The LisbOn KInetics simulation tools and data

International School on Atomic and Molecular Data Evaluation and Curation

A Tejero-del-Caz[1,2], T C Dias[2], V Guerra[2], M Lino da Silva[2], L Marques[3], N Pinhão[2], C D Pintassilgo[2,4] and L L Alves[2]

[1] *Departamento de Física, Facultad de Ciencias, Universidad de Córdoba, Córdoba, SPAIN*
[2] *Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, PORTUGAL*
[3] *Centro de Física das Universidades do Minho e do Porto, Braga, PORTUGAL*
[4] *Departamento de Engenharia Física, Faculdade de Engenharia, Universidade do Porto, Porto, PORTUGAL*

Introduction: data and tools

We started years ago the development of simulation tools for Low Temperature Plasmas (LTP), addressing quick and simple simulations for large and complex plasma systems: the LisbOn KInetics simulation tools, a suite for plasma chemistry simulations (LoKI) written in MATLAB and a Monte Carlo code for electron kinetics simulations (LoKI-MC) written in C++, resorting to the well-grounded scientific foundations of the Portuguese group N-PRiME.

The LoKI tools [1] are being developed with a clear ontology in terms of data handling. For example, LoKI-B and LoKI-MC require electron scattering cross sections as input data, which are parsed adopting a format compliant with the open-access website LXCat [2]. The decision of publishing data in a public database is advantageous for both users and developers, as it separates tools and data, ensures the open access to data, promotes using validated (recommended) data, and encourages adopting a standardised classification and organization of data.

Today, LXCat provides mainly electron scattering cross sections and swarm parameters 'required for modelling low temperature plasmas'. The database was developed more than a decade ago, and its current structure needs updating in terms of handling both data and metadata.

- **LoKI-B** (**released as open-source code** [3-5]) 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.

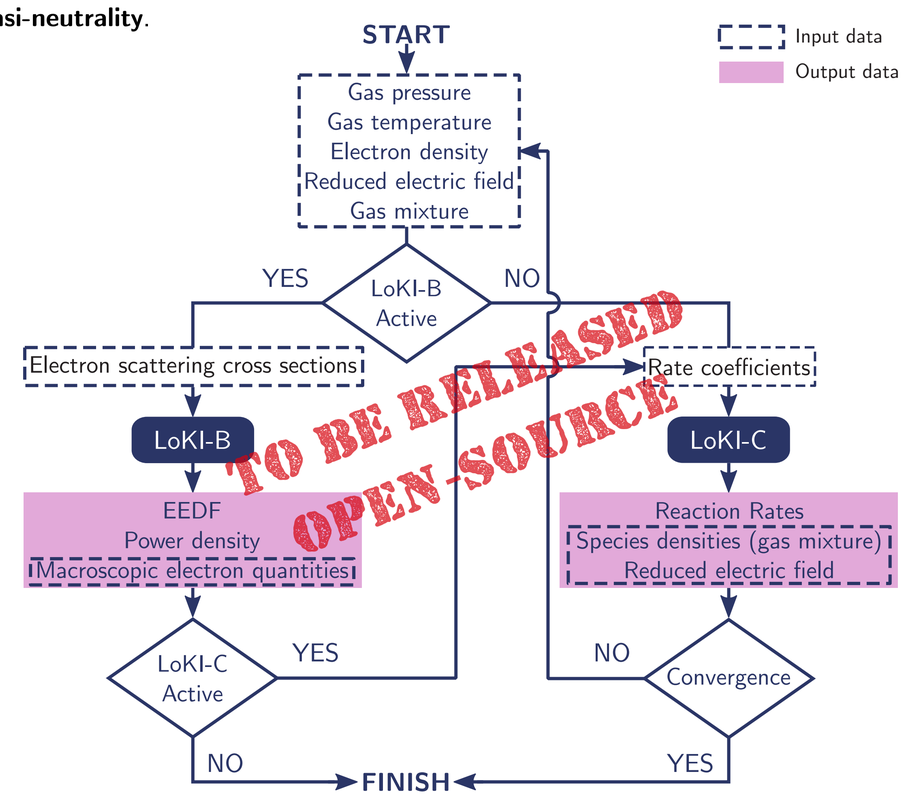
- **LoKI-C** (**to be released as open-source code**) solves the system of zero-dimensional (volume average) rate balance equations for the most relevant charged and neutral species in the plasma, receiving as input the kinetic schemes for the gas/plasma system under study. LoKI-C uses several modules (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** [6,7]) 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, 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 [8], as well as DC magnetic fields [9].

LisbOn KInetics

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 [3] 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).

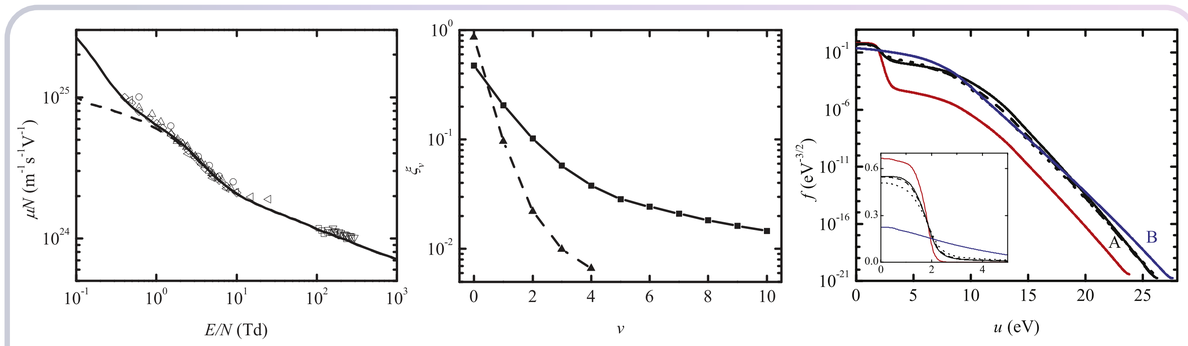


Figure 1 Figure 2 Figure 3

LoKI-MC showcases

To illustrate the main use of LoKI-MC we show modelling results [6] 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.

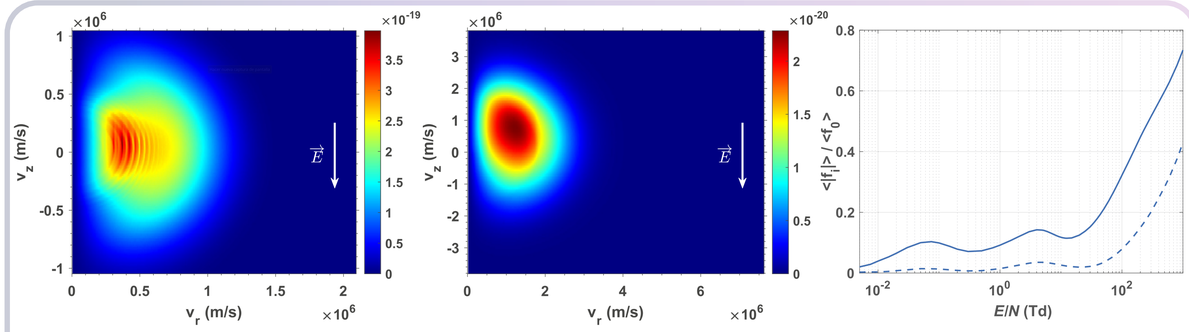


Figure 4 Figure 5 Figure 6

LoKI-C showcases

To illustrate the main use of LoKI-C we show modelling results [10] 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.

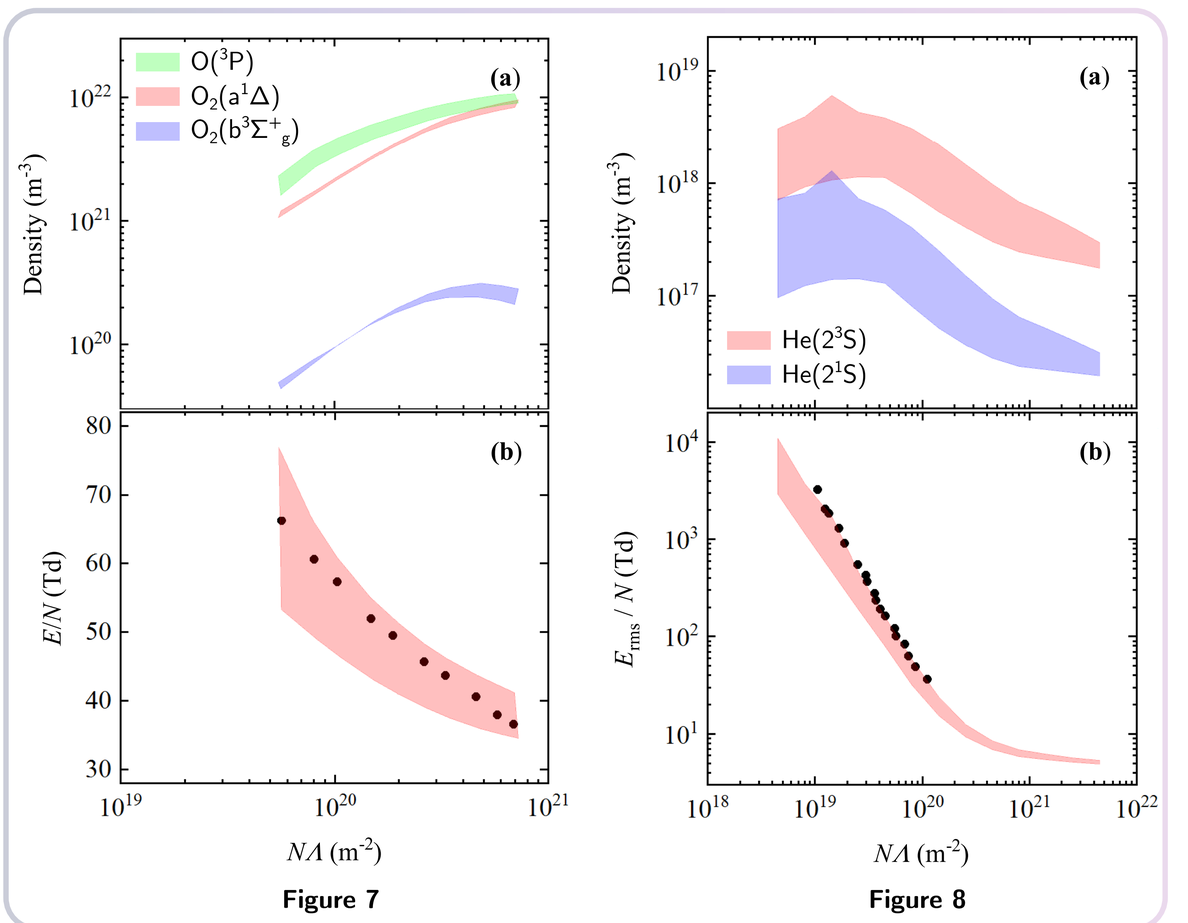


Figure 7 Figure 8

Prospectives

Presently, the development of the LisbOn KInetics 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.

The future LXCat 3.0 will allow (i) detailing the internal structure (electronic / vibrational / rotational) of both target and product species; (ii) extending the set of electron cross sections to the scattering by excited states; (iii) providing unambiguous classifications for every type of cross section; and (iv) direct communication of codes (namely LoKI-B) with the database, via an API. This evolution will facilitate the state-to-state description of the electron kinetics and promote the path to host chemistry schemes.

References

[1] LoKI website htts://nprime.tecnico.ulisboa.pt/loki/
[2] LXCat website https:lxcat.net
[3] A. Tejero-del-Caz, et al. *Plasma Sources Science and Technology*, **28**(4):(2019) 043001.
[4] A. Tejero-del-Caz, et al. *Plasma Sources Science and Tecnology*, **30**(6):(2021) 065008.
[5] IST-Lisbon. LoKI-B repository on GitHub. https://github.com/IST-Lisbon/LoKI
[6] Dias, T. C. et al. *Computer Physics Communications* **282**:(2023), 108554.
[7] IST-Lisbon. LoKI-B repository on GitHub. https://github.com/IST-Lisbon/LoKI-MC
[8] Dias, T. C. and Guerra, V. Assessment of time-locality assumptions on the modelling of nanosecond-pulsed discharges. XXXVth ICPIG (2023).
[9] Pintassilgo, C. D. et al. Effect of the magnetic field on the electron kinetics under AC/DC electric fields. XXXVth ICPIG (2023).
[10] L. L. Alves and A. Tejero-del-Caz *Plasma Sources Science and Technology*, **32**:(2023) 054003.

Acknowledgements

This work was partially funded by the Portuguese Foundation for Science and Technology under projects 2022.04128.PTDC (doi.org/10.54499/2022.04128.PTDC), UIDB/50010/2020 and UIDP/50010/2020.

FCT Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

Multimedia

Scan with your smartphone to access multimedia content.

Download this poster

Go to our website

International School on Atomic and Molecular Data Evaluation and Curation, 22nd-25th October 2023, Valladolid (SPAIN)