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Simplifying elaborate model building and refinement for neutron reflectivity data

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Neutron reflectometry is used by a wide community of scientific groups addressing questions in many different fields, including materials science, magnetism, polymer physics and biophysics. The analysis of reflectivity data from instruments around the world is traditionally performed either with computer programs that use a graphical user interface for building simple slab models of the interface, or with more sophisticated packages that require the writing of code for the description of models with higher complexity that incorporate functional dependencies and constraints in the model's parametrisation. In the present contribution we discuss the advantages of a newly introduced software package (anaklasis) [1] that attempts to simplify the definition of elaborate interfacial models by permitting the definition of constraints and layer features (sld, thickness, roughness etc.) directly as symbolic mathematical expressions involving parameters. Through a set of representative examples that include polarised and multi-contrast data, we showcase the abilities of the package for the generation of reproducible, easily readable and statistically accurate analyses.

[1] A. Koutsioubas, J. Appl. Cryst. (2021). 54, 1857–1866

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