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LXCat TNG — A Status Report and Sneak Preview

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The LXCat project is one of the most popular sources of data for low-temperature plasma (LTP) physics. This community-driven project provides cross sections, swarm data and intra-molecular potentials, with an emphasis on electron-impact processes [1]. In recent years the project has been starting to feel the limitations of the aging software stack and the lack of a formally specified data model. More recently, work has started on a new design and implementation of LXCat [2, section 6]. In the present contribution we will provide a sneak preview of this possible future LXCat replacement.

In the first part of the presentation the proposed data model will be discussed. The primary design challenge has been the wish to support both types of data that appear in LTP physics. LXCat has traditionally been focusing on 'self-consistent data sets', or reaction 'mechanisms' that typically involve reactions and species with a somewhat fuzzy meaning (such as the proverbial He*). Such sets are specifically meant to be used with a 2-term Boltzmann solver such as BOLSIG+ [3], yielding excellent values for electronic transport coefficients and reaction rates. The data model continues to support this type of data (backward compatibility tops our list of design criteria) but provides much better support for state-to-state processes involving species in precisely defined states.

The project builds on a newly developed extensible LTP type library, that has been written in TypeScript [4, 5]. The library facilitates the creation of 'schema' for the data files, which are written in JSON [6,7]. A second important decision has been the choice for the ArangoDB database [8,9]. The advantages of combining the graph and document-store capabilities of this multi-model database for the modeling of species and reactions will be discussed.

Finally, the layered design (database, API, front-ends) of the software stack will be presented. This has distinct advantages in terms of maintainability, and facilitates the creation of other front-ends than the traditional website. This is demonstrated using two open source software packages: the open-source Boltzmann solver LoKI-B [10,11] and the potential integrator MagnumPI (under development at Eindhoven University of Technology). Both applications are continuously being updated to track the data format and to test the retrieval of input data by directly interacting with the platform. The presentation concludes with an assessment of the wider applicability the software stack, for example for the realization of a database for more general plasma-chemistry data sets.

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