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Key Insights on disseminating Multidimensional Rietveld Refinement

Our group specializes in the development of neutron powder diffraction methods, primarily utilizing the neutron time-of-flight diffractometer POWTEX, which was developed in collaboration with Forschungszentrum Jülich at FRM-II in Garching. As part of the DAPHNE4NFDI project, we are expanding these methodologies to enhance their applications, with a strong emphasis on sustainability.

We are actively engaged in researching multidimensional data reduction and Rietveld refinement techniques that are applicable not only to POWTEX but also to large-area detector TOF diffractometers such as POWGEN and SNAP at SNS, ORNL in the USA, as well as future TOF diffractometers at ESS. Recent advancements have allowed for efficient multidimensional data reduction using the Mantid software. Furthermore, we have incorporated multidimensional refinement routines into a customized version of GSAS-II, which is currently undergoing refactoring and testing with real samples.

Our successful trials have already demonstrated the application of these methods on the POWTEX detector operated at POWGEN (SNS, ORNL), as published [1]. However, to extend these methodologies to other instruments effectively, the availability of instrument-specific information is crucial; unfortunately, this information is often not readily provided.

To address this issue, we propose creating a nexus file that serves as a centralized repository for all metadata related to an experiment—including essential instrument-specific details. This nexus file could also encompass information about any related files necessary during data reduction and versioning of algorithms used for this process. By ensuring that refinement software is properly adjusted, separate files for instrument parameters would become superfluous, thereby streamlining the analysis of measurement data.

Building on these concepts, we have developed a sample nexus file that incorporates some of the aforementioned features. It contains fundamental instrument parameters along with links to related files. These links can then be utilized during data reduction in Mantid through a slightly modified version of our algorithm PowderReduceP2D. Additionally, this algorithm automatically generates instrument parameter files that would otherwise need to be downloaded separately.

This integrated approach enhances both efficiency and accessibility in neutron powder diffraction research while supporting our commitment to sustainability and broadening the applicability of our methods across various instruments.

[1] Houben, Andreas; Meinerzhagen, Yannick; Nachtigall, Noah; Jacobs, Philipp; Dronskowski, Richard (2023): POWTEX visits POWGEN. In J Appl Cryst 56 (3), pp. 633–642. DOI: 10.1107/S1600576723002819.

Primary author: Dr MEINERZHAGEN, Yannick (RWTH Aachen)

Co-author: HOUBEN, Andreas (RWTH Aachen)

Presenter: Dr MEINERZHAGEN, Yannick (RWTH Aachen)

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