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Library of models for fitting Quasi Elastic Neutron Scattering data

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We report on a library of models for Quasi Elastic Neutron Scattering (QENS) data. This development, initiated by SINE2020 Workpackage 10 on Data Treatment, was to develop an exhaustive library of dynamical models in order to increase interoperability and modularity for rapid prototyping. Different building blocks are provided to users and can be combined, convoluted and plugged into different frameworks, such as Mantid Workbench [1], for visualizing and fitting. A similar approach was used for Small Angle Scattering with SasView, SasModels and its marketplace [2].

The library has been developed under an open-source license. The models are written in Python for easy integration in workflows. In order to help users, a few examples of data analysis using different standard fitting engines are provided as Jupyter notebooks [3]. Tools are also provided to help those interested in adding models or sharing examples of data treatment to the project.

[1] O. Arnold, et al., Nuclear Instruments and Methods in Physics Research A 764, 156 (2014)

[2] www.sasview.org and marketplace.sasview.org/

[3] jupyter.org/

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