The LisbOn KInetics LoKI-B+C simulation tool

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The LisbOn KInetics LoKI-B+C [1] is a simulation tool for plasma chemistry that couples two main calculation blocks: a Boltzmann solver (LoKI-B) [2,3] and a Chemical solver (LoKI-C), developed / 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 (released as open-source code [4] 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 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, yielding the coverage of available/occupied sites at the surface while describing the interplay between surface and volume kinetics.

The solution of LoKI-B+C follows a workflow embedding four iterative cycles: (i) over the initial mixture composition, to obtain the user-prescribed *pressure*; (ii) over the reduced electric field, to satisfy the plasma *neutrality*, for an user-prescribed electron density (or some equivalent parameter, see below); (iii) over the densities of the most relevant excited states afecting the electron Boltzmann equation, to *globally* converge over the electron energy distribution function (EEDF) and the electron macroscopic parameters; and (iv) over the electron density, to obtain the user-prescribed *discharge current* (or *power density*). As output, LoKI-B+C self-consistently calculates the EEDF and the associated electron macroscopic parameters, the densities of species, the reaction creation/destruction rates, and the reduced electric field.

This contribution presents a status report of the LoKI-B+C simulation tool, and is intended to also receive comments and suggestions from the low-temperature plasmas community, in preparation of its release as open-source code. Presently, evolutions of LoKI-B+C under the supervision of the N-PRiME group, comprise mostly: (i) the development of LoKI-B++, the C++ version of LoKI-B; (ii) the inclusion

of an additional heating operator in LoKI-B, describing the combined ohmic-stochastic interaction of electrons with the applied electric field; (iii) the inclusion in LoKI-B of a DC magnetic field, at arbitrary angles; (iv) the time-dependent coupling between LoKI-B and LoKI-C; (v) the use of the hdf5 format to write output results; and (vi) the optimization of the iterative calculation cycles.

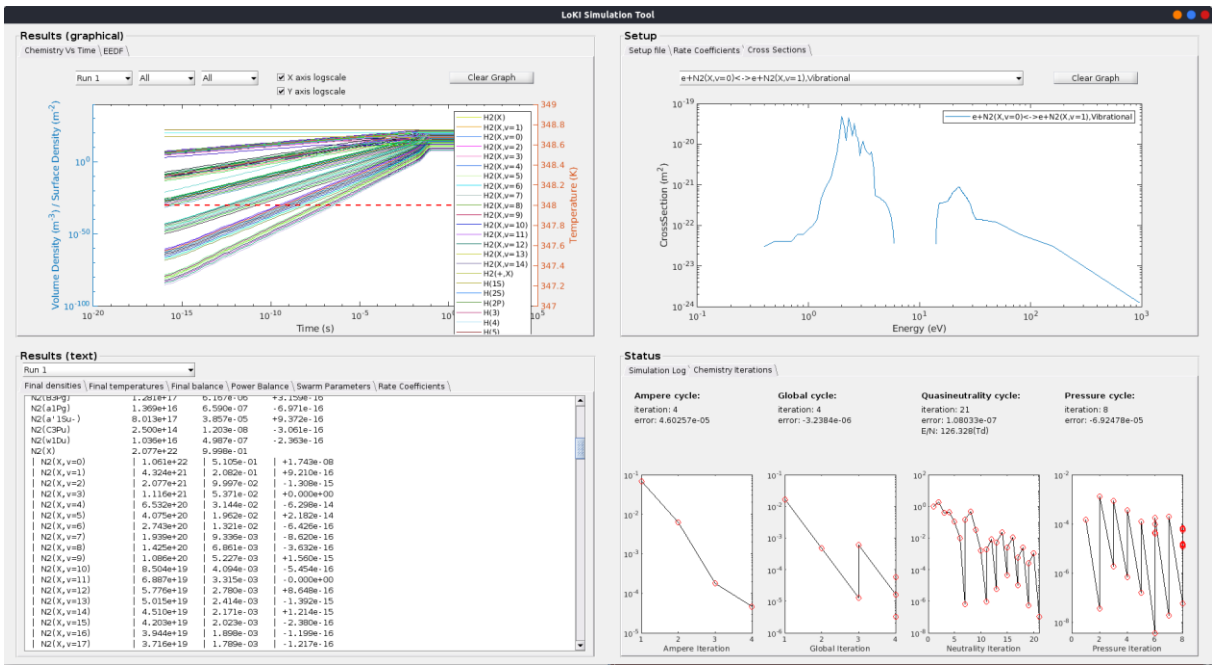

Fig. 1: Example of the Graphical User Interface display after a complete LoKI-B+C simulation.

Figure 1 presents an example of the Graphical User Interface (GUI) display after a complete LoKI-B+C simulation, for a situation where the working conditions impose the discharge current. The updated version of the GUI shows: in the lower-right corner, the four convergence cycles, from right to left, for the pressure, the neutrality, the global densities, and the discharge current; in the lower-left corner, the summary of the output results, in text format (the figure shows the results for the densities of species); in the upper-left corner, the summary of the output results, in graphical format (the figure shows the results for the densities of species, as a function of the calculation time); and in the upper-right corner, the summary of the input data (the figure depicts a vibrational cross section used in the calculations).

The current efforts in the development of LoKI-B+C are focused on replacing the pressure cycle by a different handling of the in/out-flows, and on generalizing the neutrality cycle so that it iterates over the reduced electric field to directly obtain the electron density, the discharge current or the power density imposed by the user.

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