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LOKI-B C++: AN OPEN-SOURCE BOLTZMANN SOLVER FOR REPRODUCIBLE ELECTRON BOLTZMANN CALCULATIONS

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Abstract. Boltzmann solvers are crucial in the simulation of low-temperature plasmas, where the electron energy distribution function (EEDF) is typically not Maxwellian, and thus needs to be computed separately. Input is provided in the form of a set of cross sections that measure the probability of the corresponding electron impact process as a function of the electron energy. Subsequently, output is in the form of swarm parameters, which in turn consist of transport and rate coefficients. These coefficients can then e.g. be used for further plasma modeling.

The Lisbon KInetics Boltzmann solver (LoKI-B), is a Boltzmann solver that is originally written in Matlab, see Tejero-del-caz et al. 2019. The project is open-source and available under a copyleft license on GitHub (`https://github.com/IST-Lisbon/LoKI`). The development of LoKI-B was instigated for two main reasons. The first reason is the desire to handle complex molecular gas mixtures that require explicit treatment of the ro-vibrational substructure of electronically excited states. LoKI-B solves this problem by explicitly treating the ro-vibrational substate relations, which allows for the user to assign population distributions to specific populations of states. The second reason is to provide a transparent and open-source alternative to the existing offer.

The choice for Matlab is understandable, as it is a high-level language that is often taught as part of a physics degree at university. However, it is also limiting, as it is hard to implement custom, performant algorithms, and to interop with complementary simulation tools that are not written in the same language. Moreover, usability is hampered as a Matlab license is required, and, whereas the code is open-source, LoKI-B is thus not free software. These observations lead to the development of a C++ version of LoKI-B.

This work presents LoKI-B C++, which will be open-source at the time of the conference. The code focuses on sound open-source practices, including test driven development, usage of code coverage metrics, and continuous integration and deployment. Community contributions are welcome and even encouraged. Additionally, this work presents benchmarks, numerical improvements; such as exploratory work on a nonuniform discretization of the electron energy, and improvements regarding data management and accessibility.

More specifically, usability and ease-of-access are strongly improved by providing a fully featured, free instance of LoKI-B C++ directly in the browser. This feat is made possible by compilation to WebAssembly. These developments, when combined with the recent developments in LXCat3 (Carbone et al. 2021, `https://github.com/LXCat-project/LXCat`), realize the capability to perform fully transparent and reproducible electron Boltzmann computations.

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