The LisbOn KInetics simulation tools

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International Conference on Phenomena in Ionized Gases
XXXVth edition, July 9th to 14th 2023
Fully in person
Egmond aan Zee, The Netherlands

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N PRiME

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.

Predictive tools for non-equilibrium low-temperature plasmas should properly describe the **kinetics of both the electrons and the heavy-species**, the former responsible for inducing plasma reactivity and the latter providing the pathways for reaction mechanisms.

In this context, we started years ago the development of a set of simulation tools addressing quick and simple simulations for large and complex plasma systems: the **LisbOn KInetics simulation tools** [1], a suite for plasma chemistry simulations (LoKI) and a Monte Carlo code for electron kinetics simulations (LoKI-MC), developed adopting an ontology that separates tools and data, resorting to the well-grounded scientific foundations of the Portuguese group N-PRiME.

Implementation

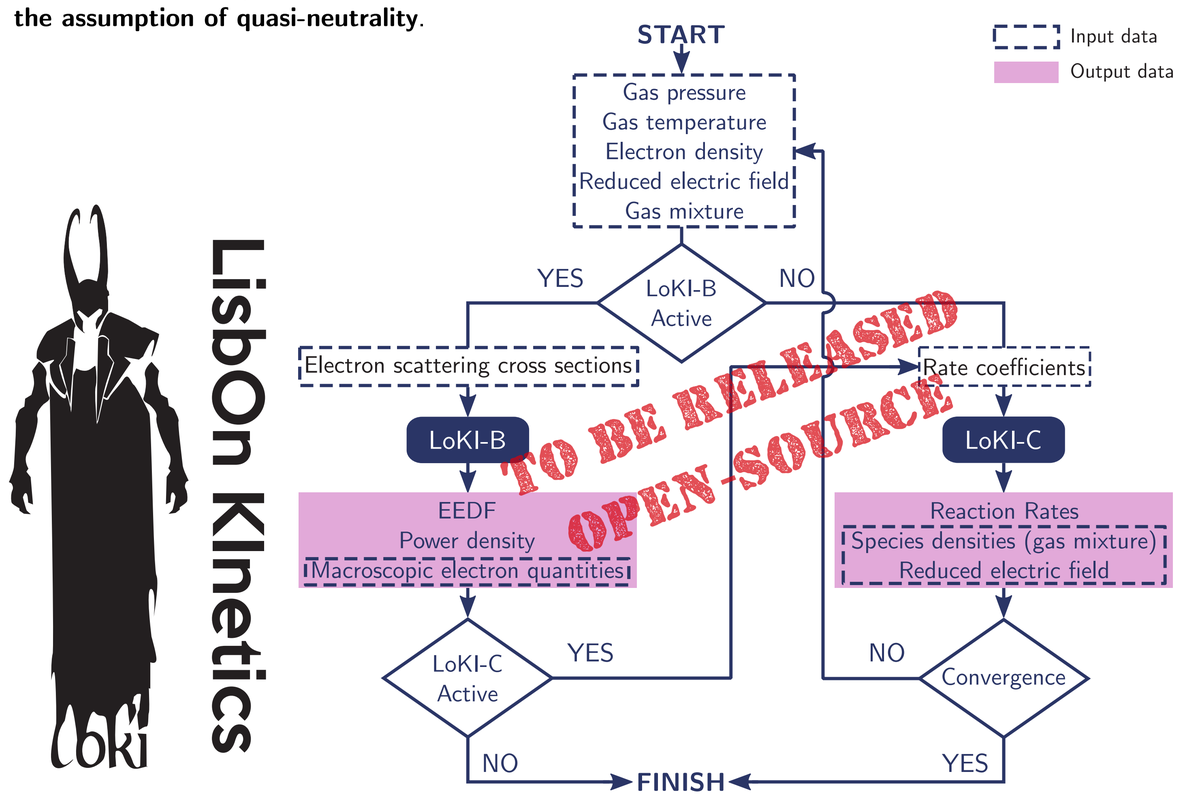
- **LoKI-B** (**released as open-source code** [2-4]) solves the space independent form of the two-term electron Boltzmann equation for non-magnetised non-equilibrium low-temperature plasmas, excited by DC/HF electric fields or time-dependent (non-oscillatory) electric fields from different gases or 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** (**to be released as open-source code**) 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.

- **LoKI-MC** (**released as open-source code** [5,6]) solves the electron kinetics for plasmas excited by uniform DC electric fields from different gas mixtures, using Monte Carlo techniques independent from the two-term approximation. The code, written in C++, follows an object-oriented structure and a data organization similar to LoKI-B, including as output the electron velocity distribution function and related macroscopic parameters. Recently, the LoKI-MC formulation was extended to further include AC/time-dependent electric fields [7], as well as DC magnetic fields [8].

LoKI workflow

The following flowchart describes the **workflow of LoKI**. For stationary discharges, **when both modules are activated**, the **reduced maintenance electric field** (or an equivalent parameter, such as the electron temperature) is **self-consistently calculated** as an eigenvalue solution to the problem, **under the assumption of quasi-neutrality**.



LoKI-B showcases

To illustrate the main use of LoKI-B we show modelling results [2] for a Nitrogen-Oxygen discharge:

- Figure 1: swarm analysis (for the reduced mobility) for a 80% Nitrogen - 20% Oxygen discharge: considering a Boltzmann distribution at T_g = 300 K for the vibrational and rotational distribution functions for the ground-states of both Nitrogen and Oxygen (solid); not considering rotational transitions (dashed); experimental measurements (symbols).

- Figure 2: Vibrational distribution functions for $N_2(X,v)$ (solid curve and squares), corresponding to a Treanor-Gordiets distribution at T_g = 300 K and T_{vib} = 4000 K, and for $O_2(X,v)$ (dashed and triangles), corresponding to measurements in an ICP.

- Figure 3: Electron energy distribution functions, calculated at E/N = 30 Td, considering different N_2–O_2 mixtures with the VDFs in Figure 2: 100% – 0% (black solid); 80% – 20% (black dashed); 50% – 50% (black dotted); 0% – 100% (blue). The red curve is the EEDF calculated for 80% – 20%, collapsing the VDFs to the ground-states $N_2(X, v=0)$ and $O_2(X, v=0)$.

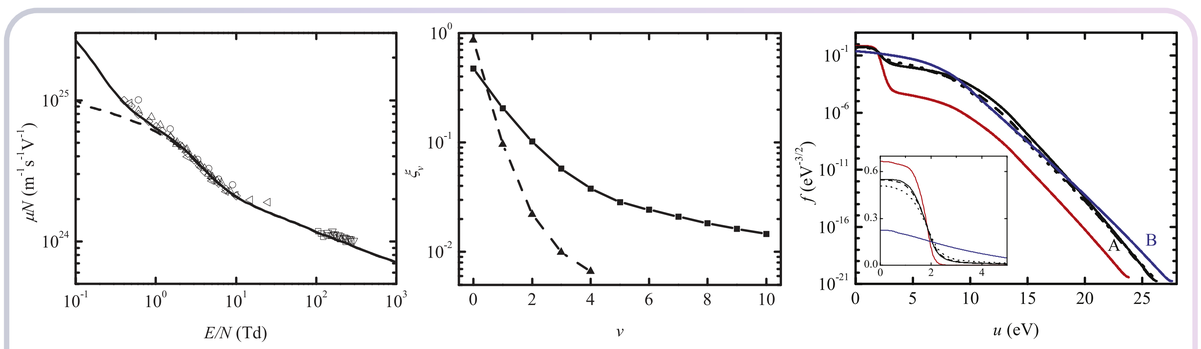


Figure 1 Figure 2 Figure 3

LoKI-MC showcases

To illustrate the main use of LoKI-MC we show modelling results [5] for a pure Oxygen DC discharge:

- Figure 4 (10 Td) / Figure 5 (500 Td): Electron velocity distribution functions for low/high reduced electric fields.

- Figure 6: velocity-average anisotropy ratios as a function of the reduced electric field.

LoKI-MC is preferred over LoKI-B in cases characterized by high anisotropies in the velocity space, which typically arise when the reduced electric field is high or when inelastic collisions significantly outweigh elastic collisions.

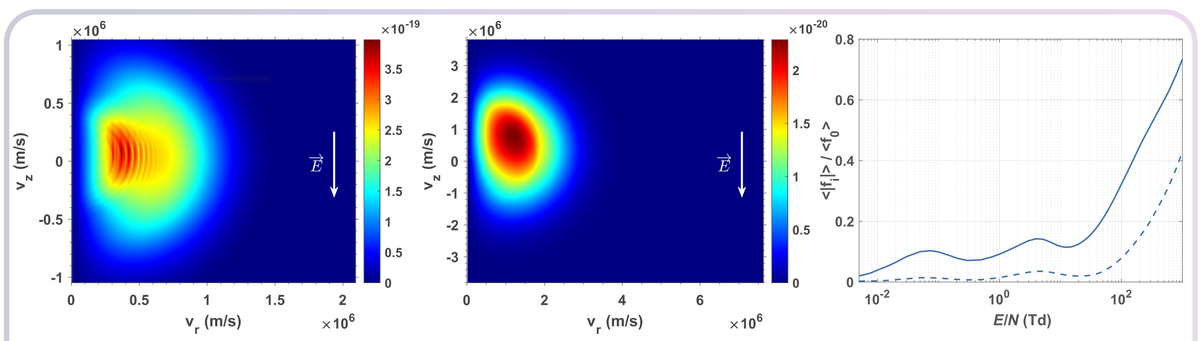


Figure 4 Figure 5 Figure 6

LoKI-C showcases

To illustrate the main use of LoKI-C we show modelling results [9] for:

- Figure 7: a low pressure pure Oxygen DC discharge with 1 cm radius and 52.5 cm in length for a self-consistently calculated gas temperature and for an interelectrode current of 40 mA.

- Figure 8: a high pressure pure Helium 2.45 GHz Surface-Wave Discharge with 0.3 cm radius for a gas temperature of 1000 K and an electron density of 5×10^{18} m^{-3}.

For both figures we show the densities of the main heavy-species (a) as well as the maintenance reduced electric field (b) as a function of $N\Lambda$ (N being the gas density and Λ the characteristic diffusion lenght) calculated considering different models for the transport of ions. Bands represent modelling results and points experimental measurements.

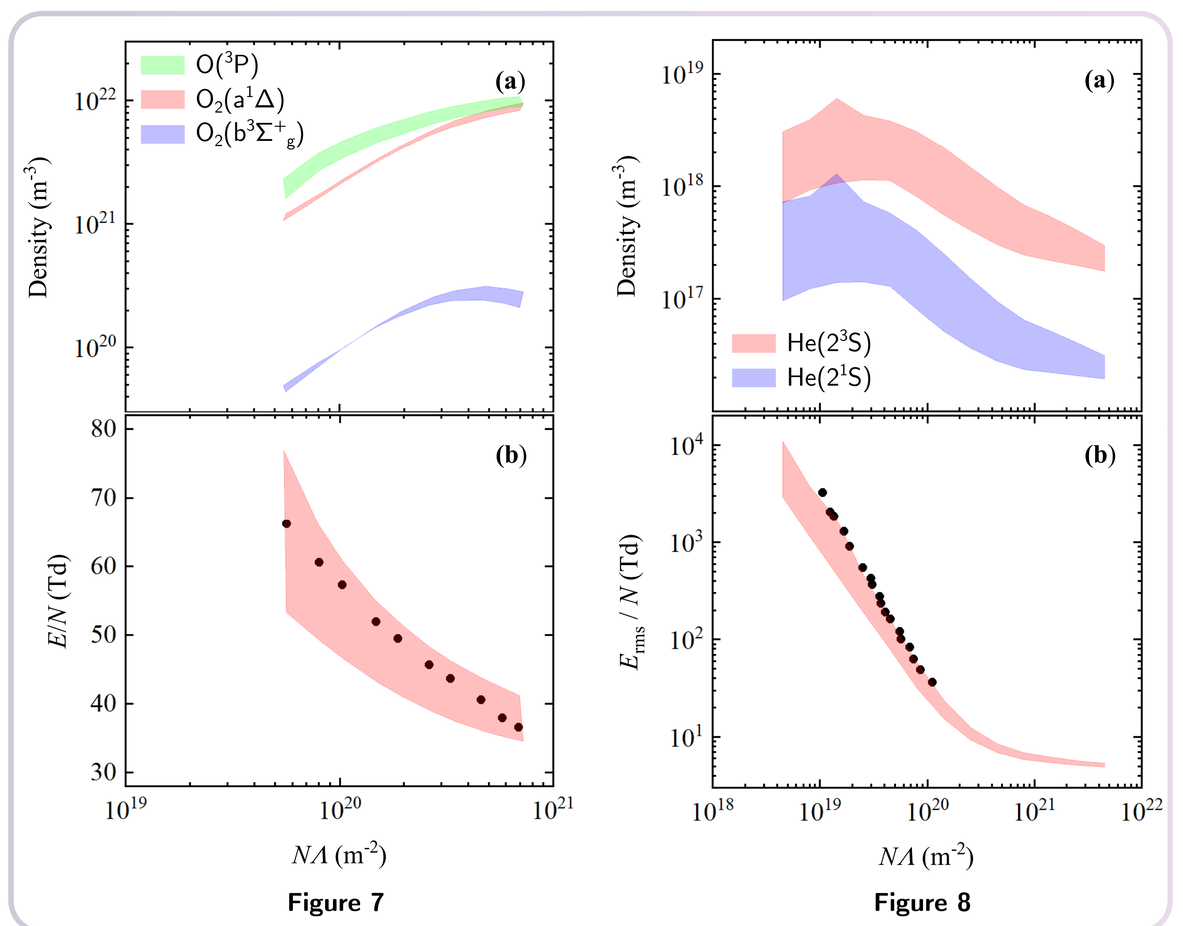


Figure 7 Figure 8

Conclusions

The LisbOn KInetics simulation tools are a set of user-friendly, scalable and upgradable codes. They enable users to **easily perform plasma simulations** accounting for both electrons and heavy species kinetics in any complex gas mixture.

Presently, the development of the different simulation tools comprises: (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 time-dependent coupling between LoKI-B and LoKI-C. LoKI is planned to be fully released as open-source code in the near future.

References

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Acknowledgements

This work was partially funded by the Portuguese Foundation for Science and Technology under projects 2022.04128.PTDC, UIDB/50010/2020 and UIDP/50010/2020.

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