The LisbOn KInetics LoKI-B+C simulation tool

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Introduction and LoKI-B+C description

The **LisbOn KInetics LoKI-B+C** [1] is a simulation tool for plasma chemistry, developed and consolidated resorting to the well-grounded scientific foundations of the Portuguese group N-PRIME. LoKI-B+C has been originally developed with flexible and upgradable object-oriented programming under MATLAB®, to benefit from its matrix-based architecture, adopting an ontology that privileges the separation between tool and data.

LoKI-B+C couples two main calculation blocks: a **Boltzmann solver (LoKI-B)** [2-3], and a **Chemical solver (LoKI-C)** [4] that can run self-consistently coupled or as standalone tools.

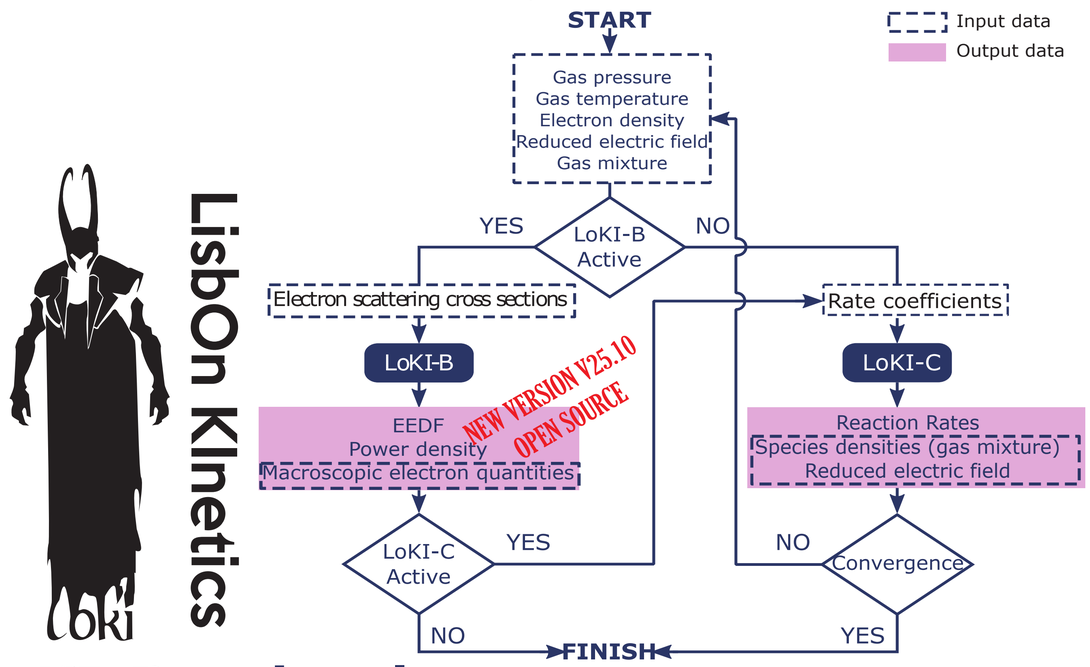
- **LoKI-B** (released as open-source code [2] licensed under the GNU GPL v3.0) solves the space-independent form of the two-term electron Boltzmann equation for non-magnetised non-equilibrium low-temperature plasmas, excited by DC/HF electric fields or time-dependent (non-oscillatory) electric fields from different gases or gas mixtures. The tool addresses glow plasmas, using 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 handles the electron kinetics in **any complex gas mixture**, describing first and second-kind electron collisions (with anisotropic effects for elastic and rotational encounters) with **any target state**, characterized by **any user-prescribed population**.

- **LoKI-C** [4] solves the system of zero-dimensional (volume average) rate balance equations for the most relevant charged and neutral species in the plasma, receiving as input the **kinetic schemes for the gas/plasma system** under study. LoKI-C uses several modules (i) to describe the mechanisms (collisional, radiative and transport) controlling the creation/destruction of species, namely various transport models for charged and neutral particles; (ii) to self-consistently calculate the gas temperature, by solving a gas/plasma thermal model; and (iii) to fully couple volume and surface kinetics, namely by solving a set of deterministic "rate-balance like" equations [5,6], accounting for different **plasma-surface interaction processes**.

This contribution presents a **status report on the development of LoKI-B+C** and is intended to also receive comments and suggestions from the low-temperature plasmas community, **in preparation of its release as open-source code**.

LoKI-B+C workflow

The solution of LoKI-B+C follows a **workflow embedding iterative cycles until convergence**. As input LoKI-B+C receives the working conditions for the experimental setup (radius and length), the gas (e.g., mixture composition, pressure, temperature, and inflow), and the excitation characteristics (electron density, or discharge current, or power density). As output, LoKI-B+C self-consistently calculates the electron energy distribution function (EEDF) and the associated electron macroscopic parameters, the densities of species, the reaction creation/destruction rates, the outflow, and the reduced electric field. Results are stored in **TXT** and/or **HDF5** format.



LisbOn KInetics

LoKI-B+C optimization of iterative cycles

The convergence algorithm of LoKI-B+C has been revised to consolidate convergence cycles, speeding up calculations and improving performance. Currently the convergence algorithm comprises **2.5 cycles**:

(i) NEUTRALITY cycle for an user prescribed electron density, discharge current or power density.

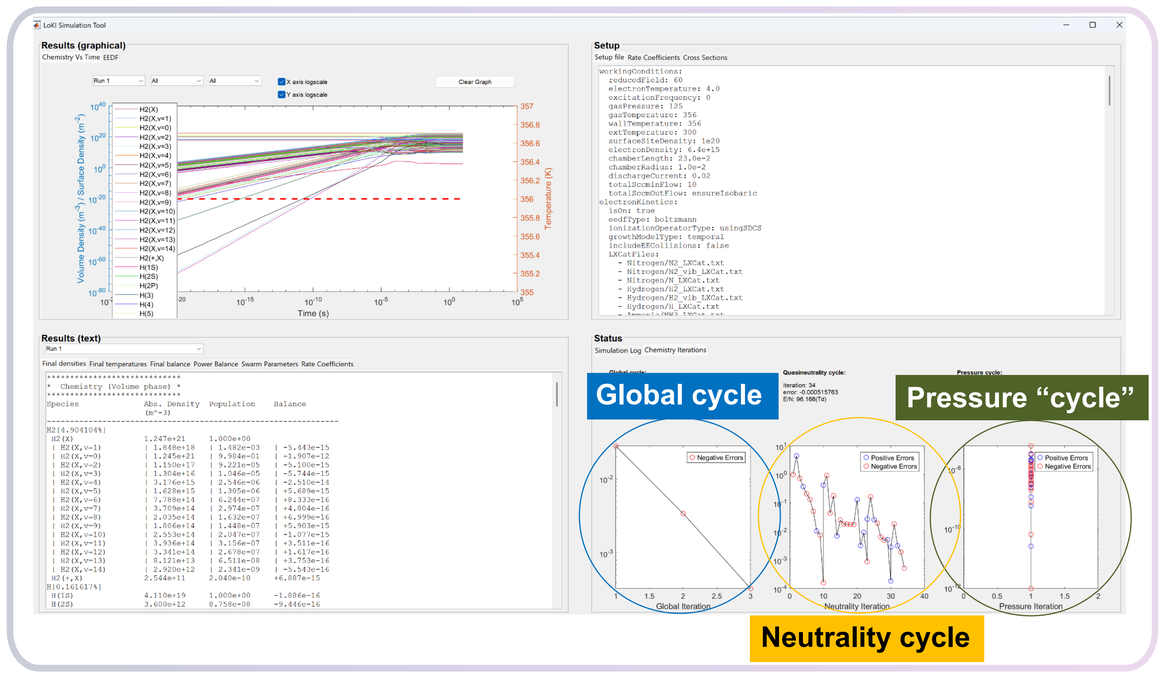
(ii) GLOBAL cycle: over the densitites of the most relevant excited states afecting the electron Boltzmann equation, to globally converge over the EEDF and the electron macroscopic parameters.

(iii) PRESSURE "cycle": to verify the user-prescribed steady-state pressure, according to the inflow/outflow conditions.

The outflow frequency is self-consistently obtained as to ensure the conservation of the number of particles ($dp/dt = 0$)

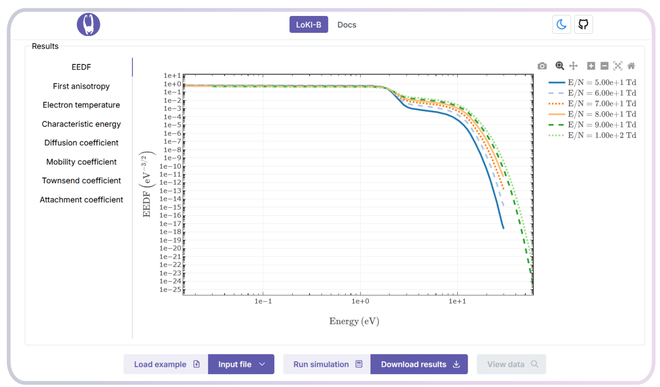
$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \left.\frac{\mathrm{d}n_i}{\mathrm{d}t}\right|_{chem} + \left.\frac{\mathrm{d}n_i}{\mathrm{d}t}\right|_{flow} = \left.\frac{\mathrm{d}n_i}{\mathrm{d}t}\right|_{chem} - k_{out} n_i$$

$$k_{out} = \frac{1}{N}\left.\frac{\mathrm{d}N}{\mathrm{d}t}\right|_{chem} + \frac{1}{T_g}\frac{\mathrm{d}T_g}{\mathrm{d}t}, \qquad \left(N = \sum_i n_i = \frac{p}{k_B T_g}\right)$$



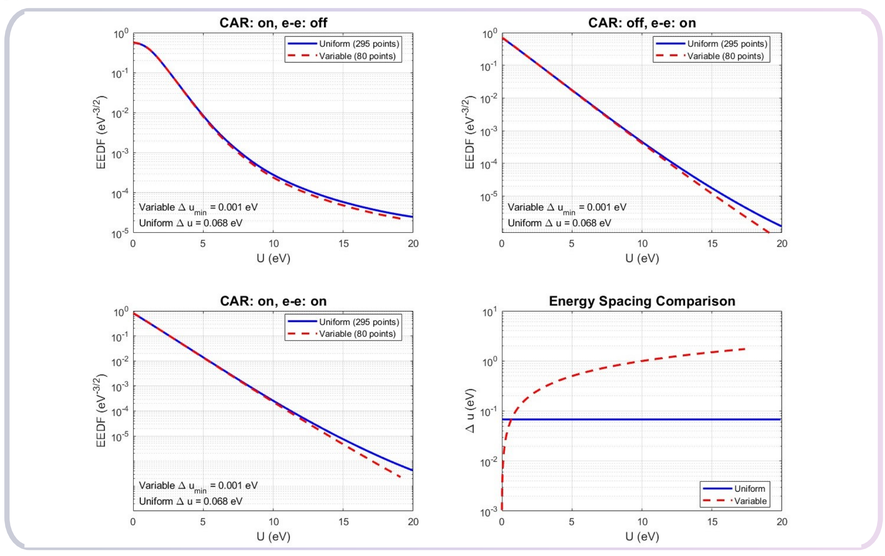
LoKI-B web solver

The **C++ version of LoKI-B** can be accessed through a standalone tool that allows users to perform **web-based calculations** [7]. Each simulation generates a unique address containing a specific identifier for the input file. This ensures that the exact same input conditions and cross-section data - obtained automatically through **LXCat 3.0** [8] - can be preserved and shared, enabling full reproducibility of the simulation.



LoKI-B on variable energy grid

Calculations on **variable energy grids** were performed in LoKI-B, using a geometric progression for the energy step. This first implementation addressed the **continuous operators**: electric field, elastic collisions, continuous approximation for rotations (CAR), and electron-electron (e-e) collisions (see below an illustration for H_2 at E/N = 10 Td). Discretization factors were introduced to ensure particle and energy conservation.



Developments in progress and releases

The **current efforts** in the development of LoKI-B+C are focused on:

(i) the inclusion of an **additional heating operator in LoKI-B**, describing the combined ohmic-stochastic interaction of electrons with the applied electric field [10]
(ii) the **implementation of time-dependent calculations**, coupling **LoKI-B and LoKI-C** under different approximations
(iii) the design and development of a **regression test suite**

(iv) the design and development of a user-friendly **GUI for setup data input**

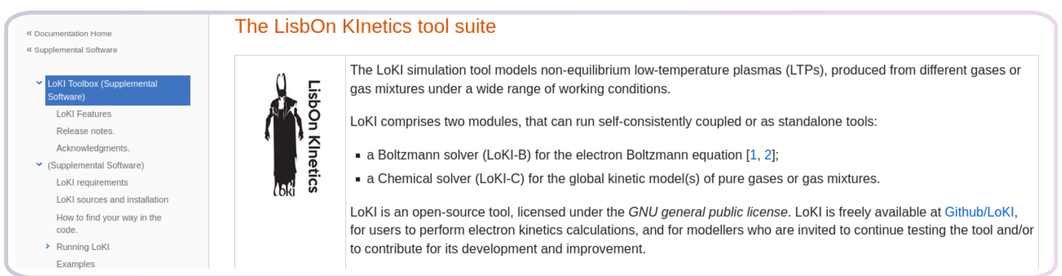
The release of LoKI-B+C as open-source is planned for 2025/2026.

New release of LoKI-B and LoKI-B++ v25.10:
- LoKI-B++**, the C++ counterpart of LoKI-B MATLAB,** developed in collaboration with **TU/e, was released as Open Source and integrated in PLASIMO 10** [11].

- New Features such as **HDF5 output** and **JSON input** support (LXCat 3.0 compliant).

LoKI-B+C as MATLAB add-on

Packaging of LoKI-B+C as a **MATLAB toolbox** [9], allowing integration with other MATLAB products for an **easy distribution, installation and a browser-based online-help.**



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[8] LXCat 3.0, https://demo.lxcat.net/
[9] https://www.mathworks.com/help/matlab/creating-help.html
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[11] PLASIMO - plasma modeling software, https://plasma-matters.nl

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