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EasyDiffraction: Making diffraction data analysis and modelling easier

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Diffraction is a key tool for structure analysis. However, currently available software for modelling and analysis of diffraction data may be, on the one hand, difficult for new users looking to apply diffraction to their field of expertise and, on the other hand, not flexible enough for domain experts.

EasyDiffraction [1] aims to lower the barrier of entry to diffraction data analysis by providing an intuitive and user-friendly graphical interface allowing for the simulation of diffraction patterns based on structural models and refinement against experimental data. It is distributed as an all-in-one package that includes all dependencies and can be installed with just a few clicks on different operating systems. For more complex problems and increased flexibility the Python library behind EasyDiffraction can be used through Jupyter notebooks and scripting.

Simple interface of EasyDiffraction can help improve the user experience and thereby make it easier to train users and students, as well as be better prepared for experiments. We plan to integrate EasyDiffraction into the full data processing workflow to increase experiment automation and make better use of beam time.

EasyDiffraction is built on the EasyScience framework [2], a platform aimed at unifying neutron scattering analysis software. In addition to diffraction, this framework has been successfully applied to reflectometry. Quasielastic neutron scattering will also be targeted in the future.

EasyDiffraction relies on existing crystallographic libraries as calculation engines to cover the necessary functionality. It is still in beta and has only some basic features of the CrysPy [3] and CrysFML [4] libraries, such as support for one-dimensional constant wavelength and time-of-flight powder neutron diffraction data. We are collaborating with LLB and ILL regarding the CrysPy and CrysFML, respectively, and more functionality will become available as the project matures.

EasyDiffraction is being developed free and open source and we hope to attract interested people to jointly contribute to this project and help us, for the benefit of everyone, in making diffraction data analysis and modelling easier.

[1] <https://easydiffraction.org>

[2] <https://easyscience.software>

[3] <https://github.com/ikibalin/cryspy>

[4] <https://code.ill.fr/scientific-software/crysfml>

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