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refnx - The Next Generation of Reflectometry Analysis Software

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refnx [1] is a next generation reflectometry analysis package, building on its predecessor, Motofit. It has undergone a large amount of collaborative development over the last five years, introducing innovative features that greatly aid the national and international neutron and X-ray reflectometry community:

- a Bayesian statistics core with comprehensive uncertainty analyses and model selection ("how many layers can the data justify").
- quantitative introduction of prior information into the modelling system (information known from other sources)
- modular construction of structural models, ranging from a basic Slab up to freeform SLD profiles and Lipid membrane leaflets. These components are easily extensible.
- co-refinement of multiple contrast datasets.
- mixed Area models.
- Python based with analyses performed in Jupyter notebooks or a Qt GUI.

Here we give a brief introduction to how these aspects advance the reflectometry technique. In addition, refnx is designed to enable reproducible research. We also discuss what reproducible research means in the context of a neutron scattering study, outlining how this is achieved with refnx, and how these practices could (should) be taken up by neutron scatterers in general.

[1] Nelson, Andrew RJ, and Stuart W. Prescott. "refnx: neutron and X-ray reflectometry analysis in Python." Journal of applied crystallography 52.1 (2019): 193-200.

Level of Expertise

Expert

Presenter Gender

Man

Pronouns

Which facility did you use for your research

Australian Centre for Neutron Scattering

Students Only - Are you interested in AINSE student funding

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

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