Beitrag ID: **98** Typ: **Contributed Talk**

DAPHNE4NFDI - Improving Research data management at Neutron Facilities

Dienstag, 17. September 2024 11:50 (20 Minuten)

Advances in neutron instrumentation and techniques offer new opportunities for researchers. At the same time there is an increasing demand to make measured data accessible to the wider community through improved research (meta)data- management, and for implementation of FAIR data principles by which data should be made **F**indable, **A**ccessible, **I**nteroperable and **R**eusable. The challenge is becoming even greater due to increasing data rates, multi-dimensional data sets and in-situ / operando experiments.

The consortium DAPHNE4NFDI (DAta from PHoton and Neutron Experiments for NFDI) addresses this challenge within the German National Research Data Infrastructure (NFDI), in relation to European/worldwide initiatives [1]. Users and facilities engage to develop data solutions and infrastructure for the wider photon and neutron community. New data management and analysis schemes are established, metadata capture for re-use with searchable catalogues is deployed, and on-the-fly data analysis and reduction are developed in the consortium.

This presentation will give an overview of our activities and elaborate on our progress, showcasing progress in some of our use-cases including:

(1) Data@MLZ: Providing FAIR data combined with user friendliness, the qualified data chain is built on the metadata catalogue SciCat and an electronic laboratory notebook, including persistent sample identifiers, different interfaces and community-specific metadata specifications. For several techniques, "ML-readiness" of (meta)data will be available. The data chain is tested on virtual instruments.

(2) SECoP&DAPHNE: The flexible SECoP protocol facilitates the integration of sample environment devices into experiments and complements the FAIR metadata collection on the facility side by automatically providing metadata regarding the sample environment.

(3) Combination of simulation and experiment: The program Sassena was further developed to compute simultaneously correct small-angle and wide-angle diffractograms, and the incoherent intermediate scattering function. [2]

(4) TOF neutron diffraction: To exploit the large-area detectors on new neutron TOF diffractometers, multi-dimensional Rietveld refinement needs to be applied [3]. Based on a fundamental instrument description, all instrument parameters are provided as NeXuS files, and metadata are available for the treatment and analysis process as well as for AI aided structure solution methods.

References
[1] A. Barty et al., Zenodo, DAPHNE4NFDI - Consortium Proposal, 2023. https://doi.org/10.5281/zenodo.8040606
[2] A. Majumdar et al.: Int. J. Mol. Sci. 2024, 25(3), 1547.
[3] A. Houben et al.: POWTEX visits POWGEN, J. Appl. Cryst.56, 633–642(2023).

This work was supported by the consortium DAPHNE4NFDI in the context of the work of the NFDI e.V. The consortium is funded by the DFG - project number 460248799.

Hauptautor: SCHNEIDEWIND, Astrid (JCNS at MLZ, FZ Jülich)

Co-Autoren: AMELUNG, Lisa (DESY); BARTY, Anton (DESY); BUSCH, Sebastian (hereon at MLZ, Helmholtz-Zentrum hereon); GRUNWALDT, Jan-Dierk (KIT); GUTT, Christian (Universität Siegen); LOHSTROH, Wiebke (FRM

II at MLZ, TU München); MURPHY, Bridget (Christian-Albrechts-Universität zu Kiel); SCHREIBER, Frank (Universität Tübingen); UNRUH, Tobias (Friedrich-Alexander-Universität Erlangen)

Vortragende(r): LOHSTROH, Wiebke (FRM II at MLZ, TU München)

Sitzung Einordnung: Session 4: Instrumentation and Data Management I (Chairs: Tobias Neuwirth & Artur Gregor Glavic)

Track Klassifizierung: Instrumentation & Data Management