# Development of the LisbOn KInetics (LoKI) tool

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## Introduction

**Predictability** in plasma science and engineering based on fundamental **modelling** has been considered a requirement for the progress in the field, and the **model-based design** of plasma processes has been identified as a necessary capability to achieve **industrial goals**. Therefore, there is general agreement on the intellectual and technological importance of modelling **low-temperature plasmas** (LTPs)

Predictive tools for non-equilibrium LTPs should describe the **kinetics of both electrons and heavy-species**, the former responsible for inducing plasma reactivity and the latter providing the paths for industrial applications.

Here, we focus on plasma-based environmental and biological applications, which have recently attracted the interest of pure and applied research. In this context, we have launched a research project for delivering a KInetic Testbed for PLASMa Environmental and Biological Applications (**KIT-PLASMEBA**), embodying a MATLAB® computational tool, LisbOn Kinetics (**LoKI**) linked to a web-platform (KIT) containing state-of-the-art kinetic schemes.

## Code implementation

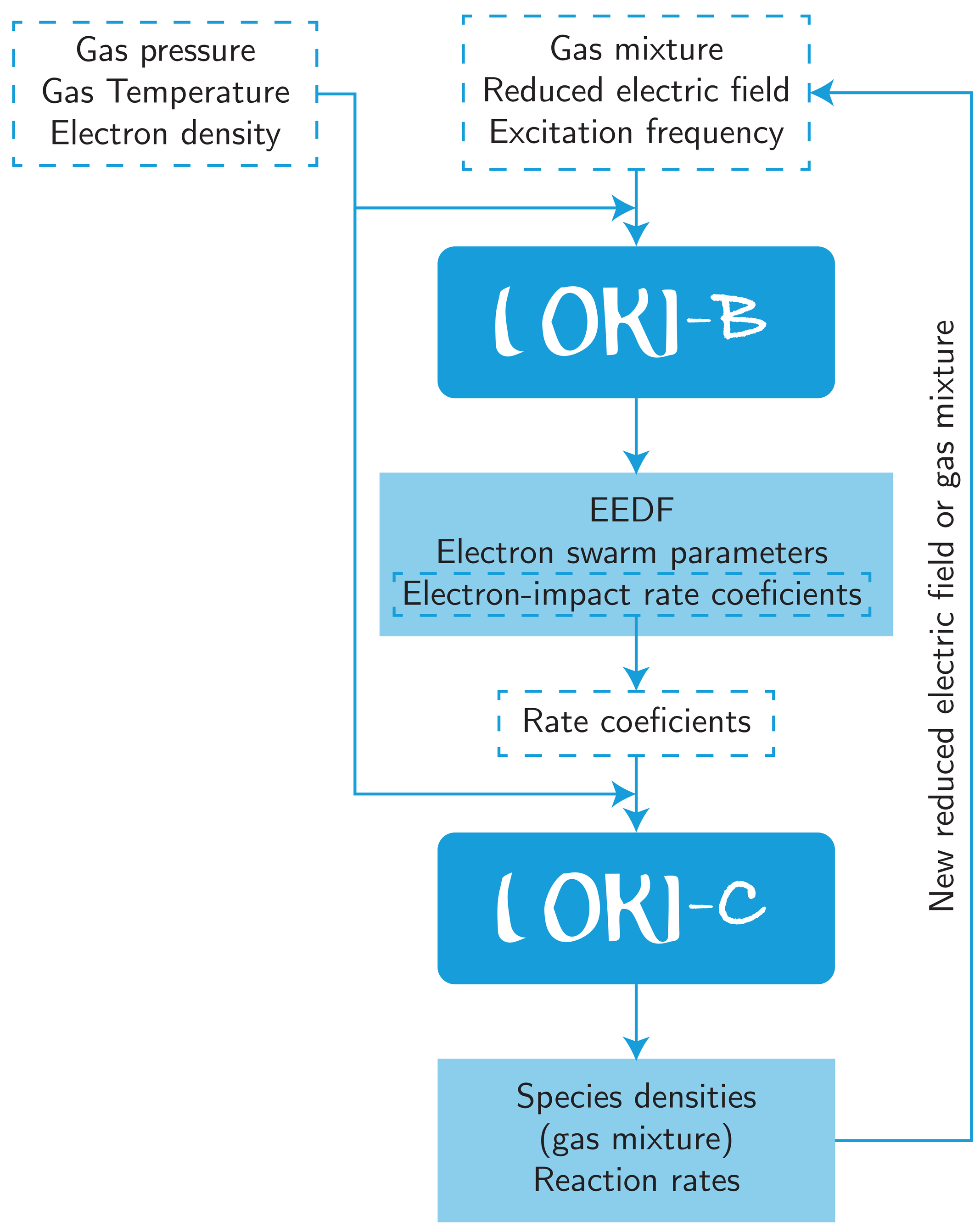
**LoKI** comprises two modules (LoKI-B and LoKI-C) that can run self-consistently coupled or as standalone tools. The foundations for developing this tool were stablished years ago [1].

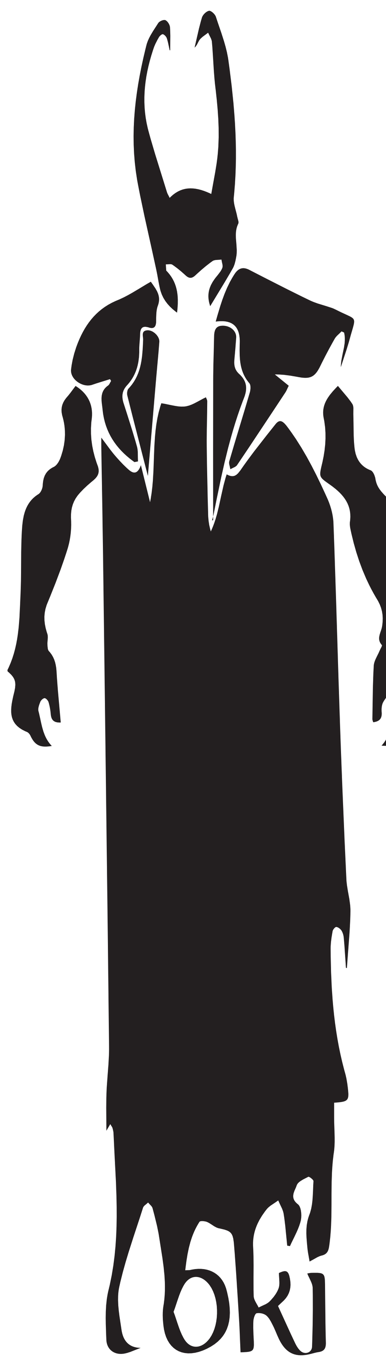
**LoKI-B** (to become open-source) provides the solution to the homogeneous **two-term electron Boltzmann equation** [2] (for a pure gas or a gas mixture, including first and second-kind collisions, as well as electron-electron collisions), using the **LXCat** open-access website [3] for obtaining electron scattering cross section data.

**LoKI-C** gives the solution to the system of **zero-dimensional rate balance equations** (volume average) for the most relevant charged and neutral species in the plasma.

The simulations can include **any gas mixture**, accounting for the **electronic, vibrational and rotational internal degrees of freedom** of the atomic /molecular excited states present in the discharge.

On **output**, LoKI yields the **electron energy distribution function** (EEDF), the **electron swarm parameters**, the **concentrations of the various plasma species**, and the corresponding **gain/loss reaction rates**.

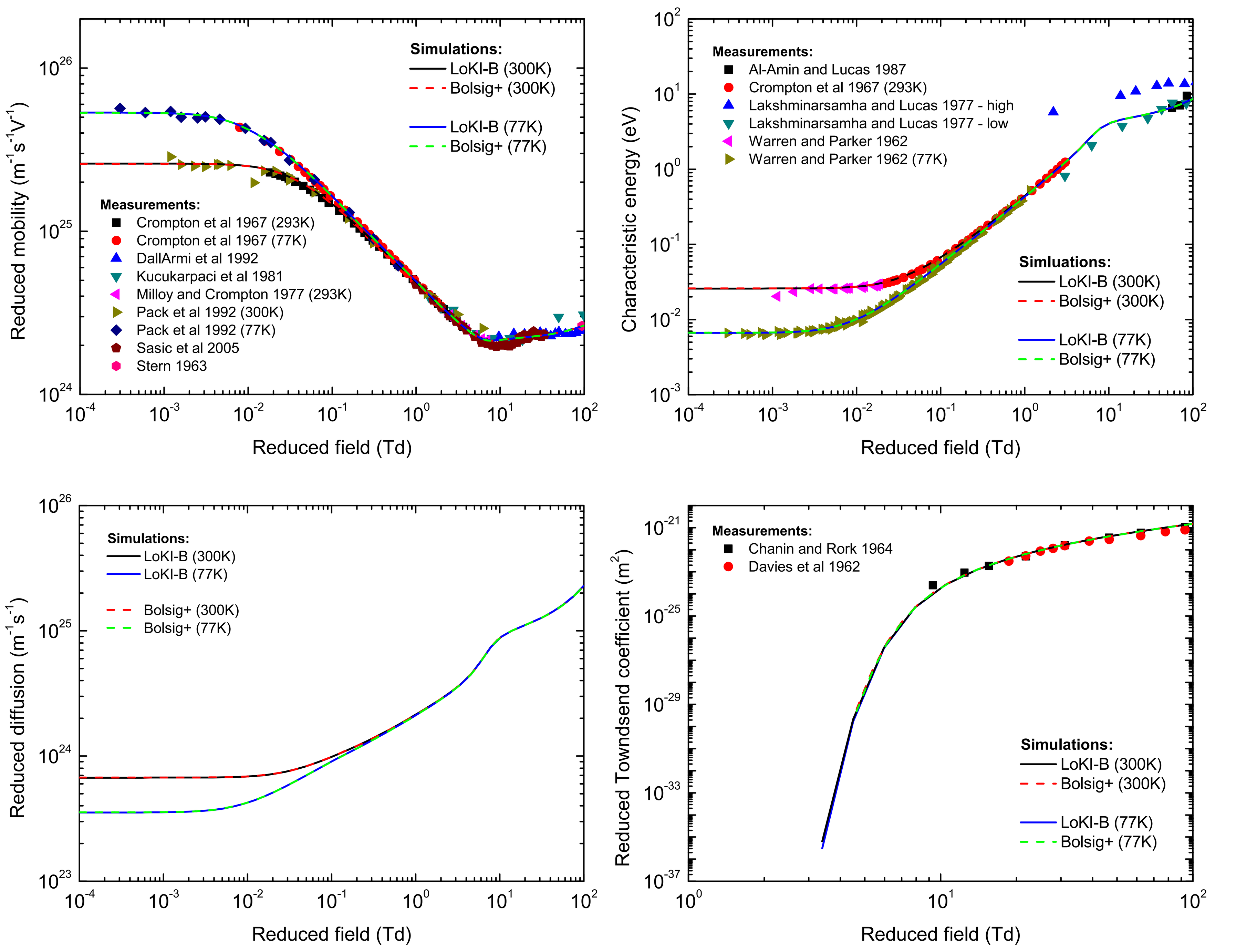



## Atomic gas (Helium, IST-Lisbon@LXCat)

**LoKI-B** has been **benchmarked** by performing a **swarm analysis** using a complete set of cross sections. First an **atomic gas**, Helium, was used. The results were compared with measurements and with the output of **Bolsig+** [4] obtained for the same set of cross sections and working conditions.

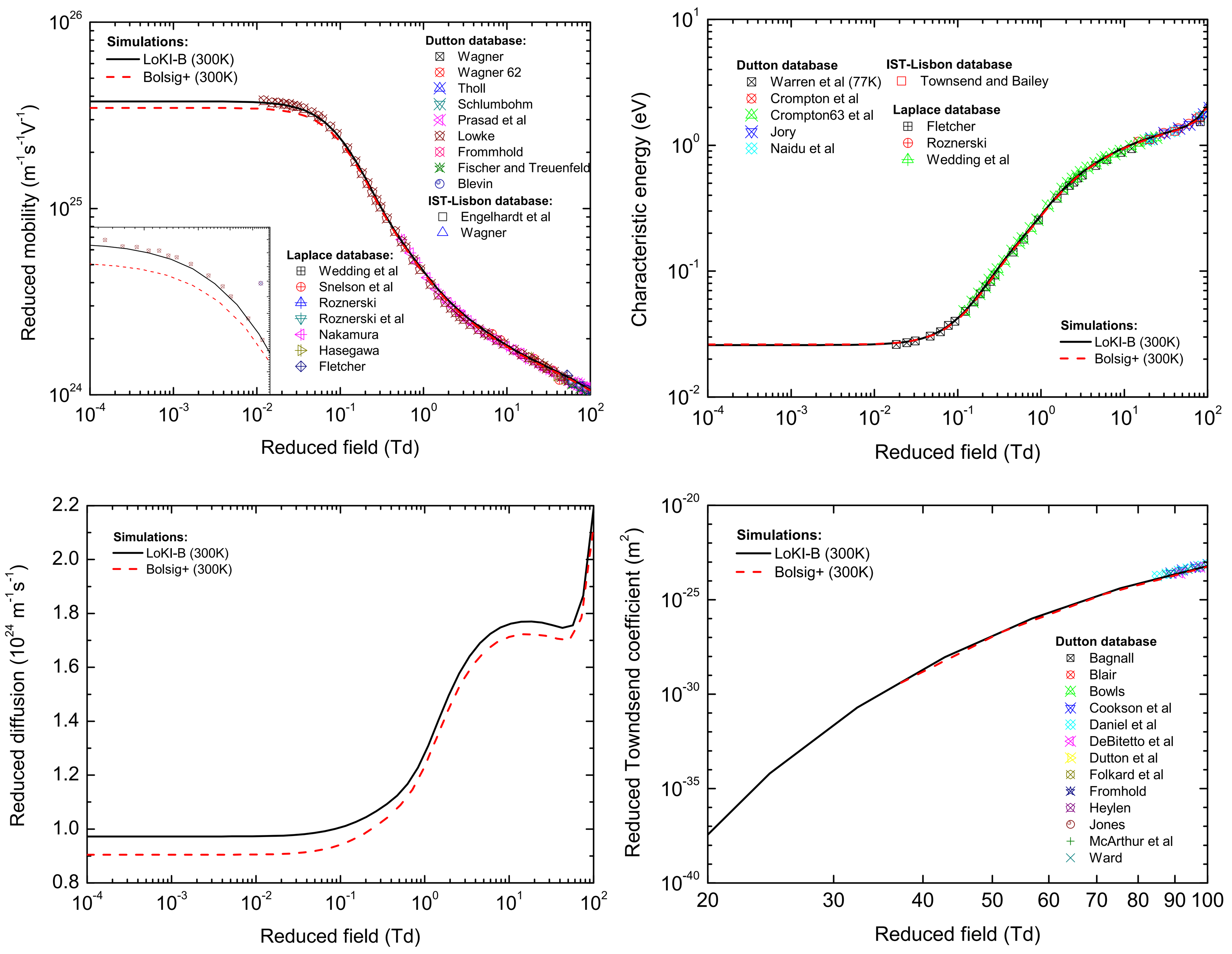
A **very good agreement** is found between the results of both codes and with the measurements.




## Molecular gas (Nitrogen, IST-Lisbon@LXCat)

When **molecular gases** are considered the **populations of the internal states** must be carefully and properly accounted for. Below, a swarm analysis perfomed for Nitrogen, using **LoKI-B** and **Bolsig+**.

Again, **good agreement** is found between both codes and the measurements. LoKI-B provides a slightly better agreement with the experiment for the electron reduced mobility.




## Definition of internal state populations

In LoKI, the **populations** of the internal states of gases and gas mixtures, *e.g.* **vibrational and rotational states** of molecular species, are **defined in a clear and adequate manner**.

LoKI input file:

```
...
population:
      - N2(X) = 1.0
      - N2(X,v=*) = boltzmannPopulation@gasTemperature
      - N2(X,v=0,J=*) = boltzmannPopulation@gasTemperature
...
```

```
N2(X) < N2(X,v=0) < N2(X,v=0,J=0)
        N2(X,v=1)   N2(X,v=0,J=1)
        N2(X,v=2)   N2(X,v=0,J=2)
N2(A)   N2(X,v=3)   N2(X,v=0,J=3)
                    N2(X,v=0,J=4)
                    N2(X,v=0,J=5)
  ⋮         ⋮           ⋮
```

## Conclusions

**LoKI** is a **user-friendly**, **scalable** and **upgradable** tool. This work discusses its current status of development, presenting basic structure, evidencing functionality and introducing test cases along with **first results of benchmarking** against other codes. LoKI development will continue focusing on its **graphical user interface**, on the introduction of **verification and validation** procedures and the integration with the **chemistry module**.

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## References

[1] Guerra V and Loureiro J, Plasma Sources Sci. Technol. **6** (1997) 373-385.

[2] Alves L L, Plasma Sources Sci. Technol. **16** (2007) 557-569.

[3] LXCat, www.lxcat.net

[4] Bolsig+, www.bolsig.laplace.univ-tlse.fr

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