(u)} \frac{df(u)}{du} , \quad (8b)$$

where (7a) and (8a) or (7b) and (8b) correspond to the isotropic and anisotropic components of the EBE, respectively, in the following approximations:

---

<sup>1</sup>As mentioned, in a HF case the quantity  $f^1(u)$  in (7b) represents the *real part* of the first-anisotropy of the electron distribution function. Indeed, in this case  $f^1(u, t) = \tilde{f}^1(u) e^{j\omega t}$  with

$$\tilde{f}^1(u) = -\gamma \sqrt{u} \frac{E_p}{N \gamma \sqrt{u} \Omega_c(u) + j\omega} \frac{df(u)}{du} = -\frac{\zeta(E/N)}{\Omega_{\text{PT}}(u)} \frac{df(u)}{du} + j \frac{\zeta(E/N) \frac{\omega/N}{\Omega_c \gamma \sqrt{u}}}{\Omega_{\text{PT}}(u)} \frac{df(u)}{du} . \quad (6)$$

- **temporal growth model:** the space-homogeneous equations (7a)-(7b), which can be used in either the DC or the HF cases, assume an exponential temporal growth of the electron density with a growth constant  $\langle \nu_{\text{eff}} \rangle \equiv \langle \nu_{\text{ion}} \rangle - \langle \nu_{\text{att}} \rangle \equiv \sum_{k,i} \delta_{k_i} [\langle \nu_{k_i, \text{ion}} \rangle - \langle \nu_{k_i, \text{att}} \rangle]$ , corresponding to the electron net creation frequency for the system under study

$$\frac{\partial n_e(t)}{\partial t} = \langle \nu_{\text{eff}} \rangle n_e(t) , \quad (9)$$

with  $\langle \nu_{\text{ion}} \rangle$  and  $\langle \nu_{\text{att}} \rangle$  the corresponding electron mean frequencies for ionisation and attachment, respectively, and where the sums extend over all levels of all gases in the mixture (see section 3). The temporal growth model was used to simulate Pulsed Townsend (PT) discharges by Tagashira *et al* [12], using the formulation of Thomas [13] for the one dimensional continuity equation of electrons under the action of an uniform electric field;

- **spatial growth model:** the time-constant equations (8a)-(8b), which can only be used in the DC case, assume an exponential spatial growth of the electron density in the direction opposite to that of the applied electric field, with a growth constant  $\alpha_{\text{eff}} \equiv \alpha - \eta \equiv \sum_{k,i} \delta_{k_i} (\alpha_{k_i} - \eta_{k_i})$ , corresponding to the effective electron Townsend coefficient

$$\frac{\partial n_e(z)}{\partial z} = \alpha_{\text{eff}} n_e(z) , \quad (10)$$

with  $\alpha$  and  $\eta$  the corresponding first and second Townsend coefficients for ionisation and attachment, respectively (see section 3). The spatial growth model is usually adopted when simulating Steady State Townsend (SST) discharges maintained with a DC electric field [12].

Note that the inclusion of growth models for the electron density is necessary if one intends a space and time independent description, yet including non-conservative collisional mechanisms such as electron ionisation and attachment. Note further that the current version of LoKI-B does not include electron recombination mechanisms.

In these equations:

- $E/N$  is the *reduced electric field*, where  $E \equiv E_p/\zeta$  (with  $\zeta = 1$  or  $\sqrt{2}$  for the DC or the HF cases, respectively);
- the quantities  $\Omega_{\text{PT}}$  and  $\Omega_{\text{SST}}$  have the dimensions of a cross section, being defined as

$$\Omega_{\text{PT}}(u) \equiv \Omega_c(u) + \frac{[1/(\gamma^2 u)] (\omega/N)^2}{\Omega_c(u)} \quad (11a)$$

$$\Omega_{\text{SST}}(u) \equiv \sigma_c(u) , \quad (11b)$$

where  $\Omega_c(u) \equiv \sigma_c(u) + [1/(\gamma \sqrt{u})] (\langle \nu_{\text{eff}} \rangle / N)$ , with  $\sigma_c(u) \equiv \sum_k \chi_k \sigma_{k,c}$  the electron-neutral total momentum-transfer cross section, for the system under study, and  $\sigma_{k,c}$  the corresponding cross section for gas  $k$ ;

- $G \equiv G_E + G_{\text{el}} + G_{\text{CAR}} + G_{ee}$  is the *upflux* function that contains power gain/loss contributions due to, in order, the applied electric-field, the elastic collisions, the rotational collisions (in the continuous approximation for rotations, CAR, with a Chapman-Cowling correction due to the gas temperature [14–17], written here for the case of homonuclear diatomic molecules), and the electron-electron collisions [16], respectively

$$G_E(u) = N \gamma \frac{u}{3} \frac{1}{\zeta} \frac{E}{N} f^1(u) \quad (12a)$$

$$G_{\text{el}}(u) = - \sum_k 2 \frac{m_e}{M_k} \nu_{k,c}^{\text{el}}(u) u^{3/2} \left[ f(u) + \frac{k_B T_g}{e} \frac{df(u)}{du} \right] \quad (12b)$$

$$G_{\text{CAR}}(u) = - \sum_k 4 B_k \nu_{0,k} u^{1/2} \left[ f(u) + \frac{k_B T_g}{e} \frac{df(u)}{du} \right] \quad (12c)$$

$$G_{ee}(u) = -2 \nu_{ee}(u) u^{3/2} \left[ I(u) f(u) + J(u) \frac{df(u)}{du} \right] , \quad (12d)$$

where  $\nu_{k,c}^{\text{el}} \equiv N_k \gamma \sqrt{u} \sigma_{k,c}^{\text{el}}$  is the electron-neutral elastic momentum-transfer collision frequency for the gas  $k$  ( $\sigma_{k,c}^{\text{el}}$  being the corresponding cross section),  $\nu_{0,k} \equiv N_k \gamma \sqrt{u} \sigma_{0,k}$  is the electron-neutral collision

frequency for the rotational excitation of gas  $k$  ( $\sigma_{0,k} \equiv 8\pi Q_k^2 a_0^2 / 15$  being the corresponding cross section, with  $a_0$  the Bohr radius),  $B_k$  and  $Q_k$  are the rotational constant and the quadrupole-moment constant (in units of  $ea_0^2$ ) of the gas  $k$ , respectively<sup>2</sup>,  $I(u)$  and  $J(u)$  are the relevant Spitzer integrals [9, 18], and  $\nu_{ee} \equiv 4\pi [e^2 / (4\pi\varepsilon_0 m_e)]^2 \ln \Lambda_c / v^3 n_e$  is the electron-electron collision frequency (with  $\varepsilon_0$  the vacuum permittivity,  $\ln \Lambda_c$  the Coulomb logarithm ( $\Lambda_c \equiv 12\pi n_e \lambda_D^3$ ) and  $\lambda_D$  the Debye length);

- $S \equiv \sum_{i,j>i} S_{i,j} + \sum_i S_{i,\text{ion}} + \sum_i S_{i,\text{att}}$  is the discrete collision operator that contains power loss/gain contributions due to inelastic/superelastic mechanisms, ionisation and attachment (as mentioned before, recombination is not yet considered), respectively

$$\begin{aligned} S_{i,j}(u) &= \delta_i [(u + V_{i,j})\sigma_{i,j}(u + V_{i,j})f(u + V_{i,j}) - u\sigma_{i,j}(u)f(u)] \\ &\quad + \delta_j \frac{g_i}{g_j} [u\sigma_{i,j}(u)f(u - V_{i,j}) - (u + V_{i,j})\sigma_{i,j}(u + V_{i,j})f(u)] \end{aligned} \quad (13a)$$

$$\begin{aligned} S_{i,\text{ion}}(u) &= \delta_i \left\{ \int_{u+V_{i,\text{ion}}}^{2u+V_{i,\text{ion}}} u'\sigma_{i,\text{ion}}^{\text{sec}}(u', u' - V_{i,\text{ion}} - u)f(u')du' \right. \\ &\quad \left. + \int_{2u+V_{i,\text{ion}}}^{\infty} u'\sigma_{i,\text{ion}}^{\text{sec}}(u', u)f(u')du' - u\sigma_{i,\text{ion}}(u)f(u) \right\} \end{aligned} \quad (13b)$$

$$S_{i,\text{att}}(u) = -\delta_i u\sigma_{i,\text{att}}(u)f(u) . \quad (13c)$$

In (13a)-(13c), the subscripts  $i, j$  and the densities  $\delta_i, \delta_j$  now refer to any state of any gas in the system;  $\sigma_{i,j}$  is the electron-collision cross section for the  $i \rightarrow j$  excitation with energy threshold  $V_{i,j}$  and statistical weights  $g_i$  and  $g_j$ , respectively (note that the third and fourth superelastic terms in (13a) were written resorting to the Klein-Rosseland relation [19]);  $\sigma_{i,\text{att}}(u)$  is the electron-collision cross section for the attachment of state  $i$ ;  $\sigma_{i,\text{ion}}^{\text{sec}}(u', u)$  is the single differential cross section (SDCS) for the ionisation of state  $i$  with energy threshold  $V_{i,\text{ion}}$ ; and

$$\sigma_{i,\text{ion}}(u) = \int_0^{(u-V_{i,\text{ion}})/2} \sigma_{i,\text{ion}}^{\text{sec}}(u, u')du' \quad (14)$$

is the integral cross section for the ionisation of state  $i$ . The SDCS takes into account the distribution of the energy available after an ionisation event, caused by a primary electron with energy  $u'$ , yielding a secondary electron born in the event with energy  $u$  and a scattered electron with energy  $u' - V_{i,\text{ion}} - u$ .

Note that the effect of rotational inelastic/superelastic mechanisms, in the electron kinetics of homonuclear diatomic molecules, can be considered by adopting either the CAR approach of (12c) or the discrete approach of the collision operator (13a), yielding similar results provided that the rotational constants  $Q_k$  and  $B_k$  are coherently matched to the rotational cross section set  $\sigma_{i,j}$  [14].

LoKI-B allows the user to choose between different descriptions of the ionisation mechanism, namely:

- **conservative:** taking ionisation as conservative a mechanism, described by the inelastic part of the collisional operator (13a), in which case the first terms in the left-hand side of (7a) and (8a) should be set to zero;
- **usingSDCS:** taking ionisation as a non-conservative mechanism, described by the collisional operator (13b) with a SDCS, and using the EBE given by (7a)-(8b);
- **oneTakesAll:** taking ionisation as a non-conservative mechanism, and prescribing no-sharing of energy between the secondary electron, introduced at  $u = 0$ , and the scattered electron, introduced at energy  $u' - V_{i,\text{ion}}$ . In this case the SDCS for the secondary electrons writes  $\sigma_{i,\text{ion}}^{\text{sec}}(u', u) = \sigma_{i,\text{ion}}(u')\delta(u)$  and the ionisation operator becomes

$$S_{i,\text{ion}}(u) = \delta_i \left[ (u + V_{i,\text{ion}})\sigma_{i,\text{ion}}(u + V_{i,\text{ion}})f(u + V_{i,\text{ion}}) - u\sigma_{i,\text{ion}}(u)f(u) + \frac{1}{\gamma} \frac{\langle \nu_{i,\text{ion}} \rangle}{N} \delta(u) \right] , \quad (15)$$

corresponding to the inelastic part of (13a) plus an extra term that describes the introduction of new electrons at zero-energy;

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<sup>2</sup>In the previous version LoKI-B\_v1.0.0, the rotational cross section  $\sigma_{0,k}$  was wrongly calculated with a linear (not quadratic) dependence on the quadrupole-moment constant  $Q_k$ . The bug is now corrected. We acknowledge Jan van Dijk and Dan Boer (TU/e, Eindhoven, The Netherlands) for pointing this out.

- **equalSharing:** taking ionisation as a non-conservative mechanism, and prescribing equal-energy-sharing between the secondary and the scattered electrons, introduced at energy  $(u' - V_{i,\text{ion}})/2$ . In this case the SDCS for the secondary electrons writes  $\sigma_{i,\text{ion}}^{\text{sec}}(u', u) = \sigma_{i,\text{ion}}(u')\delta[u - (u' - V_{i,\text{ion}})/2]$  and the ionisation operator becomes

$$S_{i,\text{ion}}(u) = \delta_i [4(2u + V_{i,\text{ion}})\sigma_{i,\text{ion}}(2u + V_{i,\text{ion}})f(2u + V_{i,\text{ion}}) - u\sigma_{i,\text{ion}}(u)f(u)] , \quad (16)$$

where the first term of  $S_{i,\text{ion}}(u)du$  describes the entrance of both the secondary and the scattered electrons at a total energy between  $2u$  and  $2u + 2du$ , produced by a primary electron with energy  $u' = 2u + V_{i,\text{ion}}$ , whereas the second term describes the exit of primary electrons with energy  $u$  after ionizing collisions.

Naturally, the attachment mechanism is taken **always** as non-conservative, meaning that, in the case of electronegative gases, the code adopts the electron-density growth-model (**temporal** or **spatial**) specified by the user.

Note that the current version of LoKI-B does not include any external sources of electrons, such as electron beam injection or photoionization. However, the model adopted in the code can be easily upgraded as to consider these effects: (i) on the right-hand side of the EBE, with the addition, to the source function  $S$ , of an energy-resolved gain-term; (ii) on the left-hand side of the EBE, with the addition of the corresponding energy-integral term, describing the growth of the electron density in a stationary situation. The inclusion of these external sources of electrons, as well as the handling of the non-conservative electron-collision mechanisms (particularly the attachment), must be carefully monitored in all cases, since they can be responsible for the development of significant anisotropies, in which case the two-term expansion of the EBE adopted here is no longer valid.

### 1.3 The time-dependent electron Boltzmann equation

The original capabilities of LoKI-B have been extended in order to obtain the solution of the EBE for plasma electrons under the action of a time-dependent (non-oscillatory,  $\omega = 0$ ) electric-field along the  $z$ -axis [2]. In this case, assuming the classical two-term expansion and a space-independent exponential temporal growth of the electron density

$$\begin{aligned} F(u, t) &\simeq [f^0(u, t) + f^1(u, t) \cos(\theta)] n_e(t) \\ \frac{dn_e(t)}{dt} &= \langle \nu_{\text{eff}} \rangle(t) n_e(t) , \end{aligned} \quad (17)$$

the EBE is updated as follows (see equations (7a)-(7b)):

$$\frac{1}{N} \frac{1}{\gamma} \sqrt{u} \frac{\partial f(u, t)}{\partial t} + \frac{1}{\gamma \sqrt{u}} \frac{\langle \nu_{\text{eff}} \rangle(t)}{N} u f(u, t) + \frac{1}{N} \frac{1}{\gamma} \frac{\partial G(u, t)}{\partial u} = S(u, t) \quad (18a)$$

$$f^1(u, t) = -\frac{(E(t)/N)}{\Omega_c(u, t)} \frac{\partial f(u, t)}{\partial u} . \quad (18b)$$

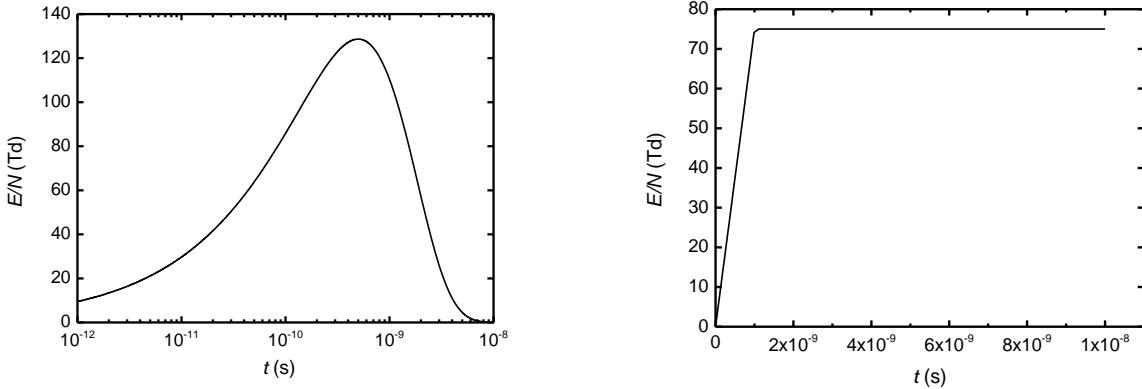


Figure 1: Example of time-dependent (non-oscillatory) reduced electric-fields that can be used in LoKI-B simulations: electric-field pulse (left) and electric-field step (right), calculated using (21a) and (21b), respectively.

In these equations, the first term on the left-hand side of (18a) accounts for the intrinsic time evolution of the isotropic component of the electron distribution function; the second term on the left-hand side of (18a) and

the time-dependent collision frequency  $\Omega_c(u, t)$  in (18b) account for the intrinsic time evolution of the electron density. In this case, the collision frequency is given by

$$\Omega_c(u, t) \equiv \sigma_c(u) + \frac{1}{\gamma\sqrt{u}} \frac{1}{N n_e(t)} \frac{dn_e(t)}{dt} = \sigma_c(u) + \frac{1}{\gamma\sqrt{u}} \frac{\langle \nu_{\text{eff}} \rangle(t)}{N} . \quad (19)$$

It is assumed a steady-state form for equation (18b), describing the first anisotropy, because the characteristic evolution time of the EEDF  $\tau$  is much larger than the characteristic evolution time of the anisotropic component, *i.e.*

$$\tau \simeq \frac{1}{\sum_k (m_e/M_k) \nu_{k,c}^{\text{el}}} \gg \frac{1}{\nu_{k,c}^{\text{el}}} . \quad (20)$$

Equations (18a)-(18b) are used to obtain the time-dependent solution of the EBE for user-prescribed electric-field forms, initial and final times, and sampling values of the field. As an example, figure 1 shows two forms of the reduced electric-field that can be used in the time-dependent solution of LoKI-B, corresponding to an electric field pulse given by

$$\frac{E(t)}{N} (\text{Td}) = \frac{E_0}{N} \sqrt{\frac{t(\text{s})}{\tau_{\text{rise}}}} \exp\left(-\frac{t(\text{s})}{\tau_{\text{rise}}}\right) \quad (21a)$$

with  $E_0/N = 300$  Td and  $\tau_{\text{rise}} = 10^{-9}$  s; and an electric-field step given by

$$\frac{E(t)}{N} (\text{Td}) = \begin{cases} \frac{E_{\text{max}}}{N} \frac{t(\text{s})}{\tau_{\text{rise}}}, & 0 \leq t(\text{s}) \leq \tau_{\text{rise}} \\ \frac{E_{\text{max}}}{N}, & t(\text{s}) > \tau_{\text{rise}} \end{cases} , \quad (21b)$$

with  $E_{\text{max}}/N = 75$  Td and  $\tau_{\text{rise}} = 10^{-9}$  s.

## 1.4 Prescribed EEDFs

LoKI-B calculations can also adopt a prescribed EEDF, corresponding to a generalized Maxwellian given by the expression [20–22]

$$f(u) = \left( \frac{2}{3k_B T_e} \right)^{3/2} \frac{\Gamma(\frac{5}{2s})^{3/2}}{\Gamma(\frac{3}{2s})^{5/2}} \exp\left(-\left[ \frac{\Gamma(\frac{5}{2s})}{\Gamma(\frac{3}{2s})} \frac{2eu}{3k_B T_e} \right]^s\right) , \quad (22)$$

where  $\Gamma$  represents the gamma-function and  $s$  is a positive real number that controls the “shape” of the EEDF. In particular, (22) yields a Maxwellian EEDF and a Druyvesteyn EEDF for  $s = 1$  and  $s = 2$ , respectively.

This setting corresponds to a local thermodynamic equilibrium framework, where the electron energy (defined by the electron temperature, given as input parameter) is dissipated exclusively in electron-neutral *conservative* collisions. Thus, in this case LoKI-B considers neither an electron-density growth model nor time-dependent calculations. Indeed, when adopting a prescribed EEDF, LoKI-B calculations are limited to evaluating (i) the EEDF for given  $T_e$ , according to (22), (ii) the electron rate coefficients for the set of cross sections defined as input data (see section 3), (iii) the most relevant electron transport parameters (see section 3), (iv) the power transferred in electron-neutral elastic/inelastic/superelastic collisions (see section 3), and (v) the *equivalent* reduced electric-field that would ensure a local equilibrium between the power gained from the field and lost in collisions (see section 3).

## 2 Numerical solution

The EBE is numerically solved in an uniform energy grid defined in the energy interval  $[0, u_{\max}]$ , with *cells*

$$u_n^{\text{cell}} \equiv u_n = (n - 1/2)\Delta u, \quad n = 1, 2, \dots, \mathcal{N} \quad (23)$$

of fixed step-size  $\Delta u = u_{\max}/\mathcal{N}$ , each cell  $n$  being limited by *nodes*  $n - 1/2$  and  $n + 1/2$ , each node  $n$  having energy

$$u_n^{\text{node}} = u_{n-1/2} = (n - 1)\Delta u, \quad n = 1, 2, \dots, \mathcal{N} + 1 \quad (24)$$

Figure 2 presents a graphic representation of the energy grid as defined in (23)-(24). The user can define the

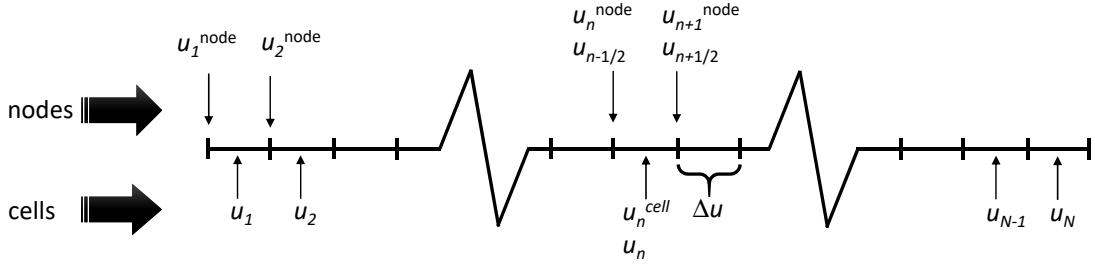


Figure 2: Graphic representation of the energy grid as defined in (23)-(24).

energy grid in two ways: (i) by setting the maximum energy  $u_{\max}$  and the number of cells  $\mathcal{N}$ ; (ii) by prescribing a number of decades in the fall of the EEDF, between  $f_1$  and  $f_{\mathcal{N}}$ , as to ensure an automatic adjustment of the energy grid. Typical values for the decade-fall are within 10 to 25, considering not only the use of double precision, but also the order of magnitude of the various quantities (kinetic energy, cross sections) multiplying the EEDF in the calculations. The user is responsible for adequately defining the energy grid, namely by noticing that small energy steps are required to resolve any relevant structure in the cross sections, such as near-threshold variations and resonances, as well as situations involving the presence of a Ramsauer minimum.

Equations (7a)-(8b) are written for each **grid-cell**, where the isotropic and anisotropic functions  $f$  and  $f^1$  are defined, with the corresponding upfluxes  $G_x$  ( $x = E, \text{el}, \text{CAR}, ee$ ) and cross sections  $\sigma_y$  ( $y = k, c; k_{(i,j)}$ ) being set on the **grid-nodes**. The cross sections are interpolated linearly from the data provided by the user, setting to zero all the values up to the corresponding energy threshold, *i.e.*  $\sigma_{y_n} = 0$  for  $n \leq \text{INT}(V_{i,j}/\Delta u)$ .

The EBE is discretised adopting the centered finite differences scheme presented in [23]. The result is a system of algebraic equations that can be written under matrix form, with tridiagonal elements coming from the left-hand sides of (7a) and (8a), and some sparse off-tridiagonal elements due to the electron-neutral collisional operator in the right-hand sides.

The emphasis of the discretization is with the definition of the upflux functions  $G(u)$  on the grid-nodes, *i.e.* on the general boundaries  $u_{n\pm 1/2}^{\text{cell}}$  of a cell  $n$  centered at energy  $u_n^{\text{cell}}$ . The discretization method can be described as a finite-volume-like procedure, by applying Gauss' theorem to an integral over a one-dimensional energy volume around  $u_n^{\text{cell}}$  as follows

$$-\frac{1}{N} \frac{1}{\gamma} \left. \frac{dG_x(u)}{du} \right|_{n; x=E, \text{el}, \text{CAR}} = -\frac{1}{N} \frac{1}{\gamma} \frac{1}{\Delta u} \int_{u_{n-1/2}^{\text{cell}}}^{u_{n+1/2}^{\text{cell}}} \frac{dG_x(u)}{du} du = -\frac{1}{N} \frac{1}{\gamma} \frac{G_{x_{n+1/2}} - G_{x_{n-1/2}}}{\Delta u} , \quad (25a)$$

and therefore

$$\begin{aligned} -\frac{1}{N} \frac{1}{\gamma} \left. \frac{dG_x(u)}{du} \right|_{n; x=E, \text{el}, \text{CAR}} &= \left\{ \frac{d}{du} \left[ g_x(u) \left( d_x f(u) + c_x \frac{df(u)}{du} \right) \right] \right\}_n \\ &\simeq g_{x_{n+1/2}} \left( \frac{d_x}{\Delta u} \int_{u_n^{\text{cell}}}^{u_{n+1}^{\text{cell}}} f(u) du + \frac{c_x}{\Delta u} \int_{u_n^{\text{cell}}}^{u_{n+1}^{\text{cell}}} \frac{df(u)}{du} du \right) \\ &\quad - g_{x_{n-1/2}} \left( \frac{d_x}{\Delta u} \int_{u_{n-1}^{\text{cell}}}^{u_n^{\text{cell}}} f(u) du + \frac{c_x}{\Delta u} \int_{u_{n-1}^{\text{cell}}}^{u_n^{\text{cell}}} \frac{df(u)}{du} du \right) \end{aligned}$$

$$\begin{aligned}
&\simeq g_{x_{n+1/2}} \left( \frac{d_x}{2} (f_n + f_{n+1}) + \frac{c_x}{\Delta u} (f_{n+1} - f_n) \right) \\
&- g_{x_{n-1/2}} \left( \frac{d_x}{2} (f_{n-1} + f_n) + \frac{c_x}{\Delta u} (f_n - f_{n-1}) \right) \\
&= \left[ \frac{g_{x_{n-1/2}}}{\Delta u} \left( \frac{c_x}{\Delta u} - \frac{d_x}{2} \right) \right] f_{n-1} \\
&- \left[ \frac{g_{x_{n+1/2}}}{\Delta u} \left( \frac{c_x}{\Delta u} - \frac{d_x}{2} \right) + \frac{g_{x_{n-1/2}}}{\Delta u} \left( \frac{c_x}{\Delta u} + \frac{d_x}{2} \right) \right] f_n \\
&+ \left[ \frac{g_{x_{n+1/2}}}{\Delta u} \left( \frac{c_x}{\Delta u} + \frac{d_x}{2} \right) \right] f_{n+1} ,
\end{aligned} \tag{25b}$$

where  $c_x$  and  $d_x$  are constants,  $g_x(u)$  can be obtained straightforwardly from (12a)-(12c), and

$$\begin{aligned}
f_n &\equiv f(u_n^{\text{cell}}) \\
g_{x_{n+1/2}} &\equiv g_x(u_{n+1/2}^{\text{cell}}) \equiv g_x(u_{n+1}^{\text{node}}) .
\end{aligned}$$

In addition to the terms proportional to  $dG_{x=E,\text{el},\text{CAR}}/du$ , equations (7a)-(8b) are further composed by terms proportional to  $f$ ,  $df/du$  and  $dG_{ee}/du$  whose discretised forms can be generally summarised as follows (the latter receiving a treatment similar to equations (25a)-(25b))

$$[a(u)f(u)]_n = a_n f_n \tag{26a}$$

$$[a'(u)f(u \pm V_{i,j})]_n = a'_n f_n \pm \text{INT}(V_{i,j}/\Delta u) \tag{26b}$$

$$\left[ b(u) \frac{df(u)}{du} \right]_n = b_n \frac{f_{n+1} - f_{n-1}}{2\Delta u} \tag{26c}$$

$$-\frac{1}{N} \frac{1}{\gamma} \frac{dG_{ee}(u)}{du} \Big|_n = \left\{ \frac{d}{du} \left[ g_{ee}(u) \left( I(u)f(u) + J(u) \frac{df(u)}{du} \right) \right] \right\}_n , \tag{26d}$$

where  $a(u)$ ,  $a'(u)$  and  $b(u)$  are generic functions of  $u$ ; and  $g_{ee}(u)$ ,  $I(u)$  and  $J(u)$  can be obtained straightforwardly from (12d).

The detailed discretized form of each term is given below, with the cross sections defined on the grid-nodes as

$$\begin{aligned}
\sigma_{y_n} &\equiv \sigma_y(u_n^{\text{node}}) \\
\sigma_y(u_n^{\text{cell}}) &= \frac{1}{2} (\sigma_{y_n} + \sigma_{y_{n+1}}) .
\end{aligned}$$

- **Time-dependent term (only for time-dependent simulations, see section 1.3)**

$$\frac{1}{N} \frac{1}{\gamma} \sqrt{u} \frac{\partial f(u, t)}{\partial t} \Big|_n = \frac{1}{N} \frac{1}{\gamma} u_n^{1/2} \frac{\partial f_n(t)}{\partial t} . \tag{27}$$

- **Temporal growth term**

$$\frac{1}{\gamma \sqrt{u}} \frac{\langle \nu_{\text{eff}} \rangle}{N} u f(u) \Big|_n = \frac{1}{\gamma} \frac{\langle \nu_{\text{eff}} \rangle}{N} u_n^{1/2} f_n . \tag{28}$$

- **Spatial growth term**

$$\frac{1}{3} \frac{\alpha_{\text{eff}}}{N} u f^1(u) \Big|_n = -\frac{1}{3} \frac{\alpha_{\text{eff}}}{N} u_n \left[ \frac{\alpha_{\text{eff}}/N}{\Omega_{\text{SST}_n}} f_n + \frac{E/N}{\Omega_{\text{SST}_n}} \frac{f_{n+1} - f_{n-1}}{2\Delta u} \right] . \tag{29}$$

- **Electric field operator**

$$g_E(u) = \frac{u}{3N} \times \begin{cases} \frac{(E/N)}{\Omega_{\text{PT}}(u)}, & \text{for a PT situation} \\ \frac{(\alpha_{\text{eff}}/N)}{\Omega_{\text{SST}}(u)}, & \text{for a SST situation} \end{cases} \quad (30a)$$

$$c_E = \begin{cases} 1, & \text{for a PT situation} \\ \frac{(E/N)}{(\alpha_{\text{eff}}/N)}, & \text{for a SST situation} \end{cases} \quad (30b)$$

$$d_E = \begin{cases} 0, & \text{for a PT situation} \\ 1, & \text{for a SST situation} \end{cases} \quad (30c)$$

For a PT situation

$$-\frac{1}{N} \frac{1}{\gamma} \frac{dG_E(u)}{du} \Big|_n = \left[ \frac{g_{E_{n-1/2}}}{(\Delta u)^2} \right] f_{n-1} - \left[ \frac{g_{E_{n-1/2}} + g_{E_{n+1/2}}}{(\Delta u)^2} \right] f_n + \left[ \frac{g_{E_{n+1/2}}}{(\Delta u)^2} \right] f_{n+1}. \quad (31)$$

For an SST situation

$$\begin{aligned} -\frac{1}{N} \frac{1}{\gamma} \frac{dG_E(u)}{du} \Big|_n &= \left[ \frac{g_{E_{n-1/2}}}{\Delta u} \left( \frac{E/N}{(\alpha_{\text{eff}}/N) \Delta u} - \frac{1}{2} \right) \right] f_{n-1} \\ &\quad - \left[ \frac{g_{E_{n-1/2}}}{\Delta u} \left( \frac{E/N}{(\alpha_{\text{eff}}/N) \Delta u} + \frac{1}{2} \right) + \frac{g_{E_{n+1/2}}}{\Delta u} \left( \frac{E/N}{(\alpha_{\text{eff}}/N) \Delta u} - \frac{1}{2} \right) \right] f_n \\ &\quad + \left[ \frac{g_{E_{n+1/2}}}{\Delta u} \left( \frac{E/N}{(\alpha_{\text{eff}}/N) \Delta u} + \frac{1}{2} \right) \right] f_{n+1} \end{aligned} \quad (32)$$

- **Elastic operator**

$$g_{\text{el}}(u) = 2u^2 \sum_k \frac{m_e}{M_k} \chi_k \sigma_{k,c}^{\text{el}}(u) \quad (33a)$$

$$c_{\text{el}} = \frac{k_B T_g}{e} \quad (33b)$$

$$d_{\text{el}} = 1 \quad (33c)$$

$$\begin{aligned} -\frac{1}{N} \frac{1}{\gamma} \frac{dG_{\text{el}}(u)}{du} \Big|_n &= \left[ \frac{g_{\text{el}_{n-1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} - \frac{1}{2} \right) \right] f_{n-1} \\ &\quad - \left[ \frac{g_{\text{el}_{n-1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} + \frac{1}{2} \right) + \frac{g_{\text{el}_{n+1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} - \frac{1}{2} \right) \right] f_n \\ &\quad + \left[ \frac{g_{\text{el}_{n+1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} + \frac{1}{2} \right) \right] f_{n+1} \end{aligned} \quad (34)$$

- **CAR operator**

$$g_{\text{CAR}}(u) = 4u \sum_k B_k \chi_k \sigma_{0,k}(u) \quad (35a)$$

$$c_{\text{CAR}} = \frac{k_B T_g}{e} \quad (35b)$$

$$d_{\text{CAR}} = 1 \quad (35c)$$

$$\begin{aligned} -\frac{1}{N} \frac{1}{\gamma} \frac{dG_{\text{CAR}}(u)}{du} \Big|_n &= \left[ \frac{g_{\text{CAR}_{n-1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} - \frac{1}{2} \right) \right] f_{n-1} \\ &\quad - \left[ \frac{g_{\text{CAR}_{n-1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} + \frac{1}{2} \right) + \frac{g_{\text{CAR}_{n+1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} - \frac{1}{2} \right) \right] f_n \\ &\quad + \left[ \frac{g_{\text{CAR}_{n+1/2}}}{\Delta u} \left( \frac{k_B T_g}{e \Delta u} + \frac{1}{2} \right) \right] f_{n+1} \end{aligned} \quad (36)$$

- **Electron-electron collisions operator**

[In the case of time-dependent simulations, see section 1.3, the electron density  $n_e(t)$  and the EEDF  $f(u, t)$  introduce a time-dependence into  $g_{ee}(u, t)$ ,  $I(u, t)$  and  $J(u, t)$ , which are written for a given  $t$ .]

$$g_{ee}(u) = \frac{2}{\gamma} \frac{\nu_{ee}(u)}{N} u^{3/2} \quad (37a)$$

$$I(u) = \int_0^u f(u') u'^{1/2} du' \quad (37b)$$

$$J(u) = \frac{2}{3} \left[ \int_0^u f(u') u'^{3/2} du' + u^{3/2} \int_u^\infty f(u') du' \right] \quad (37c)$$

$$\begin{aligned} -\frac{1}{N} \frac{1}{\gamma} \frac{dG_{ee}(u)}{du} \Big|_n &= \left\{ \frac{d}{du} \left[ g_{ee}(u) \left( I(u)f(u) + J(u) \frac{df(u)}{du} \right) \right] \right\}_n \\ &= A_{n-1} f_{n-1} - (A_n + B_n) f_n + B_{n+1} f_{n+1} \end{aligned} \quad (38)$$

$$A_n \equiv A_{I_n} + A_{J_n} = -\frac{2}{\gamma} \frac{\nu_{ee_{n+1/2}}}{N} u_{n+1/2}^{3/2} \left[ \frac{I_{n+1/2}}{2\Delta u} - \frac{J_{n+1/2}}{(\Delta u)^2} \right] \equiv \sum_{m=1}^N a_{n,m} f_m \quad (39a)$$

$$B_n \equiv B_{I_n} + B_{J_n} = \frac{2}{\gamma} \frac{\nu_{ee_{n-1/2}}}{N} u_{n-1/2}^{3/2} \left[ \frac{I_{n-1/2}}{2\Delta u} + \frac{J_{n-1/2}}{(\Delta u)^2} \right] \equiv \sum_{m=1}^N b_{n,m} f_m \quad (39b)$$

$$A_{I_n} = -\frac{2}{\gamma} \frac{\nu_{ee_{n+1/2}}}{N} u_{n+1/2}^{3/2} \frac{I_{n+1/2}}{2\Delta u} , \quad \text{etc} \quad (39c)$$

$$I_{n+1/2} = \sum_{m=1}^n f_m u_m^{1/2} \Delta u \quad (39d)$$

$$J_{n+1/2} = \frac{2}{3} \left[ \sum_{m=1}^n f_m u_m^{3/2} \Delta u + u_{n+1/2}^{3/2} \sum_{m=n+1}^N f_m \Delta u \right] \quad (39e)$$

$$a_{n,m} = -\frac{2}{\gamma} \frac{\nu_{ee_{n+1/2}}}{N} u_{n+1/2}^{3/2} \times \begin{cases} \frac{1}{2} u_m^{1/2} - \frac{2}{3} \frac{u_m^{3/2}}{\Delta u} , & m \leq n \\ -\frac{2}{3} \frac{u_{n+1/2}^{3/2}}{\Delta u} , & m > n \end{cases} \quad (39f)$$

$$b_{n,m} = \frac{2}{\gamma} \frac{\nu_{ee_{n-1/2}}}{N} u_{n-1/2}^{3/2} \times \begin{cases} \frac{1}{2} u_m^{1/2} + \frac{2}{3} \frac{u_m^{3/2}}{\Delta u} , & m \leq n-1 \\ \frac{2}{3} \frac{u_{n-1/2}^{3/2}}{\Delta u} , & m > n-1 \end{cases} . \quad (39g)$$

- **Discrete collision operator**

$$S_n = \sum_{i,j>i} S_{(i,j)_n} + \sum_i S_{(i,\text{ion})_n} + \sum_i S_{(i,\text{att})_n} \quad (40a)$$

$$l_{i,j} \equiv \text{INT}(V_{i,j}/\Delta u) \quad (40b)$$

$$\sigma_{i,\text{ion}}(u_n^{\text{cell}}) = \sum_{m=1}^{(n-l_{i,\text{ion}})/2} \sigma_{(i,\text{ion})_{(n,m)}}^{\text{sec}} \quad (40c)$$

$$\begin{aligned} S_{(i,j)_n} &= \delta_i \left[ u_{n+l_{i,j}} \frac{\sigma_{(i,j)_{n+l_{i,j}}} + \sigma_{(i,j)_{n+l_{i,j}+1}}}{2} f_{n+l_{i,j}} - u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_n \right] \\ &+ \delta_j \frac{g_i}{g_j} \left[ u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_{n-l_{i,j}} - u_{n+l_{i,j}} \frac{\sigma_{(i,j)_{n+l_{i,j}}} + \sigma_{(i,j)_{n+l_{i,j}+1}}}{2} f_n \right] \end{aligned} \quad (41a)$$

$$S_{(i,\text{ion})_n} = \delta_i \left\{ \sum_{m=n+l_{i,\text{ion}}+1}^{2n+l_{i,\text{ion}}} u_m \sigma_{(i,\text{ion})_{(m,m-n-l_{i,\text{ion}})}}^{\text{sec}} f_m \Delta u \right\}$$

$$+ \sum_{m=2n+l_{i,\text{ion}+1}}^N u_m \sigma_{(i,\text{ion})_{(m,n)}}^{\text{sec}} f_m \Delta u - u_n \frac{\sigma_{(i,\text{ion})_n} + \sigma_{(i,\text{ion})_{n+1}}}{2} f_n \Bigg\} \quad (41\text{b})$$

$$S_{(i,\text{att})_n} = -\delta_i u_n \frac{\sigma_{(i,\text{att})_n} + \sigma_{(i,\text{att})_{n+1}}}{2} f_n . \quad (41\text{c})$$

The previous equations are subjected to the following conditions [23]:

- the flux boundary conditions  $G(0) = G(u_{\max}) = 0$ , which imply  $g_{x_{1/2}} = g_{x_{N+1/2}} = 0$  and  $A_0 = A_N = B_1 = B_{N+1} = 0$ ;
- the imposition of a Maxwellian EEDF for  $dG_{ee}/du = 0$ , which is ensured by setting  $a_{n,m} = \sqrt{a_{n,m} \times a_{m-1,n+1}}$ ;
- the energy conservation condition for  $dG_{ee}/du$ , which yields  $b_{m,n} = a_{n,m}$ ;

After discretisation, the isotropic part of the EBE can be written as  $\sum_{m=1}^N C_{n,m}(f) f_m = 0$ , which is solved coupled to the normalisation condition  $\sum_{m=1}^N f_m \sqrt{u_m} \Delta u = 1$ .

Note that the EBE is solved as a balance equation written as (see below and in section 5.2, details about the solution method and the numerical calling of the algorithm)

- for the direct solution method (successively applied in the presence of nonlinear terms), when using `mixingDirectSolutions` as algorithm:

- when adopting a temporal growth model

$$0 = -\frac{1}{\gamma \sqrt{u}} \frac{\langle \nu_{\text{eff}} \rangle}{N} u f(u) \Big|_n - \frac{1}{N} \frac{1}{\gamma} \frac{dG(u)}{du} \Big|_n + S_n ; \quad (42\text{a})$$

- when adopting a spatial growth model

$$0 = -\frac{1}{3} \frac{\alpha_{\text{eff}}}{N} u f^1(u) \Big|_n - \frac{1}{N} \frac{1}{\gamma} \frac{dG(u)}{du} \Big|_n + S_n ; \quad (42\text{b})$$

- for the relaxation method, when using `temporalIntegration` as algorithm:

- when adopting a temporal growth model and/or in the case of time-dependent simulations

$$\frac{\partial f(u,t)}{\partial t} \Big|_n = -N \frac{\langle \nu_{\text{eff}} \rangle}{N} f(u) \Big|_n - \frac{1}{\sqrt{u}} \frac{dG(u)}{du} \Big|_n + N \gamma \sqrt{u} \frac{1}{u} S_n ; \quad (42\text{c})$$

- when adopting a spatial growth model

$$\frac{\partial f(u,t)}{\partial t} \Big|_n = -\frac{1}{3} \gamma \sqrt{u} N \frac{\alpha_{\text{eff}}}{N} f^1(u) \Big|_n - \frac{1}{\sqrt{u}} \frac{dG(u)}{du} \Big|_n + N \gamma \sqrt{u} \frac{1}{u} S_n . \quad (42\text{d})$$

For electropositive gases, when choosing `ionizationOperatorType` as `conservative` (see sections 1.2 and 5.2), the first term on the right-hand side of the previous equations is set to zero.

The matrix  $C(f)$  is nonlinear due to the presence of the following terms.

- The temporal/spatial growth-term of the electron density, associated with non-conservative mechanisms, involves either the effective ionisation rate coefficient  $\langle \nu_{\text{eff}} \rangle/N$  or the effective Townsend reduced coefficient  $\alpha_{\text{eff}}/N$ , both being functions of the EEDF (see section 3).
- The expression of the electron-electron upflux  $G_{ee}$  involves linear functions of the EEDF, as confirmed by (12d) and (39a)-(39b).

The solution method adopted in solving the EBE depends on its linear/nonlinear features.

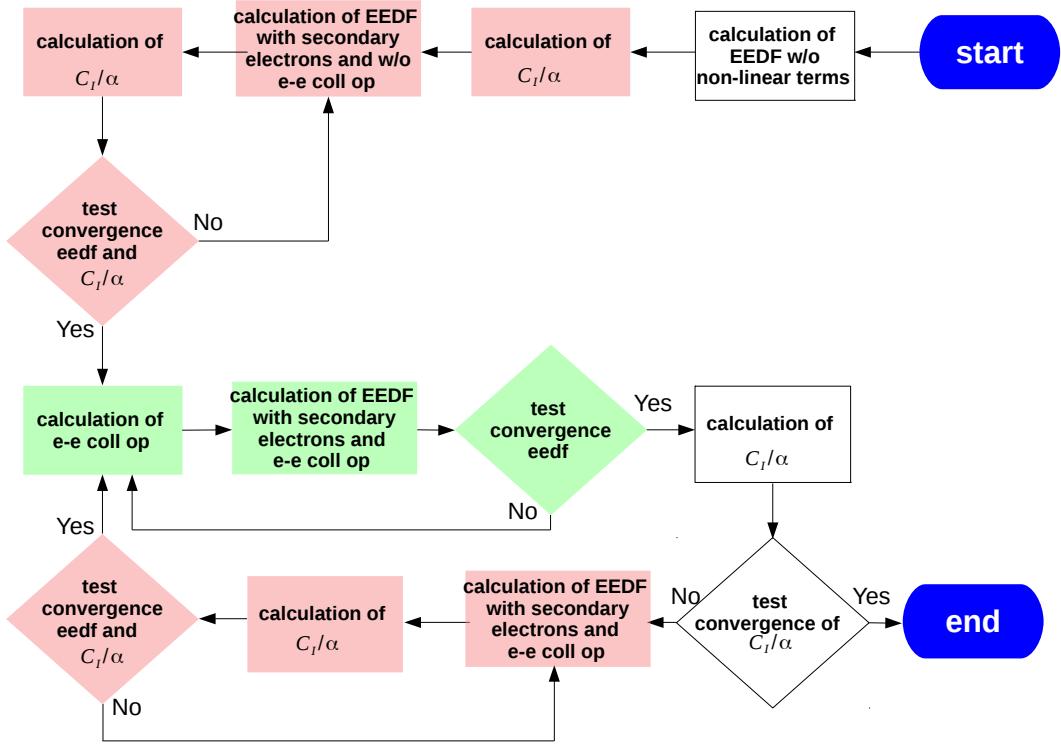


Figure 3: Simplified flowchart of LoKI-B, in the case of weak nonlinear effects. In red are the steps done within the ionization routine. In green are the steps done within the electron-electron collisions routine.

- In the absence of nonlinear effects (*e.g.*, for electropositive gases, with the ionization taken as a conservative mechanism and no electron-electron collisions), the EBE is solved adopting a very effective direct solution method. In this case the first equation of the Boltzmann system is added to the normalisation condition of the EEDF, *i.e.*  $\sum_{m=1}^N C_{1,m} f_m = \sum_{m=1}^N \sqrt{u_m} \Delta u f_m = 1$ , and the resulting non-homogeneous equation system becomes ready for direct inversion.
- When the matrix  $C(f)$  contains nonlinear terms, the EBE is solved using an iterative method.
  - In the case of weak nonlinear effects (*e.g.*, low electronegativity and low ionization degree), the solution can be obtained by using two iterative algorithms, based on successive direct solutions. The algorithm is represented in the simplified flowchart of figure 3, and it adopts:
    - \* a mixing of solutions to converge over the temporal growth parameter  $\langle \nu_{\text{eff}} \rangle / N$  or the spatial growth parameter  $\alpha_{\text{eff}} / N$ . In this case the convergence criterion looks for relative differences, between two consecutive iterations, below  $10^{-10}$  for the growth parameter and below a user-prescribed value (typically  $10^{-9}$ ) for the EEDF;
    - \* a Newton-Raphson-based approach to converge over the electron-electron collision operator. In this case the convergence criterion looks for relative differences, between two consecutive iterations, below  $\sim 10^{-9} - 10^{-10}$  for the ratio of the power “dissipated” in electron-electron collisions to the reference power  $\Theta_{ee}/\Theta_{\text{ref}}$  (see section 3 for the definition of  $\Theta_{\text{ref}}$ ), and below a user-prescribed value (typically  $10^{-9}$ ) for the EEDF.

When both algorithms are needed, the code ensures that the relative differences between the final EEDFs, obtained in each of the algorithms, are below a user-prescribed value for the EEDF.

- in the presence of strong nonlinear effects, the user is recommended to choose a relaxation method. In this case the EBE is solved with a time-dependent algorithm, using MATLAB’s ordinary differential equation solver `ode15s` [24], and the user can specify the (optional) parameters contained in the structure of the solver, *e.g.* maximum step-size (typical value  $10^{-7}$ ). The default convergence criterion demands relative variations of the EEDF below a user-prescribed value (typically  $10^{-9}$ ), between two consecutive iterations.

The solution of the time-dependent EBE adopts also a relaxation method, using MATLAB's ordinary differential equation solver `ode15s` [24]. When electron-electron collisions are included in the calculations, LoKI-B can solve the system of equations

$$\frac{\partial f(t)}{\partial t} = C[f(t)]f(t) \quad (43a)$$

$$\frac{dn_e(t)}{dt} = \langle \nu_{\text{eff}}(t) \rangle n_e(t) , \quad (43b)$$

subjected to some initial conditions  $f(t = 0) \equiv f_0$  and  $n_0$ . **Although this is implemented in LoKI-B, the option is not available by default. If needed, it can be easily activated by the user directly in the code.** The solver adopts a variable-step, variable-order algorithm suited for stiff problems, based on a set of highly-stable implicit integration formulas of orders 1 to 5 (optionally, it can also use the backward differentiation formulas). Specifically, the integrator estimates the error at each iteration and then adjusts the timestep  $\Delta t$  to improve either the accuracy (*i.e.* by decreasing the timestep) or the efficiency (*i.e.* by increasing the timestep). At each time  $t$  the solution is updated using  $f(t) = f(t - \Delta t) + (\partial f(t)/\partial t)\Delta t$  and  $n_e(t) = n_e(t - \Delta t) + (dn_e(t)/dt)\Delta t$ . Again, the user can specify the (optional) parameters contained in the structure of the solver, *e.g.* absolute tolerance (typical value  $10^{-300}$ ), relative tolerance (typical value  $10^{-6}$ ) and maximum step-size (typical value  $10^{-7}$ ), which are applied by the solver to adjust  $\Delta t$  for each instant  $t$ . The relative tolerance works as convergence criterion, imposing the maximum value of the relative variations of the EEDF, between two consecutive iterations.

### 3 Simulation output

On output, LoKI-B calculates the isotropic and the anisotropic parts of the electron distribution function, in addition to various electron macroscopic parameters obtained by integration over the EEDF (obtained from the solution to the EBE or adopting some other form prescribed by the user, *e.g.* a generalized Maxwellian EEDF), namely:

- swarm parameters (transport parameters and rate coefficients), which can be used to adjust complete sets of electron-scattering cross sections [25, 26] or as input parameters in macroscopic (fluid / global) plasma models [11, 27, 28];
- power-transfer terms [11, 18], providing the distribution of power among the different collisional channels and controlling the calculation errors.

The electron mean energy (in eV) is defined as

$$\varepsilon \equiv \int_0^\infty u^{3/2} f(u) du , \quad (44)$$

and is used to introduce the kinetic temperature (in eV)

$$T_e \equiv \frac{2}{3} \varepsilon . \quad (45)$$

The DC reduced transverse free-diffusion coefficient (in  $\text{m}^{-1} \text{s}^{-1}$ ) and the DC reduced mobility (in  $\text{V}^{-1} \text{m}^{-1} \text{s}^{-1}$ ) are calculated from [11, 18]

$$D_e N = \frac{\gamma}{3} \int_0^\infty \frac{u}{\Omega_x(u)} f(u) du \quad (46a)$$

$$\mu_e N = -\frac{\gamma}{3} \int_0^\infty \frac{u}{\Omega_x(u)} \frac{df(u)}{du} du , \quad (46b)$$

with  $x = c, \text{SST}$  for temporal or spatial growth of the electron density, respectively (see (11a)-(11b)), and these quantities allow defining the electron characteristic energy (in eV)

$$u_k \equiv \frac{D_e N}{\mu_e N} . \quad (47)$$

Similarly to (46a)-(46b), the DC reduced transverse diffusion coefficient and the DC reduced mobility for energy transport (in  $\text{eV m}^{-1} \text{s}^{-1}$  and  $\text{m}^{-1} \text{s}^{-1}$ , respectively) are calculated from

$$D_\varepsilon N = \frac{\gamma}{3} \int_0^\infty \frac{u^2}{\Omega_x(u)} f(u) du \quad (48a)$$

$$\mu_\varepsilon N = -\frac{\gamma}{3} \int_0^\infty \frac{u^2}{\Omega_x(u)} \frac{df(u)}{du} du , \quad (48b)$$

with  $x = c, \text{SST}$  for temporal or spatial growth of the electron density, respectively (see (11a)-(11b)).

In the case of HF simulations at  $\omega \gg \nu_c$ , in addition to the DC parameters (46a)-(48b) that might be of interest for fluid/global models, the code evaluates the *complex* HF mobility, with the real <sup>3</sup> and the imaginary parts given by [18]

$$\Re[\mu_{\text{HF}} N] = -\frac{\gamma}{3} \int_0^\infty \frac{u}{\Omega_{\text{PT}}(u)} \frac{df(u)}{du} du \quad (49a)$$

$$\Im[\mu_{\text{HF}} N] = \frac{\gamma}{3} \int_0^\infty \frac{u}{\Omega_{\text{PT}}(u)} \frac{\omega/N}{\Omega_c \gamma \sqrt{u}} \frac{df(u)}{du} du . \quad (49b)$$

---

<sup>3</sup>In the version `LoKI-B_v1.0.0`, the `swarmParameters` datafile in the output of HF simulations was writing the DC mobility, calculated from (46b) at  $\omega = 0$ , instead of the real part of the HF mobility. We acknowledge Ilija Stefanovic (Ruhr Universität Bochum, Germany) for pointing this out.

The rate coefficients (in  $\text{m}^3 \text{ s}^{-1}$ ), for excitation / de-excitation mechanisms between states  $i$  and  $j > i$ , are given by [11]

$$C_{i,j} = \gamma \int_0^\infty u \sigma_{i,j}(u) f(u) du \quad (50\text{a})$$

$$C_{j,i} = \gamma \int_0^\infty \frac{g_i}{g_j} (u + V_{i,j}) \sigma_{i,j}(u + V_{i,j}) f(u) du . \quad (50\text{b})$$

Note that (50a)-(50b) can be applied not only to the cross sections adopted for solving the EBE, but also to the *extra* set of cross sections defined by the user as additional input data of LoKI-B (see section 5).

The ionisation and the attachment rate coefficients are defined similarly to (50a) as

$$C_{i,\text{ion}} \equiv \frac{\langle \nu_{i,\text{ion}} \rangle}{N} = \gamma \int_0^\infty u \sigma_{i,\text{ion}}(u) f(u) du \quad (51\text{a})$$

$$C_{i,\text{att}} \equiv \frac{\langle \nu_{i,\text{att}} \rangle}{N} = \gamma \int_0^\infty u \sigma_{i,\text{att}}(u) f(u) du . \quad (51\text{b})$$

In a DC case, equations (7b) and (8b) can be integrated to define the electron mean drift velocity (in  $\text{m s}^{-1}$ )

$$v_d \equiv \frac{\gamma}{3} \int_0^\infty u f^1(u) du ,$$

yielding

$$v_d = \mu_e E , \text{ for a PT situation} \quad (52\text{a})$$

$$v_d = \mu_e E - D_e \frac{1}{n_e} \frac{dn_e}{dz} = \mu_e E - D_e \alpha_{\text{eff}} , \text{ for a SST situation} , \quad (52\text{b})$$

and equation (8a) can be integrated to define the effective Townsend coefficient

$$\alpha_{\text{eff}} = \frac{\langle \nu_{\text{ion}} \rangle - \langle \nu_{\text{att}} \rangle}{v_d} = \frac{\langle \nu_{\text{eff}} \rangle}{v_d} , \quad (53)$$

where

$$\begin{aligned} \langle \nu_{\text{ion}} \rangle &\equiv \sum_{k,i} \delta_{k_i} \langle \nu_{k_i,\text{ion}} \rangle \\ \langle \nu_{\text{att}} \rangle &\equiv \sum_{k,i} \delta_{k_i} \langle \nu_{k_i,\text{att}} \rangle , \end{aligned}$$

with

$$\frac{\alpha}{N} \equiv \frac{\langle \nu_{\text{ion}} \rangle / N}{v_d} \quad (54\text{a})$$

$$\frac{\eta}{N} \equiv \frac{\langle \nu_{\text{att}} \rangle / N}{v_d} \quad (54\text{b})$$

the first and the second reduced Townsend coefficients (in  $\text{m}^2$ ) for ionisation and attachment, respectively.

For DC/HF simulations involving the time-growth of the electron density, equations (51a)-(51b) are solved within each iteration on the convergence parameter  $\langle \nu_{\text{eff}} \rangle / N$  (see section 2).

For DC simulations involving the spatial-growth of the electron density, equations (52b) and (53) can be combined to yield

$$D_e \alpha_{\text{eff}}^2 - \mu_e E \alpha_{\text{eff}} + \langle \nu_{\text{eff}} \rangle = 0 , \quad (55)$$

and in this case (55) is solved within each iteration on the convergence parameter  $\alpha_{\text{eff}}$  (see section 2).

Moreover, in the case of HF simulations the parameters (52a)-(54b) are not calculated. In this case, equation (6) can be integrated to define the *time-dependent* electron drift velocity

$$v_d(t) \equiv \frac{\gamma}{3} \int_0^\infty u f^1(u, t) du = \Re \left[ \frac{\gamma}{3} \int_0^\infty u \tilde{f}^1(u) e^{j\omega t} du \right] \equiv \Re[\mu_{\text{HF}} E_p e^{j\omega t}] \quad ,$$

hence in this case the user can obtain  $v_d(t)$  from the HF mobility (49a)-(49b)

$$v_d(t) = \Re[\mu_{\text{HF}} E_p e^{j\omega t}] = \frac{E_p}{2} \Re[\mu_{\text{HF}} e^{j\omega t} + \mu_{\text{HF}}^* e^{-j\omega t}] = \{\Re[\mu_{\text{HF}} N] \cos(\omega t) - \Im[\mu_{\text{HF}} N] \sin(\omega t)\} \frac{\zeta E}{N} \quad .$$

The balance equation for the electron power-density, per electron at unit gas density, is obtained (depending on the particular PT/SST situation and solution algorithm considered) by multiplying either (42a) or (42b) by  $u\sqrt{2e/m_e}$  and integrating it over all energies; or by multiplying either (42c) or (42d) by  $u^{3/2}/N$  and integrating it over all energies. The general result writes (in  $\text{eV s}^{-1} \text{ m}^3$ )

$$\frac{\Theta(t)}{N} = \frac{\Theta_{\text{growth}}}{N} + \frac{\Theta_E}{N} + \frac{\Theta_{\text{coll}}}{N} \quad , \quad (56a)$$

where the different terms on the right-hand side represent, in order, the variation of the power density due to non-conservative mechanisms inducing a time/space net growth of the electron density, the power density gained from the applied electric field <sup>4</sup>, and the power density gained/lost in collisional (“coll”) events, which can be separately written as (note that all “gain” terms are positively defined and all “loss” terms are negatively defined).

$$\frac{\Theta_{\text{coll}}}{N} \equiv \frac{\Theta_{\text{coll}}^{\text{gain}}}{N} + \frac{\Theta_{\text{coll}}^{\text{loss}}}{N} \quad . \quad (56b)$$

The discretized form of (56a) can be obtained using the same finite-volume-like procedure as in section 2, applying Gauss’ theorem to an integral over a one-dimensional energy volume around the  $u_n^{\text{cell}}$  (see (25a)-(25b)). The terms  $\Theta(t)/N$  and  $\Theta_{\text{growth}}/N$  are straightforwardly obtained; the  $\Theta_{x=E,\text{coll}}/N$  terms involving upflux functions  $G_x(u)$  are handled as follows

$$\begin{aligned} \frac{\Theta_{x=E,\text{el,CAR}}}{N} &= -\frac{1}{N} \sum_n \int_{u_{n-1/2}^{\text{cell}}}^{u_{n+1/2}^{\text{cell}}} u \frac{dG_x(u)}{du} du = -\frac{1}{N} \sum_n u_n [G_{x_{n+1/2}} - G_{x_{n-1/2}}] \\ &= \gamma \sum_n \left\{ u_n \left[ g_{x_{n+1/2}} \left( \frac{d_x}{2} (f_n + f_{n+1}) + \frac{c_x}{\Delta u} (f_{n+1} - f_n) \right) \right. \right. \\ &\quad \left. \left. - g_{x_{n-1/2}} \left( \frac{d_x}{2} (f_{n-1} + f_n) + \frac{c_x}{\Delta u} (f_n - f_{n-1}) \right) \right] \right\} \\ &= \gamma \left\{ \sum_{n=1}^N u_n \left[ g_{x_{n+1/2}} \left( \frac{d_x}{2} - \frac{c_x}{\Delta u} \right) - g_{x_{n-1/2}} \left( \frac{d_x}{2} + \frac{c_x}{\Delta u} \right) \right] f_n \right. \\ &\quad \left. + \sum_{n=1}^N u_n \left[ g_{x_{n+1/2}} \left( \frac{d_x}{2} + \frac{c_x}{\Delta u} \right) \right] f_{n+1} - \sum_{n=1}^N u_n \left[ g_{x_{n-1/2}} \left( \frac{d_x}{2} - \frac{c_x}{\Delta u} \right) \right] f_{n-1} \right\} \\ &= \gamma \left\{ \sum_{n=1}^N u_n \left[ g_{x_{n+1/2}} \left( \frac{d_x}{2} - \frac{c_x}{\Delta u} \right) - g_{x_{n-1/2}} \left( \frac{d_x}{2} + \frac{c_x}{\Delta u} \right) \right] f_n \right. \\ &\quad \left. + \sum_{n=2}^{N+1} u_{n-1} \left[ g_{x_{n-1/2}} \left( \frac{d_x}{2} + \frac{c_x}{\Delta u} \right) \right] f_n - \sum_{n=0}^{N-1} u_{n+1} \left[ g_{x_{n+1/2}} \left( \frac{d_x}{2} - \frac{c_x}{\Delta u} \right) \right] f_n \right\} \\ &= \gamma \left[ \sum_{n=1}^N (u_n - u_{n+1}) g_{x_{n+1/2}} \left( \frac{d_x}{2} - \frac{c_x}{\Delta u} \right) - (u_n - u_{n-1}) g_{x_{n-1/2}} \left( \frac{d_x}{2} + \frac{c_x}{\Delta u} \right) \right] f_n \end{aligned}$$

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<sup>4</sup>Note that the electron power-density gained from the applied electric field corresponds to

$$\frac{\Theta_E}{N} = \begin{cases} \mu_e N \left( \frac{E}{N} \right)^2, & \text{for DC simulations} \\ \Re[\mu_{\text{HF}} N] \left( \frac{E}{N} \right)^2, & \text{for HF simulations} \end{cases} .$$

$$= \gamma \left[ \sum_{n=1}^{\mathcal{N}} g_{x_{n+1/2}} \left( c_x - d_x \frac{\Delta u}{2} \right) - g_{x_{n-1/2}} \left( c_x + d_x \frac{\Delta u}{2} \right) \right] f_n , \quad (57a)$$

where we have used the boundary conditions  $g_{x_{1/2}} = g_{x_{\mathcal{N}+1/2}} = 0$ ; and the remainder collisional terms  $\Theta_{x=\text{coll}}/N$  are obtained as follows (for example for an inelastic collision (i,j); see (41a))

$$\begin{aligned} \frac{\Theta_{(i,j),\text{inel}}^{\text{loss}}}{N} &= \gamma \sum_n \int_{u_{n-1/2}^{\text{cell}}}^{u_{n+1/2}^{\text{cell}}} S_{(i,j)}|_{\text{inel}}(u) u du \\ &= \delta_i \gamma \sum_{n=1}^{\mathcal{N}} u_n \left[ u_{n+l_{i,j}} \frac{\sigma_{(i,j)_{n+l_{i,j}}} + \sigma_{(i,j)_{n+l_{i,j}+1}}}{2} f_{n+l_{i,j}} - u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_n \right] \Delta u \\ &= \delta_i \gamma \sum_{n=l_{i,j}+1}^{l_{i,j}+\mathcal{N}} u_{n-l_{i,j}} u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_n \Delta u - \sum_{n=1}^{\mathcal{N}} u_n u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_n \Delta u \\ &= \delta_i \gamma \sum_{n=1}^{\mathcal{N}} (u_{n-l_{i,j}} - u_n) u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_n \Delta u \\ &= -\delta_i \gamma \sum_{n=1}^{\mathcal{N}} \left[ u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_n \Delta u \right] V_{i,j} , \end{aligned} \quad (57b)$$

where we have used the boundary conditions  $\sigma_{(i,j)_n} = 0$  for  $n \leq l_{i,j}$ , and  $f_n = 0$  for  $n > \mathcal{N}$ .

Therefore, the different terms on the right-hand side of (56a) are

$$\frac{\Theta_{\text{growth}}}{N} = \begin{cases} -\frac{\langle \nu_{\text{eff}} \rangle}{N} \varepsilon \\ \rightarrow -\frac{\langle \nu_{\text{eff}} \rangle}{N} \sum_{n=1}^{\mathcal{N}} u_n^{3/2} f_n \Delta u , \text{ for a PT situation} \\ -\frac{\alpha_{\text{eff}}}{N} (\mu_\varepsilon E - D_\varepsilon \alpha_{\text{eff}}) \\ \rightarrow -\frac{\alpha_{\text{eff}}}{N} \frac{\gamma}{3} \sum_{n=1}^{\mathcal{N}} u_n^2 \left[ -\frac{E/N}{\Omega_{\text{SST}_n}} \frac{f_{n+1} - f_{n-1}}{2\Delta u} - \frac{\alpha_{\text{eff}}/N}{\Omega_{\text{SST}_n}} f_n \right] \Delta u , \text{ for a SST situation} \end{cases} \quad (58a)$$

$$\begin{aligned} \frac{\Theta_E}{N} &= -\frac{1}{N} \int_0^\infty u \frac{dG_E(u)}{du} du \\ &\rightarrow \gamma \sum_{n=1}^{\mathcal{N}} \left[ g_{E_{n+1/2}} \left( c_E - d_E \frac{\Delta u}{2} \right) - g_{E_{n-1/2}} \left( c_E + d_E \frac{\Delta u}{2} \right) \right] f_n \end{aligned} \quad (58b)$$

$$\begin{aligned} \frac{\Theta_{x=\text{el,CAR}}}{N} &= -\frac{1}{N} \int_0^\infty u \frac{dG_x(u)}{du} du \\ &\rightarrow \gamma \sum_{n=1}^{\mathcal{N}} \left[ g_{x_{n+1/2}} \left( c_x - d_x \frac{\Delta u}{2} \right) - g_{x_{n-1/2}} \left( c_x + d_x \frac{\Delta u}{2} \right) \right] f_n \end{aligned} \quad (58c)$$

$$\begin{aligned} \frac{\Theta_{x=\text{el,CAR}}^{\text{gain}}}{N} &= \gamma \int_0^\infty u \frac{d}{du} \left[ g_x(u) c_x \frac{df(u)}{du} \right] du \\ &\rightarrow \gamma \sum_{n=1}^{\mathcal{N}} c_x [g_{x_{n+1/2}} - g_{x_{n-1/2}}] f_n \end{aligned} \quad (58d)$$

$$\frac{\Theta_{x=\text{el,CAR}}^{\text{loss}}}{N} = \frac{\Theta_{x=\text{el,CAR}}}{N} - \frac{\Theta_{x=\text{el,CAR}}^{\text{gain}}}{N} \quad (58e)$$

$$\begin{aligned} \frac{\Theta_{ee}}{N} &= -\frac{1}{N} \int_0^\infty u \frac{dG_{ee}(u)}{du} du \\ &\rightarrow \gamma \sum_{n=1}^{\mathcal{N}} (A_n - B_n) f_n (\Delta u)^2 \end{aligned} \quad (58f)$$

$$\frac{\Theta_{ee}^{\text{gain}}}{N} = \gamma \int_0^\infty u \frac{d}{du} \left[ g_{ee}(u) J(u) \frac{df(u)}{du} \right] du$$

$$\rightarrow \gamma \sum_{n=1}^N (A_{J_n} - B_{J_n}) f_n (\Delta u)^2 \quad (58g)$$

$$\frac{\Theta_{ee}^{\text{loss}}}{N} = \frac{\Theta_{ee}}{N} - \frac{\Theta_{ee}^{\text{gain}}}{N} \quad (58h)$$

$$\begin{aligned} \frac{\Theta_{\text{sup}}^{\text{gain}}}{N} &= \gamma \sum_{i,j>i} \int_0^\infty S_{i,j}|_{\text{sup}}(u) u du = \sum_{i,j>i} \delta_j C_{j,i} V_{i,j} \\ &\rightarrow \sum_{i,j>i} \delta_j \gamma \frac{g_i}{g_j} \sum_{n=1}^N \left[ u_{n+l_{i,j}} \frac{\sigma_{(i,j)_{n+l_{i,j}}} + \sigma_{(i,j)_{n+l_{i,j}+1}}}{2} f_n \Delta u \right] V_{i,j} \end{aligned} \quad (58i)$$

$$\begin{aligned} \frac{\Theta_{\text{inel}}^{\text{loss}}}{N} &= \gamma \sum_{i,j>i} \int_0^\infty S_{i,j}|_{\text{inel}}(u) u du = - \sum_{i,j>i} \delta_i C_{i,j} V_{i,j} \\ &\rightarrow - \sum_{i,j>i} \delta_i \gamma \sum_{n=1}^N \left[ u_n \frac{\sigma_{(i,j)_n} + \sigma_{(i,j)_{n+1}}}{2} f_n \Delta u \right] V_{i,j} \end{aligned} \quad (58j)$$

$$\begin{aligned} \frac{\Theta_{\text{ion}}}{N} &= \gamma \sum_i \int_0^\infty S_{i,\text{ion}}(u) u du = - \sum_i \delta_i C_{i,\text{ion}} V_{i,\text{ion}} \\ &\rightarrow \gamma \sum_i \sum_{n=1}^N S_{(i,\text{ion})_n} u_n \Delta u \end{aligned} \quad (58k)$$

$$\begin{aligned} \frac{\Theta_{\text{att}}}{N} &= \gamma \sum_i \int_0^\infty S_{i,\text{att}}(u) u du \\ &\rightarrow \gamma \sum_i \sum_{n=1}^N S_{(i,\text{att})_n} u_n \Delta u \end{aligned} \quad (58l)$$

In these equations, the labels “inel” and “sup” refer to inelastic and superelastic collisions, respectively, associated with electronic, vibrational and rotational excitation / de-excitation mechanisms.

The left-hand side of (56a) is

$$\frac{\Theta(t)}{N} = \begin{cases} 0, & \text{for stationary simulations} \\ \frac{1}{N} \frac{\partial \varepsilon(t)}{\partial t}, & \text{for time-dependent simulations (see section 1.3)} \end{cases}. \quad (59)$$

The quantity  $\Theta(t)/N$  is numerically calculated by summing all the power terms on the right-hand side of (56a), and on output the value of this quantity is tagged as *Power balance* (see section 5.4).

In stationary simulations, the code evaluates the relative power balance equation, dividing (56a) by the *reference power-density* (per electron at unit gas density)  $\Theta_{\text{ref}}/N$ , with the latter defined as the sum of all power-gain terms. Usually, the stationary power balance is satisfied to at least  $\sim 10^{-10}\%$ , and the user can define a threshold value for the relative power balance above which the code returns a warning message (see section 5.2).

In time-dependent simulations, equation (56a) is as accurate as the numerical solution of the EBE, being satisfied to at least  $\sim 1\%$  (according to the relative tolerance imposed as parameter to the ode solver, see section 5.2).

As mentioned, LoKI-B can also adopt a generalized Maxwellian EEDF prescribed by the user (see section 1.4). In terms of output, the previous expressions hold for all swarm parameters, but are taken in a slightly different way for the power-transfer terms.

For the latter, the following applies

- the electron power density gained from the applied electric field is deduced from the (stationary) power balance equation, obtained from (56a)-(56b) at  $\Theta(t)/N = \Theta_{\text{growth}}/N = 0$

$$\frac{\Theta_E}{N} = -\frac{\Theta_{\text{coll}}}{N} \equiv -\frac{\Theta_{\text{coll}}^{\text{gain}}}{N} - \frac{\Theta_{\text{coll}}^{\text{loss}}}{N}, \quad (60a)$$

with the  $\Theta_{\text{coll}}^{\text{gain}}/N$  and  $\Theta_{\text{coll}}^{\text{loss}}/N$  obtained from the different terms (58c)-(58k), calculated for the prescribed EEDF (22);

- the *equivalent* applied reduced electric-field is deduced from

$$\frac{E}{N} = \sqrt{\frac{-\Theta_{\text{coll}}/N}{(\Theta_E/N)/(E/N)^2}} , \quad (60\text{b})$$

where the expression in the denominator corresponds to (58b) divided by the square of the reduced electric-field <sup>5</sup>;

- the electron power density transferred in collisional events is calculated assuming conservative mechanisms only, *i.e.* treating ionization as an excitation mechanism and setting to zero the power-transfer due to attachment.

For this reason, **selecting `prescribedEedf` for studying electronegative gases is not recommended.**

---

<sup>5</sup>In practice, the *equivalent* applied reduced electric-field is deduced from

$$\frac{E}{N} = \begin{cases} \sqrt{\frac{-\Theta_{\text{coll}}/N}{\mu_e N}} , & \text{for DC simulations} \\ \sqrt{\frac{-\Theta_{\text{coll}}/N}{\Re[\mu_{\text{HF}} N]}} , & \text{for HF simulations} \end{cases}$$

## 4 The “How to...” basics

This section provides basic information enabling a user to quickly obtain and run LoKI-B for the first time.

### 4.1 How to obtain the code

You can obtain the last version of the code from the github URL

<https://github.com/IST-Lisbon/LoKI>

by downloading the LoKI-B\_v2.2.0 zip-file and extract it to your local repository.

### 4.2 How to find my way in the code

The LoKI-B\_v2.2.0 folder contains

1. A subfolder **Documentation** containing the user manual and relevant papers.
2. A subfolder **Code** containing
  - (a) Several **\*.m** files corresponding to the MATLAB® code, of which **'lokibcl.m'** is the main file.
  - (b) A subfolder **Input**, containing the input files required for the simulations, organised as follows
    - i. Default configuration files **'default\_lokib\_setup.in'** and **'default\_lokib\_pulse\_setup.in'** (see sections 4.3 and 5).
    - ii. A subfolder **Databases** with **'\*.txt'** files, containing different properties (masses, energies of states, atomic/molecular constants, ...) for the gases used in the simulations.
    - iii. Several subfolders **Helium**, **Nitrogen**, ... with **'\*.txt'** files, containing the electron-scattering cross sections for the different gases used in the simulations, usually obtained from the open-access website LXCat (<http://www.lxcat.net/>; see section 6).
  - (c) A subfolder **PropertyFunctions**, with several **\*.m** auxiliary functions for calculating the values of universal constants, some predefined distribution of states (Boltzmann, Treanor, ...), the energy of the states according to some models, etc. (see section 7.1).
  - (d) A subfolder **OtherAuxFunctions**, with several **\*.m** auxiliary functions that provide the calculations of other properties, rate coefficients, working conditions, etc. (see section 7.2).
  - (e) A subfolder **Output** (eventually), where LoKI-B will write the output files resulting from the simulations (see section 5.4).

### 4.3 How to run the code

LoKI-B is developed under MATLAB®, to benefit from its matrix-based architecture. The minimum requirements to run the code is a computer with an installation of MATLAB® (recommended version R2017b; we cannot ensure that all the features of LoKI-B will work properly under different versions).

LoKI-B runs upon calling the MATLAB® function **lokibcl(setupFile)**. The end user interacts with the code by specifying a particular “setup” for the simulation. This setup is sent to the **lokibcl()** function through the *required* input argument **setupFile**. As mentioned in section 4.2, the setup files should be located in **[repository folder]/LoKI-B\_v2.2.0/Code/Input/** with a **.in** extension (this is just a recommendation in order to keep the input folder organised; the setup files are just plain text files).

The distribution of LoKI-B includes a couple of default configuration files (**'default\_lokib\_setup.in'** and **'default\_lokib\_pulse\_setup.in'**), for the benefit of the user. By using one of these files, it is very easy to make a first run of the code, just following the sequence of steps below. For example, using the **'default\_lokib\_setup.in'** setup file:

1. Open MATLAB®
2. Navigate to the **Code** folder of your local copy of the repository:  
`>> cd [repository folder]/LoKI-B_v2.2.0/Code/`

3. Execute the following command in the MATLAB® console:  
`>> lokibcl('default_lokib_setup.in')`
4. The graphical user interface (GUI) should appear showing the solution(s) for the default setup file, represented in figure 4.

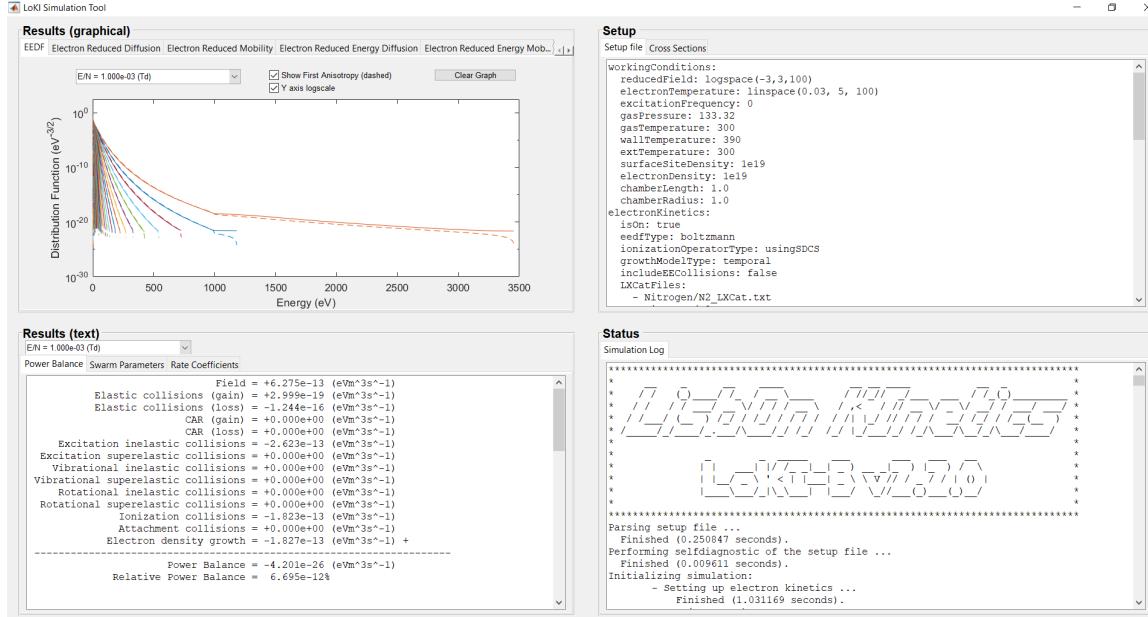


Figure 4: Graphical user interface output, for the default setup-file of LoKI-B (stationary simulations).

**Congratulations! You have now concluded your first LoKI-B simulation.**

Now, in order to run the code for different simulations, you just have to call the `lokibcl()` function with a different setup file, or a modified version of the default ones. The details on how to configure the setup file according to your needs are given in section 5.

#### 4.4 How to contact us

After downloading LoKI-B, and especially if you intend to interact with us, you are invited to send a short message

to [loki@tecnico.ulisboa.pt](mailto:loki@tecnico.ulisboa.pt)

with subject LoKI-B

just giving your name and affiliation.

#### 4.5 How to reference the code

LoKI-B is the result of the efforts of the Portuguese group N-PRiME, that decided to share the outcome of its research with the members of the Low-Temperature Plasmas community.

When using LoKI-B in your work, please give proper credits to the main developers, by adding the following citations

- Tejero A *et al* *The LisbOn KInetics Boltzmann solver* 2019 *Plasma Sources Sci. Technol.* **28** 043001.
- Tejero A *et al* *On the quasi-stationary approach to solve the electron Boltzmann equation in pulsed plasmas* 2021 *Plasma Sources Sci. Technol.* **30** 065008.

## 5 The setup file

The setup file is the main input file of LoKI-B, as well as the main User Interface (UI) with the code.

The setup file is an **indentation structured file**, *i.e.* it follows the “Off-side rule” [29] like in some programming languages such as Python. This means that it is **mandatory** that all the subfields within a field share the same level of indentation, otherwise the behaviour of the code is undefined.

In this file, the user can provide / select relevant information, namely

- about physical parameters
  - working conditions
  - collisional data
  - atomic and molecular data
  - species populations
- about physical models
  - mode of energy-sharing in ionisation collisions
  - type of growth model for the electron density
  - inclusion of electron-electron collisions
- about numerical details
  - energy grid for LoKI-B
  - nonlinear algorithm(s) to adopt in the simulations
  - convergence criteria for iterative cycles
  - integration times

The setup file is organised according to the following syntax rules.

- The setup file can include comments, signaled by the character **%**.
- Some of the fields in the setup file can accept either one or more values.  
When only one value is to be specified, it can be given in the same line of the field, right after the colon, for example:

```
mass: Databases/masses.txt
```

Alternatively, when more than one value are to be specified, one can use several lines starting with a dash, for example

```
LXCatFiles: % cross section files
- Nitrogen/N2_LXCat.txt
- Nitrogen/N2_rot_LXCat.txt
```

Note that the value(s) of certain fields in the setup file can be defined specifying an “auxiliary input file” or a “property function”. All the “auxiliary input files” (*i.e.* LXCat files or property files) specified in the setup file should be located inside the input folder ([repository folder]/LoKI-B\_v2.2.0/Code/Input), eventually organised in subfolders with self-explanatory names (*e.g.* Nitrogen, Databases; see section 4.2). In this case, the name of the subfolder should be specified in the setup file (see examples above for `mass` and for `LXCatFiles`). For more information about auxiliary input files see section 6. All the “property functions” specified in the setup file should be located in the property functions folder ([repository folder]/LoKI-B\_v2.2.0/Code/Property Functions; see section 4.2). For more information about property functions see section 7.1.

The setup file is organised into four different main fields, with self-explanatory designations:

- `workingConditions`
- `electronKinetics`
- `gui`
- `output`.

The next subsections present these fields in detail, using nitrogen as example.

## 5.1 Working conditions

In this field of the setup file the user can specify the values of the different working parameters for the simulation. Code 1 shows the section of the '`default_lokib_setup.in`' file that handles this configuration.

```
% --- configuration of the working conditions ---
workingConditions:
  reducedField: logspace(-3,3,100)          % in Td
  electronTemperature: linspace(0.03, 5, 300) % in eV
  excitationFrequency: 0                     % in Hz
  gasPressure: 133.32                        % in Pa
  gasTemperature: 300                         % in K   (average gas temperature)
  wallTemperature: 390                        % in K   (wall temperature)
  extTemperature: 300                         % in K   (external temperature)
  surfaceSiteDensity: 1e19                    % in m^-2 (used for surface kinetics)
  electronDensity: 1e19                       % in m^-3
  chamberLength: 1.0                          % in m
  chamberRadius: 1.0                         % in m
```

Code 1: Configuration of the working conditions of the simulation

### IMPORTANT NOTES:

- The `reducedField` corresponds to  $E/N$ , where
  - $E = E_p$  is the amplitude of the applied electric field, in a DC case;
  - $E = E_p/\sqrt{2}$  is the root-mean-square (RMS) amplitude of the applied electric field, in a HF case.
- The `reducedField` can also contain information about a non-oscillatory ( $\omega = 0$ ) electric-field pulse, in which case it reads

```
% --- configuration of the working conditions ---
workingConditions:
  reducedField: pulse@reducedFieldPulse, 1e-18, 2e-6, logspace, 200, 1e-6, 50
  % reducedField: pulse@reducedFieldRamp, 1e-18, 1e-8, logspace, 200, 1e-9, 75
  % pulse@functionName, firstStep, finalTime, samplingType, samplingPoints, additionalParameters
```

Code 2: Configuration of the reducedField for an electric-field pulse

where the field parameters are, in order,

- the name of the pulse function (providing  $E/N$  values in Td, as a function of time) The current distribution of LoKI-B includes the following pulse functions:

\* `pulse@reducedFieldPulse`, corresponding to

$$\frac{E(t)}{N}(\text{Td}) = \frac{E_0}{N} \sqrt{\frac{t}{\tau_{\text{rise}}}} \exp\left(-\frac{t}{\tau_{\text{rise}}}\right) . \quad (61)$$

\* `pulse@reducedFieldRamp`, corresponding to

$$\frac{E(t)}{N} (\text{Td}) = \begin{cases} \frac{E_0/N}{\tau_{\text{rise}}} t, & 0 \leq t \leq \tau_{\text{rise}} \\ \frac{E_0}{N}, & t > \tau_{\text{rise}} \end{cases} . \quad (62)$$

- the first time step (in s) for the simulation output
- the final time (in s) for the simulations and the simulation output
- the type of sampling for the time steps used in the output (`logspace` or `linspace`)
- the number of sampling points in the simulation output
- any additional parameters (optional) assisting the construction of the pulse function (*e.g.* the values of variables  $E_0/N$  and  $\tau_{\text{rise}}$  in equations (61) and (62)).

Note the following, when adopting an electric-field pulse:

- the `excitationFrequency` **MUST** be set to zero;
- the simulation runtimes can rapidly increase, especially for very long pulse-times, and/or high gas pressures, and/or a very large number of sampling points. User discretion is advised, when defining these parameters (the set of working conditions presented above for the `reducedField` is a good compromise example);
- users should be aware that keeping the graphical user interface activated (see section 5.3) can also degrade the simulation runtimes;
- it is recommended to adopt a constant energy grid (see 5.2), chosen as to ensure the correct description of the EEDF for both the minimum  $E(t)/N$  value in the simulations (considering low threshold mechanisms), and the maximum  $E(t)/N$  value in the simulations (considering the bulk-to-tail drop in the EEDF);
- it is recommended to activate the optional parameters for the ode solver adopted in the `temporalIntegration` algorithm (see sections 2 and 5.2): absolute tolerance, relative tolerance, and maximum step-size. Users should understand the role of these parameters before activating them in the simulations.

- The user can choose simulations that solve the EBE or that adopt a generalized Maxwellian EEDF (see section 1.4 and section 5.2 for details on how to select the type of simulation for the EEDF):
  - the parameter `reducedField` is activated when the “boltzmann” simulation is selected;
  - the parameter `electronTemperature` is activated when the “prescribedEedf” simulation is selected.

For the parameters `reducedField` and `electronTemperature`, it is possible to specify a single value, for a single simulation, or an array of values, for several simulations corresponding to the different values prescribed. The array of values can be defined using any expression understood by MATLAB® (*e.g.* `logspace(-4,1,100)`, `linspace(0,100,10)`, `[0 10 20 50]`, etc.), with the exception of those adopting the colon character “`:`” (*e.g.* `1:10` is not supported). In future releases of LoKI-B, this feature will probably be extended to other parameters.

- The `excitationFrequency` corresponds to the linear oscillation frequency  $\omega/(2\pi)$ .
- Not all the parameters in Code 1 are used in all the simulations. Indeed, the `gasTemperature`  $T_g$  is needed to calculate the elastic and the CAR operators (12b) and (12c), whereas the `gasPressure`  $p$  is required to calculate the total gas density only in the particular case of HF excitations (for obtaining the reduced frequency  $\omega/N$ ) and/or if electron-electron collisions are considered in the calculations (for obtaining the ionisation degree  $n_e/N$ , in which case it is also necessary to provide the `electronDensity`  $n_e$ ). Moreover, the parameters `wallTemperature`, `extTemperature`, `surfaceSiteDensity`, `chamberLength` and `chamberRadius` are not used in LoKI-B simulations.  
The user can comment the line(s) of Code 1 that specify the value(s) of parameter(s) not used in the simulations. Alternatively these lines can be kept uncommented, but in this case **it is mandatory to specify the values of the corresponding parameters**, regardless the fact that they are not used in the simulations (the values of these parameters will have no impact in the final results).
- Again, the code uses SI units for all physical quantities, except the energies that are expressed in eV (electron-volt) and the reduced fields that are expressed in Td (Townsend; 1 Td =  $10^{-21}$  V m<sup>2</sup>).

## 5.2 Electron kinetics

In this field of the setup file the user can define all the details related to the electron kinetics. Code 3 shows the section of the '`default_lokib_setup.in`' file that handles this configuration.

```
% --- configuration of the electron kinetics ---
electronKinetics:
    isOn: true                      % true or false (to activate or deactivate the electron kinetics)
    eedfType: boltzmann               % boltzmann or prescribedEedf (generalized expression Maxwellian/Druyvesteyn)
%   shapeParameter: 1      % prescribedEedf shape parameter from 1 (Maxwellian) to 2 (Druyvesteyn)
    ionizationOperatorType: usingSDCS % conservative, oneTakesAll, equalSharing or usingSDCS
    growthModelType: temporal        % temporal or spatial
    includeEECollisions: false       % true or false (to include / remove e-e collisions)
    LXCatFiles:                      % cross section files
        - Nitrogen/N2_LXCat.txt
        - Nitrogen/N2_rot_LXCat.txt
%   LXCatFilesExtra: extra_LXCat.txt % extra cross section files
%   effectiveCrossSectionPopulations: % see doc
%       - N2_effectivePop.txt
%   CARGases:                      % gases for which CAR is activated
%       - N2
gasProperties:                  % properties of the gases (S.I. Units)
    mass: Databases/masses.txt
    fraction:
        - N2 = 1
    harmonicFrequency: Databases/harmonicFrequencies.txt
    anharmonicFrequency: Databases/anharmonicFrequencies.txt
    rotationalConstant: Databases/rotationalConstants.txt
    electricQuadrupoleMoment: Databases/quadrupoleMoment.txt
    OPBParameter: Databases/OPBParameter.txt
stateProperties:                 % properties of the states (S.I. Units except for the energy [eV])
    energy:
        - N2(X,v=*) = harmonicOscillatorEnergy
        - N2(X,v=0,J=*) = rigidRotorEnergy
    statisticalWeight:
        - N2(X,v=*) = 1.0
        - N2(X,v=0,J=*) = rotationalDegeneracy_N2
population:
    - N2(X) = 1.0
    - Nitrogen/N2_vibpop.txt
    - N2(X,v=0,J=*) = boltzmannPopulation@gasTemperature
numerics:                         % configuration of numerical details of the simulation
    energyGrid:                     % properties of the energy grid (in eV)
    maxEnergy: 1                   % (use 18-20 for time-dependent simulations)
    cellNumber: 1000                % (use 1800-2000 for time-dependent simulations)
    smartGrid:                      % configuration of the smart grid
        minEedfDecay: 20            % minimum number of decade-fall for the EEDF
        maxEedfDecay: 25            % maximum number of decade-fall for the EEDF
        updateFactor: 0.05           % factor used to increase or decrease the maximum value of the energy grid
maxPowerBalanceRelError: 1e-9
% threshold for the relative power balance warning message (use at least 100 for time-dependent simulations)
nonLinearRoutines:
    algorithm: mixingDirectSolutions % mixingDirectSolutions or temporalIntegration
    mixingParameter: 0.7             % mixingDirectSolutions mixing parameter from 0 to 1
    maxEedfRelError: 1e-9 % maximum rel. variation for EEDF between two iterations (stop criterion)
%   odeSetParameters:             % optional parameters for ode solver of "temporalIntegration" algorithm
%       AbsTol: 1e-300
%       RelTol: 1e-6
%       MaxStep: 1e-7
```

Code 3: Configuration of the electron kinetics of the simulation

### IMPORTANT NOTES:

- The `isOn` allows the user to activate (`true`) or deactivate (`false`) the simulations of LoKI-B.
- The `eefdfType` allows the user to specify the type of simulation for the EEDF:
  - `boltzmann`, corresponding to the solution of the EBE under the classical two-term approximation;
  - `prescribedEedf`, corresponding to a prescribed generalised Maxwellian EEDF at given electron temperature  $T_e$  (see sections 1.4 and 5.1)
- The `shapeParameter` allows the user to specify the shape parameter  $s$ , when a `prescribedEedf` is selected (see section 1.4).
- The `ionizationOperatorType` allows the user to choose the type of ionisation operator with the EBE. The possible configurations are (see section 1.2):
  - `conservative`: the ionisation is treated as an excitation process;
  - `oneTakesAll`: the ionisation is treated as a non-conservative mechanism, with the new-born secondary electron introduced at zero kinetic-energy and the scattered electron taking the remaining energy after an ionisation event.
  - `equalSharing`: the ionisation is treated as a non-conservative mechanism, with the remaining energy after the event being equally shared between the scattered and the secondary electrons.
  - `usingSDCS`: the ionisation is treated as a non-conservative mechanism, described by considering a Single Differential Cross Section (SDCS) that depends on the energies of the primary and the secondary electrons.

In general, the available experimental data for SDCS is scarce and often measured for only a few energy values of the primary electron. Here, we have adopted the comprehensive set of measurements of Opal *et al* [30], for the double differential cross section of different gases, resolved on both the energy and the angle of the secondary electron. This pioneering work proposes differential ionization cross sections with a very reliable shape [31], which can be normalized from available experimental data for the corresponding integral cross sections (see (14)). Indeed, after integration over the angles, and by comparing the energy distributions of the secondary electrons for different energies of the primary electrons, these authors proposed a fitting expression for the SDCS

$$\sigma_{i,\text{ion}}^{\text{sec}}(u', u) = \frac{\sigma_{i,\text{ion}}(u')}{w \arctg [(u' - V_{i,\text{ion}})/(2w)]} \frac{1}{1 + (u/w)^\beta} , \quad (63)$$

where  $\beta \simeq 2$  and  $w$  is a parameter close to the ionisation threshold  $V_{i,\text{ion}}$ , which is set for each gas according to the original estimates [30]. Note that (63) satisfies exactly the expression (14) for the integral cross section  $\sigma_{i,\text{ion}}$ , and therefore it is used in LoKI-B to describe the energy distribution of the electrons involved in ionisation events, using available data and mitigating possible normalisation errors.

The value of  $w$  is introduced via the `OPBParameter`, in the `gasProperties` section (see below), and should be provided by the user if the choice of the `ionizationOperatorType` is `usingSDCS`. If no value is provided for this parameter, the code will take  $w$  for each state equal to the corresponding ionisation potential.

- The `growthModelType` allows the user to specify the configuration of the growth model, `spatial` or `temporal`, for the electron density (see section 1.2);

The parameter `growthModelType` is **mandatory**, being used if the choice of the `ionizationOperatorType` is different than `conservative`, and/or in the case of electronegative gases (with non-conservative attachment mechanisms).

When choosing `growthModelType` equal to `spatial` the user **MUST** adopt a DC applied electric field, hence `excitationFrequency` must be set equal to 0 in this case.

Note that all non-conservative modes (`oneTakesAll`, `equalSharing`, `usingSDCS` and the presence of attachment collisions) activate non-linear operators for the creation / destruction of electrons, hence code performance is expected to decrease in these cases.

- The `includeEECollisions` allows the user to activate (`true`) or deactivate (`false`) the electron-electron collision operator in LoKI-B.

The parameter `includeEECollisions` is **mandatory**.

Note that the inclusion of electron-electron collisions activates a non-linear operator, hence code performance is expected to decrease in this case.

When performing time-dependent simulations, it is possible to handle electron-electron collisions considering a time-dependent electron-density  $n_e(t)$ , calculated according to the solution of equation (43b) (see section 2), for an initial value  $n_0$  defined by the parameter `electronDensity` in the `workingConditions`. The calculation of  $n_e(t)$  is activated through the expression

```
boltzmann.eDensIsTimeDependent = true
```

in function `obtainTimeDependentSolution(boltzmann)` with the `Boltzmann.m` class. To deactivate this calculation the user should select the logical parameter `false`, instead.

Note that the previous expression only activates the calculation of  $n_e(t)$ . To use the time-evolution of the electron density in the electron-electron collisions operator, the user must further activate electron-electron collisions by setting `includeEECollisions: true` in the setup file.

- In `LXCatFiles` the user can specify the text files (along with the corresponding path) containing the electron-scattering cross sections for the different gases used in the simulations, usually obtained from the open-access website LXCat (<http://www.lxcat.net/>). From these files, the code obtains also information about all the gases and all the states that are targets and/or products in the electron collisions.

**Note that not every cross section datafile obtained from LXCat is accepted, since it must comply with certain format requirements for LoKI-B to retrieve the relevant data; see section 6.1 for more information.**

- When `LXCatFilesExtra` is activated, the user can specify the text files (along with the corresponding path) containing information on “extra” electron-scattering cross sections. The “extra” refers to **cross sections that are not used in the solution to the EBE**, but only in the evaluation of the corresponding rate coefficients by integration over the EEDF.

**Usually, the “extra” files are obtained from the open-access website LXCat (<http://www.lxcat.net/>), provided they comply with certain format requirements for LoKI-B to retrieve the relevant data; see section 6.1 for more information.**

- The `effectiveCrossSectionPopulations` allows the user to specify some particular populations to evaluate an “elastic” momentum-transfer cross section from an “effective” one. The populations can be provided through one or more “property files”, located in the input folder or in any subfolder within it (see section 6.2).

For a gas  $k$ , the electron-neutral momentum-transfer cross section  $\sigma_{k,c}(u)$  is constructed by weighting the contributions of the different types of collisional mechanisms to give

$$\sigma_{k,c}(u) = \sum_i \xi_{k_i} \sigma_{k_i,c}^{\text{el}}(u) + \sum_{i,j>i} [\xi_{k_i} \sigma_{k_{(i,j)},c}(u) + \xi_{k_j} \sigma_{k_{(j,i)},c}(u)] \quad , \quad (64)$$

where  $\sigma_{k_i,c}^{\text{el}}$ ,  $\sigma_{k_{(i,j)},c}$  and  $\sigma_{k_{(j,i)},c}$  are the electron-neutral momentum-transfer cross sections for the elastic scattering of state  $k_i$ , the inelastic excitation  $k_i \rightarrow k_j$ , and the superelastic de-excitation  $k_j \rightarrow k_i$ , respectively. The latter cross sections, whose magnitudes are usually much smaller than those of  $\sigma_{k_i,c}^{\text{el}}$ , are often taken assuming an isotropic scattering (also due to the lack of data), in which case one can identify the momentum-transfer cross section with the integral cross section (integrated over all scattering angles), i.e.  $\sigma_{k_{(i,j)},c} \simeq \sigma_{k_{(j,i)},c}$ . Also, the elastic momentum-transfer cross section is usually identified with that of the highly-populated ground-state of the gas. Therefore

$$\sigma_{k,c}(u) \simeq \sigma_{k,c}^{\text{el}}(u) + \sum_{i,j>i} [\xi_{k_i} \sigma_{k_{(i,j)}}(u) + \xi_{k_j} \sigma_{k_{(j,i)}}(u)] \quad . \quad (65)$$

Note that electron-neutral anisotropic scattering can indeed be handled in a two-term Boltzmann solver by using momentum-transfer cross sections in (11a)-(11b) and (64), **for mechanisms with low excitation thresholds** (such as rotational excitations / deexcitations) [32]. The IST-Lisbon database on LXCat provides momentum-transfer cross sections for these mechanisms in the case of some gases (see section 6.1).

The solution of the EBE requires information on both the “elastic” and the “total” momentum-transfer cross sections for **all** the electronic target-states of the gas, but the way to obtain it depends on the

momentum-transfer data available for each gas. If the “elastic” momentum-transfer cross section is available, equation (65) can be used directly to deduce the corresponding “total”  $\sigma_{k,c}$ , knowing the electron-scattering inelastic / superelastic cross sections for the transitions considered together with the relevant populations, to be self-consistently determined (if possible) within a kinetic model. Conversely, if the data available is for a “total” momentum-transfer cross section, which in databases is usually termed as “effective”  $\sigma_{k,c}^{\text{eff}}$ , then the elastic momentum-transfer cross section can be deduced from

$$\sigma_{k,c}^{\text{el}} = \sigma_{k,c}^{\text{eff}} - \sum_{i,j>i} \left[ \xi_{k_i}^{\text{prescribed}} \sigma_{k(i,j)} + \xi_{k_j}^{\text{prescribed}} \sigma_{k(j,i)} \right] , \quad (66)$$

where the populations  $\xi_{k_i}^{\text{prescribed}}$  and  $\xi_{k_j}^{\text{prescribed}}$  correspond to prescribed distributions for the vibrational states with the electronic ground-state of the gas and for the rotational states with the vibrational ground-state of the electronic ground-state of the gas. Ideally, the distributions should be coherent with the measured / estimated data of  $\sigma_{k,c}^{\text{eff}}$ , allowing to obtain a *unique* result (density independent) for the elastic cross section.

**The prescription of populations  $\xi_{k_i,j}^{\text{prescribed}}$  by the user is strongly discouraged and should be taken with extreme care, since the values of these populations are directly used in (66) without any checking or processing. In any case, this feature is to be used only when an “effective” momentum-transfer cross section is provided, instead of an “elastic”. By default, LoKI-B adopts a Boltzmann distribution at 300 K for  $\xi_{k_i,j}^{\text{prescribed}}$ , but the user can modify this choice.**

Note also the following:

- when the collisional data for a gas includes an electron-impact “effective” momentum-transfer cross section, the code evaluates an elastic momentum-transfer cross section and uses this **same** cross section for **all** the electronic target-states of the gas;
- when the collisional data for a gas includes an electron-impact “elastic” momentum-transfer cross section (*e.g.* for the ground-state of the gas), the user must provide **individual** elastic momentum-transfer cross sections for **each** electronic target-state of the gas.
- In **CARgases** the user can specify the gas or gases (indicated as a list of gas names) for which the continuous approximation for rotations (CAR) [14] should be activated in the simulations (see section 1.2). When the CAR is not to be used, this field must be removed or commented.
- Note that the CAR approach of (12c), to describe the effect of rotational inelastic/superelastic mechanisms, is valid only for some homonuclear diatomic molecules, such as N<sub>2</sub> and O<sub>2</sub> for which it was tested. In general, for rotations, the discrete approach of the collision operator (13a) should be adopted instead.
- In **gasProperties** the user can specify the relevant properties of the different gases used in the simulations, such as

```
mass
fraction
harmonicFrequency
anharmonicFrequency
rotationalConstant
electricQuadrupoleMoment
OPBParameter
```

- It is **mandatory** to specify the values of **mass** and **fraction**. The latter should add to 1, when summed over all gases used in the simulations.
- **harmonicFrequency** and **anharmonicFrequency** are optional, and are used to evaluate the energy of the different vibrational states by assuming an harmonic / anharmonic oscillator model.
- **rotationalConstant** is optional, and is used to evaluate the energy of the different rotational states by assuming a rigid-rotor model.

- `rotationalConstant` and `electricQuadrupoleMoment` are optional, and are used when adopting the CAR approach for homonuclear diatomic molecules. In the latter case the code returns an error message if these parameters are not specified.
- `OPBParameter` is optional and corresponds to the value of the  $w$  parameter to be used in (63), when adopting the `usingSDCS` mode for the ionisation operator.

The values of the different gas properties can be specified using one of the following methods:

- “Direct input” (see example below).

```
N2 = 1
```

**When using the “direct input” method, properties must be set only for those gases used in the simulations, i.e. those listed in the specified LXCat files.**

- “Property file” (see example below; for more information about “property files” see section 6.2).

```
mass: Databases/masses.txt
```

**When using the “property file” method, it is possible to specify the properties of gases that are not used in the simulations. LoKI-B handles input files as “databases”, where it searches only for the information required.**

- In `stateProperties` the user can specify the properties of the states of the different gases used in the simulations, in accordance with the information retrieved from the LXCat files. The properties available are

```
energy
statisticalWeight
population
```

- `energy` and `statisticalWeight` are optional, and can be used for the code to evaluate the population of some set of states, for example adopting a given distribution.
- `statisticalWeight` is **mandatory** for those states appearing in the LXCat files as involved in second-kind collisions (mechanisms tagged with a double-arrow  $\leftrightarrow$ ), in which case the Klein-Rosseland relation [19] is used to obtain the superelastic cross section from the corresponding inelastic.

In general, the `statisticalWeight` of a state corresponds to the product of the statistical weights  $g$  associated with the different partition functions (electronic, vibrational, rotation) of this state. For example, the statistical weight of states  $N_2(X, v=0, J)$  should be set as  $g[N_2(X, v=0, J)] = g_x \times g_{v=0} \times g_J = 1 \times 1 \times 3 [1 + \frac{1}{2} (1 + (-1)^J)] (2J + 1)$ , where the rotational statistical weight  $g_J$  includes also the contribution of the hyperfine splitting resulting from the coupling between the electron and the nuclear spin. Note, however, that the statistical weights are used only to handle second-kind collisions (see (13a), (41a), and (50b)) and to define prescribed distributions of populations (e.g, see (73) and (76) in section (7.1)), where they always appear as ratios  $g_j/g_i$  with  $i, j$  corresponding to sibling states (i.e. both electronic, or both vibrational or both rotational). Therefore, the results are not changed if the `statisticalWeight` of a state is defined only for the partition function *intrinsic* to that state; for example, the statistical weight of *rotational* states  $N_2(X, v=0, J)$  can be defined simply as  $g[N_2(X, v=0, J)] = g_J = 3 [1 + \frac{1}{2} (1 + (-1)^J)] (2J + 1)$  (see also section (7.1)).

- It is **mandatory** to specify the values of population for all states considered as **targets of electron-scattering mechanisms**, e.g. the vibrational distribution of an electronic ground-state. The user should **not** define populations for the states that are only involved in electron-scattering extra collisions (included in the `LXCatFilesExtra`), since the corresponding cross sections are not used in the calculation of the EEDF.
- The values of the different populations should be properly normalized to 1, when summed over all sibling states.

The values of the different properties of states can be specified using one of the following methods (note that the syntax supports the wildcard character \*):

- “Direct input” (see example below)

```
N2(X,v=*) = 1.0
```

- “Property functions” (see example below; for more information about “property functions” see section [7.1](#)).

```
N2(X,v=*) = harmonicOscillatorEnergy
```

**When using the “direct input” method or the “property functions” method, properties must be set only for those gases and states used in the simulations, *i.e.* those listed in the specified LXCat files.**

- “Property file” (see example below; for more information about “property files” see section [6.2](#)).

```
Nitrogen/N2_vibpop.txt
```

**When using the “property file” method, it is possible to specify the properties of gases and states that are not used in the simulations. LoKI-B handles input files as “databases”, where it searches only for the information required.**

- In numerics the user can specify the numerical details of the simulations. The configuration parameters available are

```
energyGrid
maxPowerBalanceRelError
nonLinearRoutines
```

- The `energyGrid` allows the user to specify the properties of the energy grid for simulations in LoKI-B (see section [2](#)):

- \* `maxEnergy`, corresponding to the value of  $u_{\max}$  (in eV) (this is a **mandatory** parameter);
- \* `cellNumber`, is an integer corresponding to the number of cells  $\mathcal{N} > 0$  of the energy grid (this is a **mandatory** parameter);
- \* `smartGrid`, activating a “smart grid” that will automatically adjust the maximum energy of the grid, as to ensure a user-prescribed number of decades in the fall of the EEDF, between  $f_1$  and  $f_{\mathcal{N}}$  (this is an optional parameter). This option is particularly relevant for simulations spanning different values of  $E/N$  or  $T_e$ . The configuration parameters are:
  - `minEedfDecay`, is an integer corresponding to the minimum number of decade-fall for the EEDF;
  - `maxEedfDecay`, is an integer corresponding to the maximum number of decade-fall for the EEDF ( $\text{maxEedfDecay} > \text{minEedfDecay}$ );
  - `updateFactor`, corresponding to the factor by which the `maxEnergy` is increased or decreased, in the automatic adjustment of the energy grid ( $0 < \text{updateFactor} < 1$ ).

Note that the “smart grid” is as “smart” as the user that control its properties. So, if you have doubts on how this works, it is better to ignore this feature. However, if you decide to activate the “smart grid”, you should consider the following:

1. When the smart grid is activated, the `maxEnergy` parameter is the initial value for the maximum energy of the grid. Please try to provide the best possible approximation for it, in order to avoid unnecessary iterations that will degrade the run time.
2. Do not specify very restrictive conditions for the EEDF, for example by setting `minEedfDecay` to 20 and `maxEedfDecay` to 21, since this condition can only be satisfied by imposing a very-small `updateFactor`, which will also degrade the run time. Typical values for the decade-fall are within 10 to 25, considering not only the use of double precision, but also the order of magnitude of the various quantities (kinetic energy, cross sections) multiplying the EEDF in the calculations.
3. Use a “reasonable” value for the `updateFactor` parameter. Very-small values will decrease the performance of the code, whereas very-large values will make extremely difficult for the code to satisfy the decade-fall imposed for the EEDF. Recommended values are usually between 0.05 and 0.2.

- The `maxPowerBalanceRelError` allows the user to specify the threshold value for the error of the relative power balance, above which the code **returns a warning message**. The typical threshold value is  $10^{-9}$ . (This is a **mandatory** parameter). Note that this parameter is not active in time-dependent simulations, in which case the “power balance” corresponds to the value of the intrinsic time-change of the electron mean energy, at unit gas density (see section 3).
- In `nonLinearRoutines` the user can specify several parameters for the configuration of the algorithms with the non-linear routines, dealing with the non-conservative collision operators (ionisation and attachment) and the electron-electron collisions operator (see section 2).
  - \* `algorithm`: the user can choose the nonlinear algorithm to adopt in the simulations. (This is a **mandatory** parameter).
    - `mixingDirectSolutions`, which uses two nested iterative algorithms, based on successive direct solutions.  
This algorithm is recommended in general.
    - `temporalIntegration`, which uses a relaxation method.  
This algorithm is recommended only in the case of strong nonlinear effects (*e.g.* high electronegativity and/or high ionization degrees).
    - This algorithm **MUST** be chosen for time-dependent simulations, *e.g.* when LoKI-B runs independently for electrons subjected to a pulsed electric-field.
  - \* `mixingParameter`: the user **MUST** define the value (between 0 and 1) of a mixing parameter, when choosing the `mixingDirectSolutions` algorithm.  
**Note that the mixing parameter should not be zero**, as the non-linear operators will not converge, in this case.
  - \* `maxEedfRelError`: the user can define the stop criterion for the `nonLinearRoutines`, by defining the maximum value for the relative variations of the EEDF, between two consecutive iterations. The typical value is  $10^{-9}$ . (This is a **mandatory** parameter). Note that this parameter is not active in time-dependent simulations, in which case the convergence criterion is defined by the relative tolerance `RelTol`, imposed as parameter of the `temporalIntegration` solver (see section 1.3).
  - \* `odeSetParameters`: this is an optional field where the user can define specific options for the `temporalIntegration` solver. A detailed description of the different options can be found in the MATLAB documentation [33]. Example of useful options are given below.
    - `AbsTol`: is the value of the absolute tolerance for the `temporalIntegration` algorithm. The typical value is  $10^{-300}$ .
    - `RelTol`: is the value of the relative tolerance for the `temporalIntegration` algorithm. The typical value is  $10^{-6}$ .
    - `MaxStep`: is the maximum value for the step of the advancing parameter with the `temporalIntegration` algorithm. The typical value is  $10^{-7}$ .

### 5.3 Graphical user interface

In this field of the setup file the user can set the configuration of the Graphical User Interface (GUI). Code 4 shows the section of the '`default_lokib_setup.in`' file that handles this configuration.

```
% --- configuration of the graphical user interface ---
gui:
 .isOn: true
 refreshFrequency: 1
```

Code 4: Configuration of the GUI of the simulation

#### IMPORTANT NOTES:

- The `ison` parameter allows the user to activate (`true`) or deactivate (`false`) the GUI.
- In `refreshFrequency` the user can control the frequency with which the GUI is refreshed. The value of this parameter corresponds to the number of required simulations for the GUI to be updated, hence the larger this value the less frequently the GUI is updated.

Note that a very frequent update of the GUI can considerably degrade the run time. Note further that the GUI is optimized for Full HD screen resolution. Adopting different resolutions may result in anomalous displays.

When running LoKI-B for time-independent simulations (DC or HF cases) with the GUI activated (`isOn: true`), the graphic interface appears as in figure 4.

- On the left-hand upper corner, for each value of  $E/N$  (or  $T_e$ ) adopted in the simulations and depending on the selected tab, the GUI displays the **Results (graphical)** that can be found in the output files, namely
  - in *EEDF*, the plot of the EEDF and the corresponding first anisotropy;
  - in *Electron Reduced Diffusion*, the plot of  $D_e N$  as a function of  $E/N$  (or  $T_e$ );
  - in *Electron Reduced Mobility*, the plot of  $\mu_e N$  (and also  $\Re[\mu_{HF} N]$  and  $-\Im[\mu_{HF} N]$  in a HF case), as a function of  $E/N$  (or  $T_e$ );
  - in *Electron Reduced Energy Diffusion*, the plot of  $D_\varepsilon N$  as a function of  $E/N$  (or  $T_e$ );
  - in *Electron Reduced Energy Mobility*, the plot of  $\mu_\varepsilon N$  as a function of  $E/N$  (or  $T_e$ );
  - in *Electron Energies*, the plot of  $T_e \equiv (2/3)\varepsilon$  and  $u_k$ , as a function of  $E/N$  (or  $T_e$ );
  - in *Townsend Coefficient*, the plot of  $\alpha/N$  as a function of  $E/N$  (or  $T_e$ );
  - in *Attachment Coefficient*, the plot of  $\eta/N$  as a function of  $E/N$  (or  $T_e$ );
  - in *Power Channels*, the plot of the electron energy transferred in different channels, relative to the reference power,  $\Theta_x/\Theta_{\text{ref}}$ , as a function of  $E/N$  (or  $T_e$ ) (see section 3).

In all the graphs (except for *EEDF* and *Power Channels*), the user can select/unselect a *X axis logscale* and/or a *Y axis logscale*.

- On the left-hand lower corner, for each value of  $E/N$  (or  $T_e$ ) adopted in the simulations and depending on the selected tab, the GUI displays a summary of the **Results (text)** that can be found in the output files (see section 5.4), namely
  - in *Power balance*, details about the electron power balance;
  - in *Swarm Parameters*, a summary of the electron swarm parameters (the Townsend coefficient, the attachment coefficient, and the drift velocity are only calculated and displayed in a DC case);
  - in *Rate Coefficients*, a summary of the inelastic/superelastic electron rate coefficients, calculated using both the cross sections adopted for solving the EBE and the *extra* set of cross sections defined by the user as additional input data of LoKI-B (see section 5). It also displays the description of each mechanism.
- On the right-hand upper corner, depending on the selected tab, the GUI displays a summary of the input **Setup**, namely
  - in *Setup file*, the uncommented lines of the setup file;
  - in *Cross Sections*, the graphs of the cross sections uploaded for the simulations (including both those adopted for solving the EBE and the *extra* cross sections defined by the user as additional input data of LoKI-B). Here, the user can select in the appropriated tab which cross section(s) to display.
- On the right-hand lower corner, the GUI will display a summary of the **Status** of the *Simulation Log*, with information documenting events relevant to the code execution.

When running LoKI-B for time-dependent simulations (e.g. considering a time-dependent, non-oscillatory ( $\omega = 0$ ) electric field) with the GUI activated (`isOn: true`), the graphic interface looks similar to that of figure 4. In this case

- the **Results (graphical)** and the **Results (text)** are displayed as a function of the time  $t$  (instead of  $E/N$  or  $T_e$ );
- the GUI displays also a *Pulse temporal integration progress bar* that depicts the progress of the simulation as a function of the *Integration time*, indicating also the current *Computational time*.

## 5.4 Output

In this field of the setup file the user can define the details of the simulation output. Code 5 shows the section of the '`default_lokib_setup.in`' file that handles this configuration.

```
% --- configuration of the output files ---
output:
  isOn: false
  folder: simulation1
  dataFiles:
%   - inputs
    - log
    - eedf
    - swarmParameters
    - rateCoefficients
    - powerBalance
    - lookUpTable
```

Code 5: Configuration of the output of the simulation

### IMPORTANT NOTES:

- LoKI-B provides `log` information documenting events relevant to the code execution, that are displayed in the command window. This information can also be displayed in the GUI (if activated) and/or saved as text file according to the `output` configuration (see below).
- The `isOn` parameter allows the user to activate (`true`) or deactivate (`false`) the output.
- In `folder` the user can specify the folder where the datafiles of the simulation output will be saved. This is an optional parameter; if `folder` is removed, the code will generate a generic name for the output folder, with a time stamp.  
The output folder(s) will be located inside `[repository folder]/LoKI-B_v2.2.0/Code/Output/`.
- When `isOn` is `true`, `dataFiles` is a **mandatory** parameter, where the user can specify the information to be saved after each simulation, characterized by
  - different  $E/N$  values, for `eedfType = boltzmann` and time-independent simulations. In this case the code generates as many output folders as the number of  $E/N$  values defined as `reducedField` in the `workingConditions`;
  - different  $t$  values, for `eedfType = boltzmann` and time-dependent simulations. In this case the code generates as many output folders as the number of “sampling points” defined within `reducedField` in the `workingConditions`;
  - different  $T_e$  values, for `eedfType = prescribedEedf`. In this case the code generates as many output folders as the number of  $T_e$  values defined as `electronTemperature` in the `workingConditions`.

The available options for `dataFiles` are (see section 3):

- `inputs`  
It copies all the input datafiles (*e.g* LXCat files; not functions) called from the setup file (and also an exact copy of the original setup file itself, including all commented / uncommented lines), using the corresponding structure of folders.
- `log`  
It writes the datafile `log.txt`, displaying the log information of the code execution.
- `eedf`  
It writes, for each `boltzmann` ( $E/N$  or  $t$ ) or `prescribedEedf` ( $T_e$ ) simulation, the datafile `eedf.txt`, with three columns displaying the kinetic energy  $u$ , the EEDF  $f$  and the first anisotropy  $f^1$  (only in the case of `boltzmann` simulations), respectively.
- `swarmParameters`  
It writes, for each `boltzmann` ( $E/N$  or  $t$ ) or `prescribedEedf` ( $T_e$ ) simulation, the datafile `swarmParameters.txt`, displaying the values of the following quantities:  
 $t$  (only for time-dependent simulations)

$E/N$

$D_e N$

$\mu_e N$

$v_d$  (only in DC case)

$\Re[\mu_{\text{HF}} N] + \Im[\mu_{\text{HF}} N] i$  (only in HF case)

$\alpha/N$  (only in DC case)

$\eta/N$  (only in DC case)

$D_\varepsilon N$

$\mu_\varepsilon N$

$\varepsilon$

$u_k$

$T_e \equiv (2/3)\varepsilon.$

– **rateCoefficients**

It writes, for each **boltzmann** ( $E/N$  or  $t$ ) or **prescribedEedf** ( $T_e$ ) simulation, the datafile **rateCoefficients.txt** displaying information on rate coefficients, organized into the following groups:

- \* e-Kinetics Rate Coefficients, including the inelastic / superelastic rate coefficients  $C_{i,j}$  and  $C_{j,i}$  calculated from the electron-impact cross sections between states  $i$  and  $j > i$  provided as input data, as well as the threshold of the cross sections and the description of the reactions;
- \* e-Kinetics Extra Rate Coefficients, including the inelastic / superelastic rate coefficients  $C_{i,j}$  and  $C_{j,i}$  calculated from the electron-impact extra cross sections between states  $i$  and  $j > i$  provided as input data, as well as the threshold of the cross sections and the description of the reactions.

– **powerBalance**

It writes, for each **boltzmann** ( $E/N$  or  $t$ ) or **prescribedEedf** ( $T_e$ ) simulation, the datafile **powerBalance.txt**, displaying the values of the following electron power-density gains/losses (per electron at unit gas density):

$\Theta_E/N$

$\Theta_{\text{el}}^{\text{gain}}/N, \Theta_{\text{el}}^{\text{loss}}/N, \Theta_{\text{el}}/N \equiv \Theta_{\text{el}}^{\text{gain}}/N + \Theta_{\text{el}}^{\text{loss}}/N$

$\Theta_{\text{CAR}}^{\text{gain}}/N, \Theta_{\text{CAR}}^{\text{loss}}/N, \Theta_{\text{CAR}}/N \equiv \Theta_{\text{CAR}}^{\text{gain}}/N + \Theta_{\text{CAR}}^{\text{loss}}/N$

$\Theta_{\text{sup}}^{\text{gain}}/N, \Theta_{\text{inel}}^{\text{loss}}/N, \Theta_{\text{ele,vib,rot}}/N \equiv \Theta_{\text{sup}}^{\text{gain}}/N + \Theta_{\text{inel}}^{\text{loss}}/N$  (for electronic, vibrational, rotational mechanisms)

$\Theta_{\text{ion}}/N$

$\Theta_{\text{att}}/N$

$\Theta_{\text{growth}}/N.$

It also writes

the power balance  $\Theta_{\text{growth}}/N + \Theta_E/N + \Theta_{\text{coll}}^{\text{gain}}/N + \Theta_{\text{coll}}^{\text{loss}}/N$  (with “coll” referring to all collision types). Recall that, in time-dependent simulations, the “power balance” corresponds to the value of the intrinsic time-change of the electron mean energy, at unit gas density (see section 3);

the relative power balance (in %)  $[\Theta_{\text{growth}}/N + \Theta_E/N + \Theta_{\text{coll}}^{\text{gain}}/N + \Theta_{\text{coll}}^{\text{loss}}/N] / [\Theta_{\text{ref}}/N] \times 100$ . Recall that, in time-dependent simulations, the “relative power balance” corresponds to the value of the intrinsic time-change of the electron mean energy divided by the reference power-density per electron (see section 3);

It also writes, for each gas in the mixture, the gain/loss/net results for the electron power-density associated with the different types of collisions.

– **lookUpTable**

It writes the following datafiles

- \* **lookUpTableSwarm.txt**, containing a table with all the data in the file(s) **swarmParameters.txt** presented in columns, as a function of  $E/N$ , or  $t$  and  $E/N$ , or  $T_e$  (according to the type of simulations);
- \* **lookUpTableRateCoeff.txt**, containing a table with all the data in the file(s) **rateCoefficients.txt** presented in columns, as a function of  $E/N$ , or  $t$  and  $E/N$ , or  $T_e$  (according to the type of simulations);

- \* `lookUpTablePower.txt`, containing a table with all the data in the file(s) `powerBalance.txt` presented in columns, as a function of  $E/N$ , or  $t$  and  $E/N$ , or  $T_e$  (according to the type of simulations);
- \* `lookUpTableEedf.txt` (**only for time-dependent simulations**) containing a table with all the data in the file(s) `eedf.txt`, where the first column displays the values of  $t$ , the first row displays the values of  $u$ , and the remainder rows display the values of  $f$  for the different simulation times. Table 2 presents an extract of a typical `lookUpTableEedf.txt` file.

Table 2: Extract of a typical `lookUpTableEedf.txt` file for a time-dependent simulation

|            | 0.005  | 0.015  | 0.025  | 0.035 | ... |
|------------|--------|--------|--------|-------|-----|
| 0.0000E+00 | 220.49 | 149.76 | 101.72 | 69.09 | ... |
| 1.0000E-18 | 220.49 | 149.76 | 101.72 | 69.09 | ... |
| 1.0233E-18 | 220.49 | 149.76 | 101.72 | 69.09 | ... |
| 1.0471E-18 | 220.49 | 149.76 | 101.72 | 69.09 | ... |
| ...        | ...    | ...    | ...    | ...   | ... |

- \* `electronDensityEvolution.txt`, containing a table with the values of the electron density  $n_e$  and the electron density variation  $dn_e/dt$  presented in columns, as a function of  $t$ . This file is written only in the case of time-dependent simulations in the presence of electron-electron collisions, considering a time-dependent electron density  $n_e(t)$  (see section 5.2).

## 6 Auxiliary input files

This section gives detailed information on the configuration of the different auxiliary input files used by LoKI-B, namely on the notation to be adopted in the description of the species and the electron-scattering mechanisms involved in the simulations.

The auxiliary input files should be located in the input folder [repository folder]/LoKI-B\_v2.2.0/Code/Input/ or in any subfolder within it. They are plain text files, although some can display extensions different than \*.txt, for the sake of folder organisation.

### 6.1 LXCat files

By default, LoKI-B uses electron-scattering cross sections obtained from the LXCat open-access website [34], in the solution to the EBE or as *extra* data for integration over the calculated EEDF, to obtain electron macroscopic parameters. The cross sections can be **assembled into a single file or given from multiple files**, and if/when **appearing duplicated in the datafiles they are considered only once by LoKI-B**.

LXCat is organised to provide “data required for modeling low temperature plasmas” [34] in the most effective way. In the case of electron-neutral scattering cross sections, LXCat provides easy access to *complete sets* of cross sections, defined as those giving a good description of all electron energy and momentum losses [35], yielding electron swarm parameters in agreement with available measured data (within experimental uncertainties), when used in a two-term Boltzmann solver [25,35]. Each *complete set* assembles cross sections for electron collisions with different neutral targets, usually associated with the electronic ground-state of each gas. To date, on LXCat these data are tagged with the name of the corresponding gas (*e.g.* Ar, N<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub>, ...) and are grouped under the category **Ground states**, where one can find cross sections for the collisions of electrons with the electronic / vibrational / rotational ground-states of a neutral gas. For example, the datasets N<sub>2</sub> may contain (i) the elastic / effective momentum-transfer cross section for N<sub>2</sub>; (ii) excitation cross sections for different electronic states (including the ionisation state), from the electronic ground-state N<sub>2</sub>(X); (iii) excitation cross sections for different vibrational states N<sub>2</sub>(X,v), from the vibrational ground-state N<sub>2</sub>(X,v=0); (iv) a global rotational excitation cross section for N<sub>2</sub>(X).

This practical organisation of LXCat can create some difficulties when a detailed discrimination and handling of data is intended. The reason is of technical nature, and it relates with the fact that, to date, electron collisions with the **Ground state** of a gas are described as a collection of mechanisms e + gas name -> ..., with no possibility to specify the internal structure of the electronic ground-state of the gas. Meaning that the information, if any, about the different species involved in each electron collision is scattered across the LXCat files, depending on the strategy adopted by each particular LXCat contributor. Obviously, this makes impossible to develop a general parser to collect the full list of species (with internal structure), for any file downloaded from LXCat.

This problem is to be solved by the developers of the platform, but meanwhile users can modify any cross section datafile downloaded from LXCat, to make it compliant with the LoKI-B parser. For this, it is important to understand how LXCat structures the metadata associated with each cross section. In an LXCat file, each cross-section-table comes with a header including the following fields:

- SPECIES
- PROCESS
- PARAM.
- COMMENT (multiple lines)
- UPDATED
- COLUMNS.

In principle, LoKI-B should check the **PROCESS** field to obtain details on the full structure of reactants and products, for each electron-impact mechanism, but again this is not available in the current structure of LXCat metadata. To circumvent this limitation, the LoKI-B parser looks for this information in the first line of the free-field **COMMENT**, which is modified to meet the following structure:

COMMENT:[<electron>+<target state><directionality><products states>, <collision type>, <collision subtype>] ...

where the square brackets and spaces are mandatory characters, and where the different elements in the expression have the following features:

- **electron**: can be represented by either characters **e** or **E** (see section [6.3](#) for more information about the description of the species involved in electron-scattering mechanisms).
- **target state**: can detail the electronic/vibrational/rotational state of the target species (see section [6.3](#) for more information about the description of the species involved in electron-scattering mechanisms).
- **directionality**: can be a forward arrow ( $\rightarrow$ ) for inelastic collisions, or a double arrow ( $\leftrightarrow$ ) for inelastic/superelastic collisions.
- **product states**: sum of all the product(s) resulting from an electron collision, including electron(s) and heavy-species, eventually with indication of the electronic/vibrational/rotational level (see section [6.3](#) for more information about the description of the species involved in electron-scattering mechanisms).
- **collision type**: one of the following collision types, supported by the LXCat database: **Elastic**, **Effective**, **Excitation**, **Vibrational**, **Rotational**, **Ionization** or **Attachment**. Note the **mandatory** capital letters, since the parser is case sensitive.
- **collision subtype**: (optional field) either empty for integral cross sections, or **momentum-transfer** for momentum-transfer cross section.  
**Note the following exception: the collision types Elastic and Effective are automatically handled as momentum-transfer, even if the collision subtype is left empty.**

The workaround described above is the practical solution to prepare any cross section datafile obtained from LXCat for compliance with the LoKI-B parser, and it is already implemented in the following files:

- the LXCat files distributed with the code, and located in [repository folder]/LoKI-B\_v2.2.0/Code/Input/ (see section [4.2](#)).  
**Before modifying any other LXCat file, the user should check the files distributed with the code, to become familiarised with the modifications needed.**
- cross section files, directly downloadable only from the IST-Lisbon database with the website LXCat, and to date only for the gases indicated below<sup>6</sup>
  - Argon: Ar, for electron excitations from the ground-state Ar(1S<sub>0</sub>);
  - Helium: He, for electron excitations from the ground-state He(1<sup>1</sup>S);
  - Nitrogen: N<sub>2</sub>, for electron excitations from the electronic ground-state N<sub>2</sub>(X) and the vibrational ground-state N<sub>2</sub>(X,v=0); N<sub>2</sub>-vib for electron excitations from vibrational states N<sub>2</sub>(X,v= 1 – 10); N<sub>2</sub>-rot for electron excitations from rotational states N<sub>2</sub>(X,v=0,J=0-30)  $\Delta J = 2$ .  
The latter two datagroups are clustered under **Nitrogen** in **State-specific and gas mixtures** at LXCat;
  - Atomic Nitrogen: N, for electron excitations from the ground-state N(<sup>4</sup>S); N-elec, for electron excitations from the excited states N(<sup>2</sup>D) and N(<sup>2</sup>P).  
These datagroups are clustered under **Nitrogen** in **State-specific and gas mixtures** at LXCat;
  - Oxygen: O<sub>2</sub>, for electron excitations from the electronic ground-state O<sub>2</sub>(X) and the vibrational ground-state O<sub>2</sub>(X,v=0); O<sub>2</sub>-vib for electron excitations from vibrational states O<sub>2</sub>(X,v= 0 – 41); O<sub>2</sub>-rot for electron excitations from rotational states O<sub>2</sub>(X,v=0,J=1-29)  $\Delta J = 2$ ; O<sub>2</sub>-elec for electron excitations from excited electronic states of O<sub>2</sub>, namely O<sub>2</sub>(a<sup>1</sup> $\Delta_g$ , b<sup>1</sup> $\Sigma_g^+$ ).  
The latter three datagroups are clustered under **Oxygen** in **State-specific and gas mixtures** at LXCat;

---

<sup>6</sup>LoKI-B is distributed with only part of the data available on the IST-Lisbon database at LXCat, namely complete sets of cross sections for electron excitations from the ground-state of gases, of interest for swarm analyses.

- Atomic Oxygen: `O`, for electron excitations from the ground-state O(<sup>3</sup>P); `O-elec` for electron excitations from excited electronic states of O, namely O<sup>-</sup>.  
These datagroups are clustered under `Oxygen` in `State-specific and gas mixtures` at LXCat;
- Ozone: `O3`, for electron excitations from the ground-state O<sub>3</sub>(X).  
This datagroup is under `Oxygen` in `State-specific and gas mixtures` at LXCat;
- Hydrogen: `H2`, for electron excitations from the electronic ground-state H<sub>2</sub>(X) and the vibrational ground-state H<sub>2</sub>(X,v=0); `H2-vib` for electron excitations from vibrational states H<sub>2</sub>(X,v= 1 – 15); `H2-rot` for electron excitations from rotational states H<sub>2</sub>(X,v=0,J=0-5) ΔJ = 2; `H2-elec` for electron recombination of ionic states H<sub>2</sub><sup>+</sup> and H<sub>3</sub><sup>+</sup>.  
The latter three datagroups are clustered under `Hydrogen` in `State-specific and gas mixtures` at LXCat;
- Atomic Hydrogen: `H`, for electron excitations from the ground-state H(1s); `H-elec`, for electron excitations from the excited states H(2s), H(2p), H(3), H(4) and H(5).  
These datagroups are clustered under `Hydrogen` in `State-specific and gas mixtures` at LXCat;
- Carbon dioxide: `CO2`, for electron excitations from the electronic ground-state CO<sub>2</sub>(X) and the vibrational ground-state CO<sub>2</sub>(X,v=000);
- Carbon monoxide: `CO`, for electron excitations from the electronic ground-state CO(X) and the vibrational ground-state CO(X,v=0); `CO-rot` for electron excitations from rotational states CO(X,v=0,J=0-17) ΔJ = 1;
- Carbon monoxide (with anisotropic scattering)<sup>7</sup>: `CO_anis`, for electron excitations from the electronic ground-state CO(X) and the vibrational ground-state CO(X,v=0), to be adopted when anisotropic scattering for rotational collisions is also considered; `CO_dipint-rot` delivering dipole-integral cross sections for electron excitations from rotational states CO(X,v=0,J=0-25) ΔJ = 1; `CO_dipmt-rot` delivering dipole-momentum-transfer cross sections for electron excitations from rotational states CO(X,v=0,J=0-25) ΔJ = 1; `CO_quadint-rot` delivering quadrupole-integral cross sections for electron excitations from rotational states CO(X,v=0,J=0-24) ΔJ = 2.  
These datagroups are clustered under `CO_anis` in `State-specific and gas mixtures` at LXCat.

In the folder `[repository folder]/LoKI-B_v2.2.0/Code/OtherAuxFunctions` the user can find the script `LXCat2LoKI.m` that interactively assists the modification of LXCat files, for compliance with the LoKI-B parser. Code 6 shows an example of a modified header, for a cross-section-table extracted from the `N2_LXCat.txt` file distributed with LoKI-B.

```

EXCITATION
N2 -> N2 (v=0 - v=1)
 3.000000e-1
SPECIES: e / N2
PROCESS: E + N2 -> E + N2 (v=0 - v=1), Excitation
PARAM.: E = 0.3 eV, complete set
COMMENT: [e + N2(X,v=0) <-> e + N2(X,v=1), Vibrational] Pitchford L C and Phelps A V 1982
COMMENT: Bull. Am. Phys. Soc. 27 109 Tachibana K and Phelps A V 1979 JCP 71 3544 Schulz G J 1962
COMMENT: Phys. Rev. 125 229 Schulz G J 1964 Phys. Rev. 135 A988 Schulz G J 1973 Rev. Mod. Phys.
COMMENT: 45 423 Engelhardt A G, Phelps A V and Risk C G 1964 Phys. Rev. 135 A1566 Pavlovic Z,
COMMENT: Boness M J W, Herzenberg A and Schulz G J 1972 Phys. Rev. A 6 676.
UPDATED: 2017-09-03 10:54:40
COLUMNS: Energy (eV) | Cross section (m2)
-----
3.000000e-1 0.000000e+0
4.000000e-1 3.000000e-23
5.000000e-1 4.000000e-23
...
9.653000e+2 1.238000e-24
9.654000e+2 0.000000e+0
1.000000e+3 0.000000e+0
-----
```

Code 6: Extract from the `N2_LXCat.txt` file distributed with LoKI-B (cf the modified `COMMENT` field)

<sup>7</sup>This complete set of cross sections is the result of the work of L. Vialeto *et al* [32], which proposes a model of anisotropic scattering for rotational collisions, to be used in a two-term Boltzmann solver.

## 6.2 Property files

Property files are text files with the properties of gases and states used in the simulations. Some property files are distributed with LoKI-B, but in general these files can be prepared by the user, considering the following rules:

- for organisation sake, all “property files” specified in the setup file should be located inside the input folder ([repository folder]/LoKI-B\_v2.2.0/Code/Input), eventually organised in subfolders with self-explanatory names (e.g. Nitrogen, Databases; see section 4.2);
- property files can include comments, signaled by the character %;
- property files **MUST** be two-column-formatted, separated by any white-space character. The first column should include the gas/state name (see section 6.3 for more information about the description of the species used in the simulations), and the second column should include the value of the property for that particular gas/state;
- property files accept basic mathematical operations (such as addition, subtraction, multiplication and division), in the second column with the value of the property (see Code 7 as an example);
- property files can include the properties of gases/states not used in the simulations. LoKI-B handles input files as “databases”, where it searches only for the information required.

Codes 7 and 8 show two examples of property files distributed with LoKI-B.

```
% masses of different gases expressed in SI units (Kg)
N3    3*14.007*1.660539040e-27
N4    4*14.007*1.660539040e-27
N2    2*14.007*1.660539040e-27
N    14.007*1.660539040e-27
O2    2*15.999*1.660539040e-27
O    15.999*1.660539040e-27
O3    3*15.999*1.660539040e-27
H2    2*1.008*1.660539040e-27
H    1.008*1.660539040e-27
CO2   (12.0107+2*15.999)*1.660539040e-27
CO    (12.0107+15.999)*1.660539040e-27
Ar    39.948*1.660539040e-27
He    4.002602*1.660539040e-27
He2   8.005204*1.660539040e-27
H20   (2*1.008+15.999)*1.660539040e-27
CH4   16.0427*1.660539040e-27
C     12.0107*1.660539040e-27
```

Code 7: Property file with the masses of different gases (Databases/masses.txt)

```
% populations of the different vibrational states of N2
N2(X,v=0)  1
N2(X,v=1)  0
N2(X,v=2)  0
N2(X,v=3)  0
N2(X,v=4)  0
N2(X,v=5)  0
N2(X,v=6)  0
N2(X,v=7)  0
N2(X,v=8)  0
N2(X,v=9)  0
N2(X,v=10) 0
```

Code 8: Property file with a vibrational distribution of N<sub>2</sub> (Nitrogen/N2\_vibpop.txt)

## 6.3 Species description

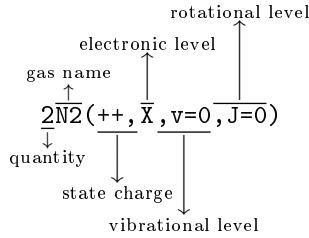
This section describes the ontology, including syntax rules, for the representation of the different species used in the simulations of LoKI-B.

LoKI-B handles two different types of species: electrons and heavy species (atomic or molecular). All species are represented by a **string without any white-space characters** and when specified in an electron collision **they are separated by plus signs (+)**.

The representation of these species follows the syntax rules below:

- **Electrons:** can be represented by either characters **e** or **E**, which can appear multiplied by an integer, *e.g.* **2e** which is equivalent to **e + e**.
- **Heavy species:** refer to the different atomic or molecular species used in the simulations. **For electron-collision target species, it is mandatory to provide information on its configuration (see below).**

The scheme below shows the general structure to adopt, when representing the configuration of a particular species:



where

- quantity: is an **optional** field composed only by integers. It represents the number of species to be considered.
- gas name: is a **mandatory** field composed by letters (English alphabet), integers and underscore characters (\\_). It can not start with an integer and is case sensitive.
- state charge: is an **optional** field composed by plus (+) and minus (-) characters. It represents the charge of an ionic state and has to terminate with a comma (,).
- electronic level: is a **mandatory** field composed by letters (English alphabet), integers, underscore characters (\\_), plus characters (+), minus characters (-), asterisk characters (\*), apostrophe characters (^), square brackets ([]), and periods (.).
- vibrational level: is an **optional** field composed by letters (English alphabet), integers, underscore characters (\\_), plus characters (+), minus characters (-) and asterisk characters (\*). It has to start with the string “,v=”.
- rotational level: is an **optional** field composed by letters (English alphabet), integers, underscore characters (\\_), plus characters (+), minus characters (-) and asterisk characters (\*). It has to start with the string “,J=” and it must necessarily come after the vibrational level field.

### IMPORTANT NOTE:

The asterisk character (\*) is supported **only** in the setup file, **not in the LXCat auxiliary input files**.

## 7 Auxiliary functions

This section describes several auxiliary functions that can be used in the simulations of LoKI-B.

### 7.1 Property functions

Property functions are `*.m` functions that can be used to specify the properties of gases and states used in the simulations. Some property functions are distributed with LoKI-B, but in general these functions can be prepared by the user, according to the needs for new functionalities. In this case, the user is advised to mimic the structure of any property function already provided with the code.

The following should be considered:

- for organisation sake, all “property functions” specified in the setup file should be located in the property functions folder (`[repository folder]/LoKI-B_v2.2.0/Code/PropertyFunctions`; see section 4.2);
- property functions receive the arguments (`state`, `argumentArray`, `workCond`), where
  - `state`: is a handle to the state-object to which the property is assigned.  
For example, when using `N2(X,v=*)` the property is assigned to all the vibrational states with the electronic ground-state of N<sub>2</sub>;
  - `argumentArray`: is an array of arguments corresponding to the list of parameters to be used in the setup file (see below);
  - `workCond`: is a handle to the working-conditions-object of the simulation.
- property functions are called from the setup file (see section 5) using the following structure:

$$\langle \text{function name} \rangle @ \underbrace{[\text{list of parameters}]}_{\text{Optional}}$$

where the `list of parameters` is a list of comma-separated values with all the parameters called by the particular property function. The parameters sent to the property functions can be mapped to the values of the different working conditions previously defined in the setup file (see Code 3 for examples, and therein the implementation of property function `boltzmannPopulation@gasTemperature`);

- property functions **MUST** be set only for those gases and states used in the simulations, *i.e.* those listed in the specified LXCat files.

Table 3 lists the property functions distributed with LoKI-B\_v2.2.0, along with the required parameters and dependencies.

The property functions in table 3 correspond to the following physical models.

#### harmonicOscillatorEnergy

It calculates the energy of (vibrational) state  $j$  of a diatomic molecule, adopting the harmonic oscillator model

$$E_j = \frac{\hbar\omega_{\text{vib}}}{e} \left( j + \frac{1}{2} \right) , \quad (67)$$

where  $\omega_{\text{vib}}$  is the `harmonicFrequency` (angular frequency) of the molecule.

#### morseOscillatorEnergy

It calculates the energy of (vibrational) state  $j$  of a diatomic molecule, adopting the Morse oscillator model

$$E_j = \frac{\hbar\omega_{\text{vib}}}{e} \left( j + \frac{1}{2} \right) - \frac{\hbar\omega_{\text{vib}}\chi_e}{e} \left( j + \frac{1}{2} \right)^2 , \quad (68)$$

where  $\omega_{\text{vib}}$   $\chi_e$  is the first `anharmonicFrequency` of the molecule (with  $\chi_e$  the anharmonicity constant).

Table 3: List of property functions distributed with LoKI-B\_v2.2.0

| Property          | Function name                        | Parameters [units]                   | Dependencies                                       |
|-------------------|--------------------------------------|--------------------------------------|--|
| energy            | harmonicOscillatorEnergy             | n/a                                  | harmonicFrequency                                  |
|                   | morseOscillatorEnergy                | n/a                                  | harmonicFrequency<br>anharmonicFrequency           |
|                   | rigidRotorEnergy                     | n/a                                  | rotationalConstant                                 |
| statisticalWeight | rotationalDegeneracy                 | n/a                                  | n/a  |
|                   | rotationalDegeneracy_N2              | n/a                                  | n/a  |
|                   | rotationalDegeneracy_H2              | n/a                                  | n/a  |
| population        | boltzmannPopulation                  | Temperature [K]                      | energy<br>statisticalWeight                        |
|                   | boltzmannPopulationRotationalCutoff  | Temperature [K]<br>J <sub>MAX</sub>  | energy<br>statisticalWeight                        |
|                   | boltzmannPopulationVibrationalCutoff | Temperature [K]<br>v <sub>MAX</sub>  | energy<br>statisticalWeight                        |
|                   | treanorPopulation                    | Temperature0 [K]<br>Temperature1 [K] | energy<br>statisticalWeight                        |
|                   | treanorGordietsPopulation            | Temperature0 [K]<br>Temperature1 [K] | energy<br>statisticalWeight<br>anharmonicFrequency |

### rigidRotorEnergy

It calculates the energy of (rotational) state  $J$  of a diatomic molecule, adopting the rigid-rotor model

$$E_J = BJ(J + 1) \quad , \quad (69)$$

where  $B$  is the rotational constant of the molecule.

These property functions should be called within the energy property of the setup file, for the corresponding vibrational and rotational states.

For example:

N2(X,v=\*) = harmonicOscillatorEnergy

to set the energies of all the vibrational states with the electronic ground-state of N<sub>2</sub>.

N2(X,v=0,J=\*) = rigidRotorEnergy

to set the energies of all the rotational states of the vibrational state v=0, with the electronic ground-state of N<sub>2</sub>.

### rotationalDegeneracy

It calculates the statistical weight of the *intrinsic* partition function of a (generic) rotational state  $J$  [14]

$$g_J = 2J + 1 \quad . \quad (70)$$

### rotationalDegeneracy\_N2

It calculates the statistical weight of the *intrinsic* partition function of a rotational state  $J$  of the N<sub>2</sub> molecule [14]

$$g_J = 3 \left[ 1 + \frac{1}{2} (1 + (-1)^J) \right] (2J + 1) \quad . \quad (71)$$

### rotationalDegeneracy\_H2

It calculates the statistical weight of the *intrinsic* partition function of a rotational state  $J$  of the H<sub>2</sub> molecule [14]

$$g_J = [2 - (-1)^J] (2J + 1) \quad . \quad (72)$$

**These property functions should be called within the `statisticalWeight` property of the setup file, for the corresponding rotational states (see also section 5.2).**

For example:

`N2(X,v=0,J=*) = rotationalDegeneracy_N2`

to set the statistical weights of all the rotational states of the vibrational state  $v=0$ , with the electronic ground-state of  $\text{N}_2$ .

#### boltzmannPopulation

It calculates the population of state  $j$ , adopting the Boltzmann distribution

$$\xi_j = \frac{g_j \exp\left(-\frac{E_j}{k_B T}\right)}{\sum_{i \in \text{siblings}} g_i \exp\left(-\frac{E_i}{k_B T}\right)}, \quad (73)$$

where  $T$  is the characteristic temperature of the distribution.

#### boltzmannPopulationRotationalCutoff

It calculates the population of rotational state  $J$ , adopting a Boltzmann distribution truncated at level  $J_{\text{MAX}}$

$$\xi_J = \frac{g_J \exp\left(-\frac{E_J}{k_B T}\right)}{\sum_{J'=0}^{J_{\text{MAX}}} g_{J'} \exp\left(-\frac{E_{J'}}{k_B T}\right)}, \quad (74)$$

where  $T$  is the characteristic temperature of the distribution.

This distribution allows defining the populations of rotational states to be considered in the solution to the electron Boltzmann calculation, irrespectively of the full list of states involved in electron collision events (for example, appearing also in extra cross section files).

#### boltzmannPopulationVibrationallCutoff

It calculates the population of vibrational state  $v$ , adopting a Boltzmann distribution truncated at level  $v_{\text{MAX}}$

$$\xi_v = \frac{g_v \exp\left(-\frac{E_v}{k_B T}\right)}{\sum_{v'=0}^{v_{\text{MAX}}} g_{v'} \exp\left(-\frac{E_{v'}}{k_B T}\right)}, \quad (75)$$

where  $T$  is the characteristic temperature of the distribution.

This distribution allows defining the populations of vibrational states to be considered in the solution to the electron Boltzmann calculation, irrespectively of the full list of states involved in electron collision events (for example, appearing also in extra cross section files).

#### treanorPopulation

It calculates the population of state  $j$ , adopting the Treanor distribution [36, 37]

$$\xi_j = \frac{g_j \exp\left(\frac{j(E_1 - E_0) - (E_j - E_0)}{k_B T_0}\right) \exp\left(-\frac{j(E_1 - E_0)}{k_B T_1}\right)}{\sum_{i \in \text{siblings}} g_i \exp\left(\frac{i(E_1 - E_0) - (E_i - E_0)}{k_B T_0}\right) \exp\left(-\frac{i(E_1 - E_0)}{k_B T_1}\right)}, \quad (76)$$

where  $T_0$  and  $T_1$  are the characteristic temperatures of the distribution.

#### treanorGordietsPopulation

It calculates the population of state  $j$ , adopting the Treanor-Gordiets distribution [36, 37]

$$\xi_j = \begin{cases} \frac{g_j \exp\left(\frac{j(E_1 - E_0) - (E_j - E_0)}{k_B T_0}\right) \exp\left(-\frac{j(E_1 - E_0)}{k_B T_1}\right)}{\sum_{i \in \text{siblings}} \xi_i}, & j \leq j^* \\ \frac{\xi_{j^*} \frac{j^*}{j}}{\sum_{i \in \text{siblings}} \xi_i}, & j > j^* \end{cases}, \quad (77)$$

where  $T_0$  and  $T_1$  are the characteristic temperatures of the distribution and

$$j^* \equiv \frac{1}{2} \left[ 1 + \frac{E_1 - E_0}{\hbar \omega_{\text{vib}} \chi_e} \frac{T_0}{T_1} \right]$$

is the vibrational level corresponding to the minimum of the Treanor distribution (with  $\omega_{\text{vib}} \chi_e$  the anharmonic frequency of the oscillator characterizing the distribution).

These property functions should be called within the population property of the setup file, for the corresponding states, using

```
boltzmannPopulation@<temperature>
boltzmannPopulationRotationalCutoff@<temperature>, <JMAX>
treanorPopulation@<temperature0>, <temperature1>
```

where temperature, temperature0, temperature1 can be temperature values or the dynamic variables gasTemperature or electronTemperature.

For example

```
N2(X,v=*) = treanorPopulation@gasTemperature,4000
```

to set the population of all the vibrational states with the electronic ground-state of N<sub>2</sub>;

```
N2(X,v=0,J=*) = boltzmannPopulation@gasTemperature
```

to set the population of all the rotational states of the vibrational state v=0, with the electronic ground-state of N<sub>2</sub>.

## 7.2 Other auxiliary functions

In OtherAuxFunctions the user can find \*.m functions

- for interactively assist the modification of LXCat files, for compliance with the LoKI-B parser. In the current distribution of LoKI-B, this function is `LXCat2LoKI.m`;
- for plotting two different EEDFs in the same MATLAB graph. In the current distribution of LoKI-B, this function is `compareEEDFs.m`;
- for calculating working conditions that can evolve during the simulations. In the current distribution of LoKI-B, this functionality is for calculating the `reducedField` in the case of step electric fields (function `reducedFieldRamp.m`) or electric field pulses (function `reducedFieldPulse.m`).

In general these functions can be prepared by the user, according to the needs for new functionalities. In this case, the user is advised to mimic the structure of any auxiliary function already provided with the code.

## 8 Validity limits and control

As any numerical tool, LoKI-B provides a mere representation of the energy distribution of the electrons in a LTP, because it is based on a specific formulation with embedded approximations. Therefore, the tool should be used only in situations fitting its validity limits, and users are advised to carefully read the extensive literature on the two-term EBE [11], for obtaining details about its solution.

The two-term approximation adopted in LoKI-B to solve the EBE is valid in a situation of small anisotropies [11], corresponding to electron-neutral mean-free-paths much smaller than any characteristic dimension of the plasma container, and an energy gain from the electric field, between collisions, much smaller than the electron kinetic energy. For a homogeneous scenario like the one described here, the latter condition is the most relevant and can be approximately written as (see (52a) and (58b))

$$\Theta_E \sim \mu_e E^2 \ll \varepsilon \nu_c , \quad (78)$$

which yields, for a Maxwellian EEDF at 1 eV temperature and a typical reduced collision frequency  $\nu_c/N \sim \sigma_c \langle v \rangle \sim 10^{-19} \times 10^6 = 10^{-13} \text{ m}^3 \text{ s}^{-1}$ ,  $E/N \ll \sqrt{m_e \varepsilon / e} (\nu_c/N) \sim 300 \text{ Td}$ . This is a conservative limit for the reduced electric-field, often exceeded in calculations because the two-term approximation yields fairly good results still.

**However, users are advised to check the EEDF results when taking  $E/N$  values much above the estimated validity limit, namely by comparing the solution obtained for the isotropic and the anisotropic parts of the electron distribution function.**

Also, HF calculations are valid only if the oscillation frequency of the electric field is much larger than the typical frequency for the electron energy relaxation, which can be approximately written as (see (12b))

$$\omega \gg (m_e/M)N(\nu_c/N) , \quad (79)$$

corresponding to  $\omega/(2\pi) \gg 20 \text{ MHz} - 20 \text{ kHz}$  for  $\nu_c/N \sim 10^{-13} \text{ m}^3 \text{ s}^{-1}$ ,  $m_e/M \sim 5 \times 10^{-5}$ ,  $T_g = 300 \text{ K}$  and  $p \sim 10^5 \text{ Pa} - 130 \text{ Pa}$ .

**Again, users are advised to check the validity of the HF approximation for the particular working conditions considered.**

LoKI-B contains several control features upon the input data and the calculation results, and in some cases it returns warning messages for the benefit of users. In particular:

- the code controls the maximum value  $u_{\max}$  of the energy grid adopted, comparing it with the cutoff energy  $u_{\text{cutoff}}$  of the electron-neutral elastic momentum-transfer cross section.  
**When  $u_{\text{cutoff}} < u_{\max}$  a warning message is returned**, and if the user accepts to proceed with the calculations these are carried out by setting to zero the values of any cross section from its corresponding  $u_{\text{cutoff}}$  and up to  $u_{\max}$ . **LoKI-B does not extrapolate cross sections beyond the cutoff energies defined in the input data-files**, again because it adopts an ontology that separates the tool and the data. The user is recommended to always careful examine the cross sections being used and, if needed, he/she should adopt adequate laws to extrapolate them, chosen according to the specific processes considered (*e.g.* dipole allowed or dipole forbidden electron excitation, ionization, etc);
- the code **returns a warning message** if the calculation of the elastic momentum-transfer cross section from the corresponding effective produces negative values for  $\sigma_{k,c}^{\text{el}}$  (see section 5.2), which is then set to zero. **In this case, users are advised to check the cross section data adopted**;
- **in stationary simulations**, the code controls the quality of the Boltzmann-matrix inversion, by monitoring the error upon the fractional electron power-balance. The latter is obtained from (56a), by normalizing this equation with respect to a *reference power-density*  $\Theta_{\text{ref}}$ ,**defined for each calculation as the sum of all power-gain terms** (see section 3).  
The relative error  $[\Theta_E + \Theta_{\text{coll}}^{\text{gain}} + \Theta_{\text{coll}}^{\text{loss}} + \Theta_{\text{growth}}] / \Theta_{\text{ref}}$  (with typical values  $\sim 10^{-9} - 10^{-10}$ , and user-defined maxPowerBalanceRelError threshold for producing a warning message, see section 5.2) degrades for very-low  $E/N$ s, due to the smallness of the power-density values for all the power-transfer channels, and for very-high  $E/N$ s, if the  $u_{\max}$  grid-limit adopted in the calculations is not large enough to prevent ill-conditioned EBE-matrices.

Concerning cross section data, the user is further advised to carefully check

- if the electron-scattering cross sections are set to zero at the threshold energy, as it is coherently assumed by LoKI-B. Note that, excluding errors, the LXCat files obtained from the IST-Lisbon database comply with this recommendation;
- the maximum value  $u_{\max}$  of the energy grid adopted, comparing it with the highest threshold  $u_{\text{th}-\max}$  of the collisional cross sections associated with reactions for which superelastic mechanisms are activated. Note that  $u_{\max} \gg u_{\text{th}-\max}$  should be ensured, to properly account for the superelastic effects.

## 9 Changelog

This is probably not very interesting for the ordinary user. But since you have made it this far, please take a moment to read a brief history of the code since its first release.

- LoKI-B\_v2.2.0 (2022/11/04):

- NEW FEATURE: general implementation of anisotropic e-impact collisions.
- NEW FEATURE: proper implementation of hf simulations for prescribed eedf .
- BUG FIX: added checking to avoid e-impact collisions types non-supported by LXCat.
- BUG FIX: improve the evaluation of power in electron-electron collisions.
- BUG FIX: solved error in the temporal growth operator, when using the time-integration algorithm.
- A few minor changes to improve stability and performance of the code.

- LoKI-B\_v2.1.0 (2022/03/04):

- NEW FEATURE: the DC reduced mobility is always evaluated and the (complex) HF mobility is only provided in the case of oscillating fields.
- NEW FEATURE: added the possibility of selecting lin/log scale for both axis on the graphs of the different swarm parameters. For the power graph only the xaxis can be toggled between lin/log scale.
- BUG FIX: solved important error in the e-e collision (`mixingDirectSolutions` scheme only) operator related with the units of the reduced field
- BUG FIX: now attachment collisions are not considered for the evaluation of a reduced field from power balance when using `PrescribedEedf`.
- BUG FIX: activated the renormalization of the eedf for the calculation of the eedf derivative.
- BUG FIX: solved an inconsistency in the evaluation of the reference power in `PrescribedEedf` with respect to `Boltzmann` class.
- Added the possibility of providing thresholds with scientific notation in LXCat files.
- A few minor changes to improve stability and performance of the code.

- LoKI-B\_v2.0.1 (2021/09/20):

- BUG FIX: solved error in the clipping of negative values of an elastic cross section (when evaluated from an effective one) to zero.

- LoKI-B\_v2.0.0 (2021/02/14):

- NEW FEATURE: Added the option to perform pulsed simulations (see sections [1.3](#) and [5](#)).
- NEW FEATURE: Added two new parameters calculated on output, the energy diffusion coefficient and the energy mobility (see section [3](#)).
- IMPORTANT CHANGE: Structure of property functions have changed from the previous version to accommodate new features. For more information see section [7.1](#).
- BUG FIX: Solved small error in the implementation of the CC-CAR operator (see section [1.2](#)).
- BUG FIX: Solved an error in the evaluation of both the Townsend coefficient and the attachment coefficient (the code now accounts for more than one of such collisions per gas).
- BUG FIX: Solved an inconsistency between the code and the documentation related with the evaluation of the reduced mobility in HF simulations The code now evaluates the real part of the HF mobility in these simulations (see section [3](#)).
- BUG FIX: Solved some inconsistencies in the evaluation of the power from the field when non linear operators were activated resulting in a wrong evaluation of the power balance in some cases.
- Removed deprecated class `Maxwellian`.
- A few minor changes to improve stability and performance of the code.

- LoKI-B\_v1.0.0 (2019/03/20):

- NEW FEATURE: The user can now use a time integration algorithm to solve the non-linear operators. For more information see section [5.2](#).
- NEW FEATURE: Added attachments collisions as non-conservative mechanisms.
- NEW FEATURE: Added power transfer plot to the GUI.
- NEW FEATURE: Added evaluation and output of the elastic/effective collision rate coefficients.
- NEW FEATURE: Added attachment collisions as non-conservative mechanism (when they are present).
- NEW FEATURE: Added the possibility for the user to change the scale of the EEDF graph in the GUI (linear/log).
- NEW FEATURE: Added evaluation of the first anisotropy
- IMPORTANT CHANGE: The reference power is now considered as the total gained power from all possible sources.
- IMPORTANT CHANGE: The configuration of the electron kinetics on the setup file has been slightly modified in order to accommodate new features. For more information see section [5.2](#).
- IMPORTANT CHANGE: Changed the “Maxwellian” EEDF type by “prescribedEedf” (generalised expression with Maxwellian/Druyvesteyn as particular cases). For more information see section [5.2](#).
- BUG FIX: fixed a problem that caused the results of the first job of a simulation to be saved outside its subfolder.
- BUG FIX: fixed small error in the morse oscillator energy formula.
- A few minor changes to improve stability and performance of the code.

- [LoKI-B\\_v0.6.3 \(2018/03/26\)](#):

- BUG FIXED: corrected a problem with the Klein-Roseland expression in the evaluation of superelastic cross sections. The bug only affected the evaluation of an elastic cross section from an effective one, and not the actual Boltzmann calculations. However, results obtained with previous versions of the code may be greatly affected (when using “effective” cross sections and superelastic mechanisms) hence it is recommended to repeat calculations with this new version.
- BUG FIXED: fixed a problem with the detailed balance in the e-e collisions. This bug only introduced a small error that affected convergence of the non-linear algorithm.

- [LoKI-B\\_v0.6.2 \(2018/01/18\)](#):

- BUG FIXED: corrected some expressions used in the evaluation of the swarm parameters, for the cases when the electron density growth is activated.
- BUG FIXED: fixed a problem with the Maxwellian type of EEDF, for which the code used to crash when trying to output (GUI or file) the power losses due to the electron density growth.

- [LoKI-B\\_v0.6.1 \(2018/01/16\)](#):

- BUG FIXED: previously the Spitzer integrals (e-e collision operator) were updated inside the routines with the operators for the electron-density growth. Now the update is done outside these routines, and convergence on both operators is completely isolated.
- BUG FIXED: previously, different EEDFs were being used to evaluate different parts of the e-e collision operator. Now, the convergence of the algorithm has been improved.
- The global cycle for the non-linear operators of the Boltzmann equation is now testing the changes in the EEDF only as convergence criterion.
- Slight improvement in the warning messages, in the cases where the non-linear operators of the Boltzmann equation do not converge.
- A few minor changes to improve stability and performance of the code.

- [LoKI-B\\_v0.6.0 \(2018/01/13\)](#):

- NEW FEATURE: The user can now select non-conservative ionization operators (“one takes all”, “equal sharing” or “using single differential cross section”) for the Boltzmann equation as well as two types of growth models (“spatial” or “temporal”) for the electron number density. For more information, see sections [1](#) and [5.2](#).

- NEW FEATURE: The user can now include the electron-electron collision operator in the Boltzmann calculations. For more information, see sections 1 and 5.2.
  - IMPORTANT CHANGE: Changes in the way the power balance is evaluated. The evaluation of the “reference power” is now fairer. The power transferred to the elastic and the CAR channels is now separated into gains and losses, and the reference power is obtained as the channel from which the electrons gain more energy.
  - BUG FIXED: fixed bug in the State.find static method, that caused errors when finding all the electronic states of a certain gas.
  - BUG FIXED: fixed bug introduced in commit 813e38f (Nov 9, 2017), that prevented the user to deactivate the output of the code.
  - A few minor changes to improve stability and performance of the code.
- LoKI-B\_v0.5.0 (2017/12/14):
    - NEW FEATURE: The electron drift velocity is now evaluated by the code. This information can be seen in the “Swarm parameters” and “Look-up-table” tabs of the GUI, as well as in the corresponding output files. (User Requested)
    - NEW FEATURE: “Extra” electron-scattering cross sections, *i.e.* cross sections that are not taken into account when solving the electron Boltzmann equation, can now be added. The corresponding rate coefficients are obtained by integrating these cross sections over the calculated EEDF. For more information, see section 5.2.
    - NEW FEATURE: The power balance is now detailed in a per-gas basis. (User Requested)
    - BUG FIXED: The output of the electron “Ionization” and “Attachment” was not being done properly.
    - IMPORTANT CHANGE: the only comment character allowed in the input files is now %, for performance reasons. The # character is NO LONGER RECOGNISED.
    - IMPORTANT CHANGE: A few changes in the way the properties of the setup file are organised. For more information, see section 4.3.
    - A few changes where introduced to improve the performance of the code:
      - \* Improved performance of the Collision.find static method, by avoiding implicit values in the loop.
      - \* Improved performance of the output.saveEedf method, by vectorizing a loop (almost 13x speedup)
    - A lot of LoKI-C code has been introduced and several changes in the structure of the code has been made in order to accommodate and integrate the chemistry module. However, LoKI-C is still not available (Coming soon!)
    - A few minor changes to improve stability and performance of the code.
  - LoKI-B\_v0.4.0 (2017/10/17):
    - NEW FEATURE: The user can now prescribe a Maxwellian EEDF. For more information, see section 5.2.
    - NEW FEATURE: The user can now specify the “refresh frequency” of the GUI, in order to speedup simulations. For more information, see section 5.3.
    - Structural changes in the calculations and aesthetical changes in the GUI, in order to speedup calculations. A huge difference is observed, when compared with previous versions.
    - BUG FIXED: the electron temperature was being calculated with the characteristic energy instead of the mean energy.
    - BUG FIXED: solved bug causing the GUI to display the same rate coefficient for direct and inverse processes.
    - A few minor changes to improve stability and performance of the code.
  - LoKI-B\_v0.3.0 (2017/09/08):
    - NEW FEATURE: The user can now specify the populations used for the evaluation of the elastic momentum-transfer cross section, from the effective. This feature must be used with care. For more information, see section 5.2.

- Added graphs in the GUI, for the reduced first Townsend and attachment coefficients vs.  $E/N$ .
  - Included the character “-” in the names of electronic states (important for some N2 states, and not supported before).
  - BUG FIXED: fixed error in the evaluation of the elastic momentum-transfer cross section from the effective. The bug affected molecular gases only.
  - BUG FIXED: fixed a completely harmless error related with the parsing of collisions. Electrons where not properly accounted for.
  - A few minor changes to improve stability and performance of the code.
- [LoKI-B\\_v0.2.0 \(2017/06/09\)](#):
- NEW FEATURE: added support for the continuous approximation for rotations (CAR). For more information, see sections [1](#) and [5.2](#).
  - BUG FIXED: the evaluation of the elastic momentum-transfer cross section from the effective is now properly done. Previously, there were some errors in the evaluation of the populations of rotational states, as well as with the inclusion of superelastic mechanisms. The problem was not affecting the simulations in which an elastic cross section was provided by the user.
  - A few minor changes to improve stability and performance of the code.
- [LoKI-B\\_v0.1.1 \(2017/04/10\)](#):
- BUG FIXED: solved error in the calculation of the reduced first Townsend coefficient. The reduced field was being used in Townsend instead of SI units, in the evaluation of the coefficient.
  - A few minor changes to improve stability and performance of the code.
- [LoKI-B\\_v0.1.0 \(2017/04/05\)](#):
- First release of the code (beta).

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