A fresh computational approach to atomic structures and processes for astro, plasma and material physics

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Owing to the recent advancements in developing new light sources and detector technologies, recent years have seen an increasing demand for atomic data. Apart from the traditional fields of astro- and plasma physics, accurate atomic data are needed today also in several other emerging areas, such as laser spectroscopy, quantum optics and metrology, VUV and x-ray lithography, or even in material science, to name just a few. In order to fulfill these demands, especially the multiconfiguration Dirac-Fock (MCDF) method has been found a versatile tool and has been implemented [1] for calculating a variety of atomic properties and processes. When compared with other many-body techniques, the MCDF method has the advantage that it can be applied quite easily to excited and open-shell structures across the whole periodic table. — Despite of its successes, however, difficulties often arise from the (open) shell structure and the large number of different processes that (may) occur in Nature, including excitation, ionization, capture of electrons as well as all the subsequent decay processes [2, 3].

In this talk, I report about a new implementation of a (Julia) code for modelling atomic properties and processes. To this end, a high-level toolbox has been designed (and already implemented to a large extent) for dealing more efficiently with complex systems. Here, I shall introduce these tools and explain by simple examples how they help provide theoretical predictions and may serve for (requests from) astro and plasma physics, or in material science.

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