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Pydidas - A modular framework for diffraction data analysis: The road towards FAIR software

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Helmholtz-Zentrum Hereon operates multiple X-ray diffraction (XRD) experiments for external users and while the experiments are very similar, their analysis is not. The variety in data analysis workflows is challenging for creating FAIR analysis workflows because a lot of the analysis is traditionally done with small scripts and not necessarily easily reproducible.

Pydidas [1, 2] is a software package developed for the batch analysis of X-ray diffraction data. It is published as open source and intended to be widely reusable. Because the wide range of scientific questions tackled with the technique of XRD, a limited number of generic tools will not be sufficient to allow all possible analysis workflows. Easy extensibility of the core analysis routines is a key requirement. A framework for creating plugin-based workflows was developed and integrated in the pydidas software package to accommodate different analytical workflows in one software tool.

Plugins are straightforward in their design to allow users/collaborators to extend the standard pydidas plugin library with tailor-made solutions for their analysis requirements. Access to plugins is handled through a registry which automatically finds plugins in specified locations to allow for easy integration of custom plugins. Pydidas also includes (graphical) tools for creating and modifying workflows and for configuring plugins, as well as for running the resulting workflows.

While pydidas was develop with the analysis of X-ray diffraction data in mind and the existing generic analysis plugins reflect this field, the architecture itself is very versatile and can easily be re-used for different research techniques.

[1] https://pydidas.hereon.de
[2] https://github.com/hereon-GEMS/pydidas

I want to participate in the youngRSE prize

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