The LisbOn KInetics LoKI-B+C simulation tool

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Introduction

With the advent of powerful hardware and readily available software, **computer simulations have become almost indispensable in all fields of research**. Low-Temperature Plasma (LTP) physics is no different, and we can find codes with approaches ranging from first-principles to model-based, running on multi-node clusters or mobile hardware.

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.

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.**

LoKI description

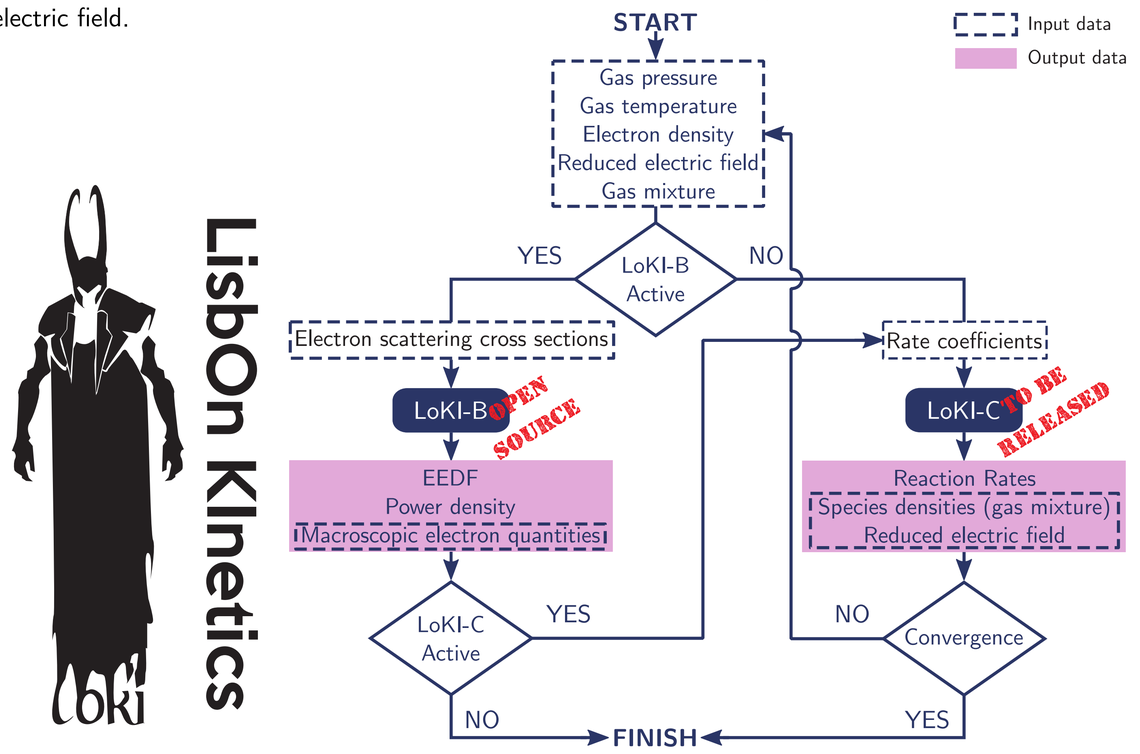
LoKI-B+C comprises two modules, a **Boltzmann solver, LoKI-B** [2-4], and a **chemistry solver, LoKI-C** [5] that can run self-consistently coupled or as standalone tools.

- **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** [5] 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 [6,7], 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.

LoKI 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 setup (radius and length), the gas (e.g., mixture composition, pressure, temperature; flow), and the excitation (electron density, or 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.



LoKI-B+C revision of convergence cycles

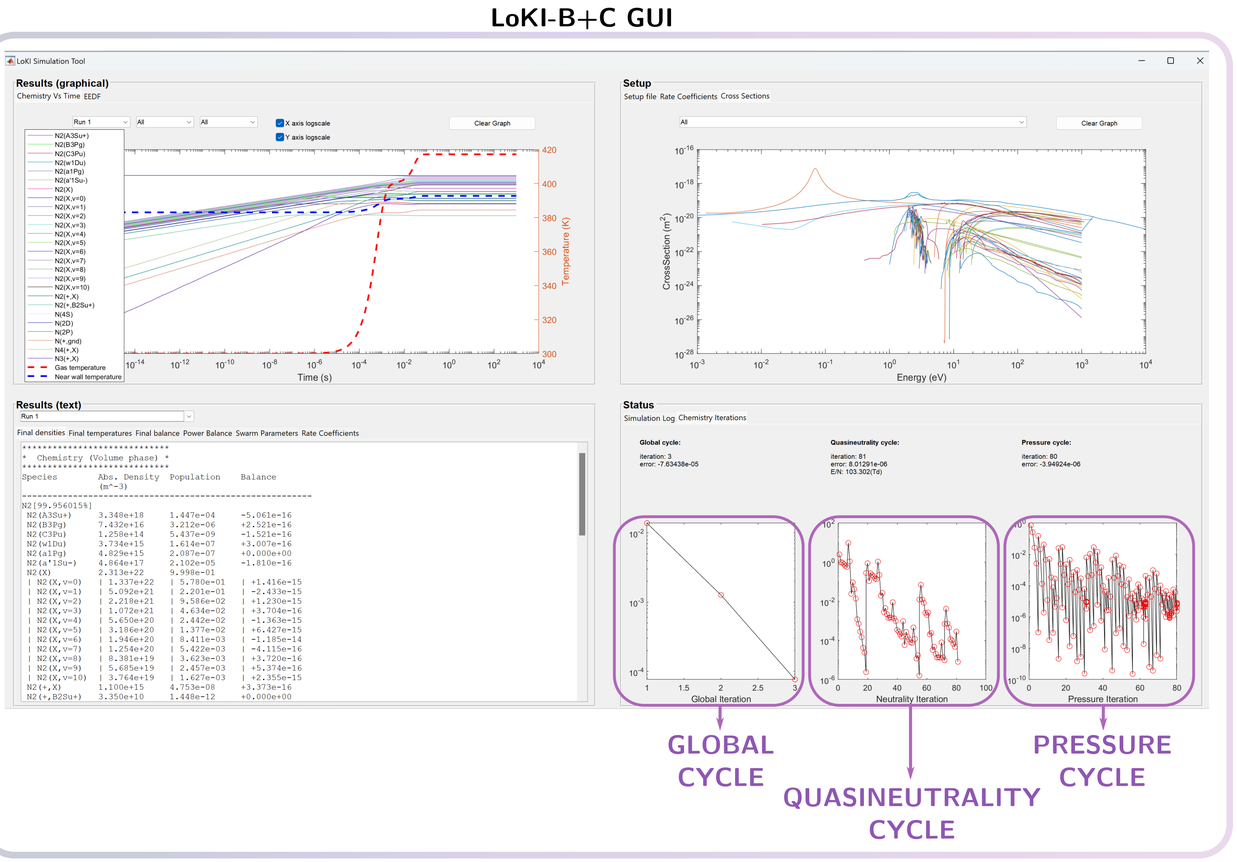
The convergence algorithm of LoKI-B+C have been revised to consolidate convergence cycles, speeding up calculations and improving performance. Currently the convergence algorithm comprises three cycles:

(i) PRESSURE cycle: over the initial pressure, to obtain the user-prescribed steady-state pressure.

(ii) QUASINEUTRALITY cycle: over the reduced electric field, to satisfy the plasma neutrality, for an user-prescribed discharge current (or power density).

(iii) GLOBAL cycle: 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.

LoKI-B+C GUI

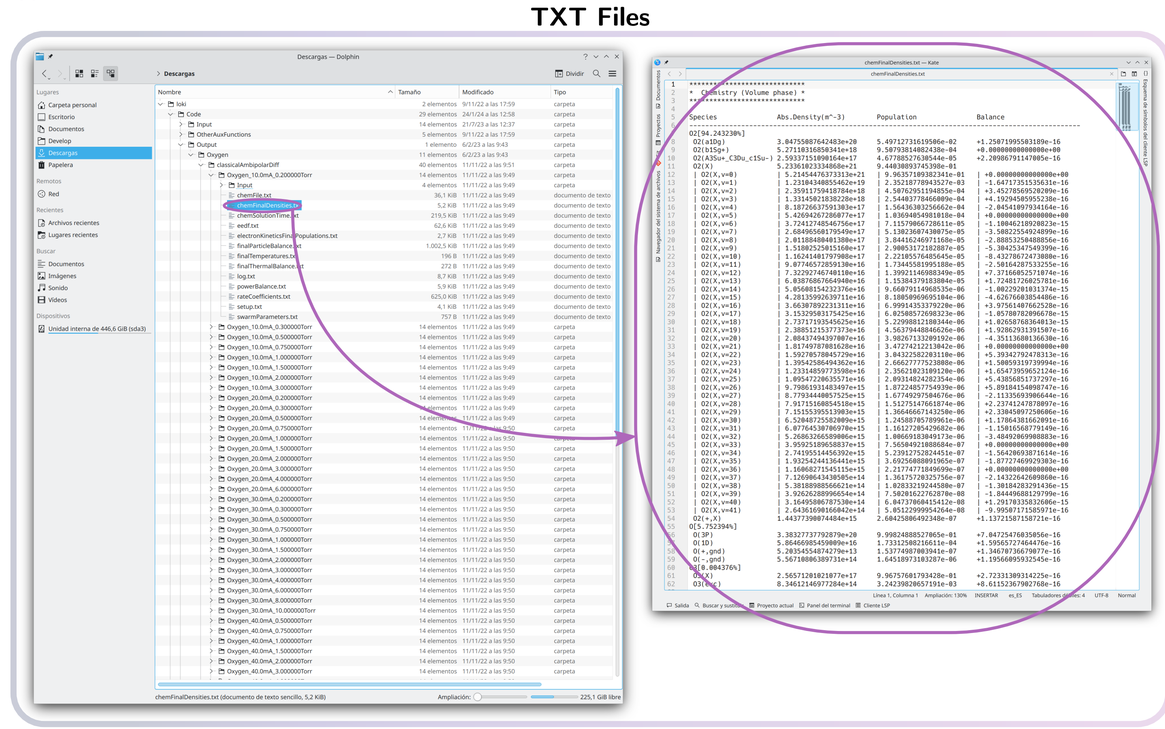


LoKI-B+C revision of output formats

The formats used in LoKI-B+C to deliver output data have been extended. Currently, LoKI-B+C supports the following output formats:

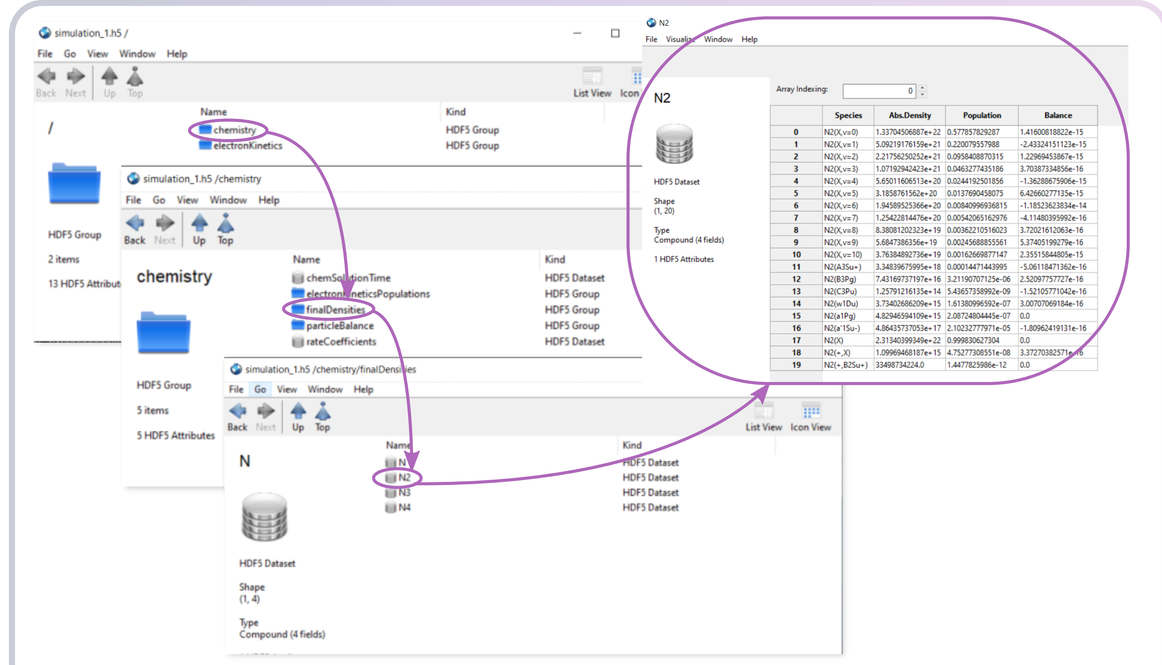
(i) TXT format: convenient and human readable, allows for quick and simple analysis of results.

TXT Files



(ii) HDF5 format [8]: cross-platform data file that supports n-dimensional datasets with complex objects, including metadata, streamlining data life-cycles and pipelines. This format enables automated analysis of output data from large amounts of simulations (LoKI-Tools).

HDF5 Files



Current status and release

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

(i) the **development of C++ version of LoKI-B** (to be released later this year).
(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) **eliminating the pressure cycle** by using a different handling of the in/out-flows.

The **release of LoKI-B+C as open-source is planned for next year**.

TENTATIVE RELEASE
OPEN-SOURCE
2025

References

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