Recent advances in reproducible plasma simulation: LXCat 3.0 and LoKI-B++

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Reproducing plasma simulation studies is notoriously difficult. There are two contributing aspects, input data and simulation tools. This work presents recent advances in both areas. The main contribution comprises LoKI-B++, a new, open-source, C++ implementation of the LoKI-B Matlab Boltzmann solver, which introduces a nonuniform energy discretization and provides a full-featured web interface. In conjunction with recent developments in LXCat 3.0, LoKI-B++ facilitates perfectly reproducible electron Boltzmann simulations.

LXCat 3.0 is the next generation of the LXCat data platform for electron and ion collisional data [1, 2]. It significantly improves data management through the introduction of a comprehensive plasma input data schema, improves reproducibility through proper versioning of data, and increases transparency by improving traceability of the data and its sources. The development of LXCat 3.0 is in the final stages before its release. Recent progress includes porting and annotating a large amount of cross section data from the current generation of LXCat, and the development of peripheral tooling. A live demo deployment is available that can be used to check on the progress [3].

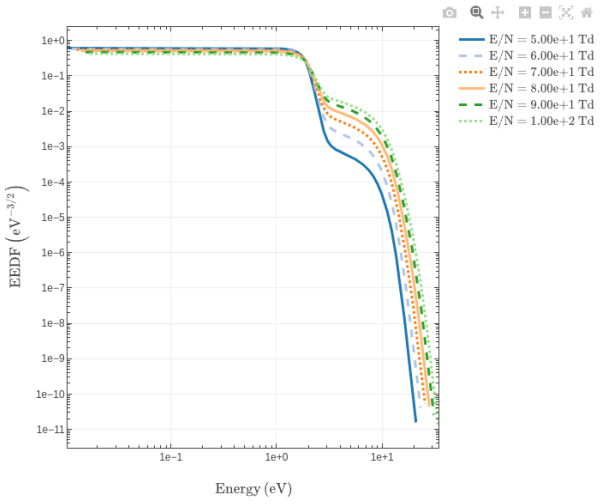

Figure 1: A screenshot of the plotting area of the LoKI-B++ web interface. The results show computed electron energy distribution functions in a N_2 plasma. The cross section data is obtained directly from the LXCat 3.0 API.

LoKI-B++ is developed in conjunction with the recent advances in plasma data management. It solves the two-term expanded Boltzmann equation for electrons and provides a fast, interoperable, and truly open-source alternative to the existing offer. The first goal is to mirror the functionality and leverage the solid scientific foundation of the original LoKI-B Matlab code [4, 5]. This led to the development of a rigid testing harness, including a comprehensive suite of unit tests, regression tests, the development of analytical solutions in the presence of inelastic collisions, and testing against LoKI-B Matlab and BOLSIG+ [6].

Furthermore, a non-uniform energy discretization is being developed, which allows to solve the Boltzmann equation on arbitrary, unstructured grids. Special attention is paid to the conservation of mass and energy in the presence of inelastic processes. In addition, a grid placement algorithm is in development that automatically arranges grid cells based on the given input data. Moreover, LoKI-B++ runs natively in the browser as a full-featured web application by compilation into WebAssembly. The web deployment of LoKI-B++ can automatically retrieve cross section data from the LXCat 3 API. The combination of LXCat 3 and the LoKI-B++ web deployment allows for perfectly reproducible studies of the electron Boltzmann equation. Full studies can be reproduced exactly by simply sharing a uniquely generated URL, paving the way for fully reproducible plasma simulation studies.

References

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