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DAPHNE4NFDI - Improving Research Data Management at Synchrotron Facilities

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Advancements in synchrotron and X-ray free-electron sources and associated developments in instrumentation and techniques offer many new possibilities for researchers. At the same time there is increasing demand and pressure to make measured data accessible to the wider community through improved research data- and metadata- management, and for implementation of FAIR data principles by which data should be made Findable, Accessible, Interoperable and Reusable.

The consortium DAPHNE4NFDI (DAta from PHoton and Neutron Experiments for NFDI) addresses this challenge within the German National Research Data Infrastructure (NFDI), and also in relation to European/worldwide initiatives [1]. DAPHNE4NFDI engages directly with the user community to develop user-driven data solutions and infrastructure for the wider photon and neutron community, based on solutions designed by and that work for the user community. Specifically, new data management and analysis schemes are developed, metadata capture for re-use with searchable catalogues is deployed, and on-the-fly data analysis and reduction is being 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) X-ray reflectivity: In addition to electronic laboratory notebooks and persistent sample identifiers, the use case has developed ML-based data analysis [2,3]. This includes "ML-readiness"of (meta)data, beamline integration, and a reference data collection for ML model training and validation.

(2) X-ray imaging for biological matter: Is serving as a test bed for integrating electronic laboratory notebooks with data collection and analysis, for both large scale facilities and laboratory measurement systems.

(3) X-ray photon correlation spectroscopy (XPCS): To automatically create a customizable and comprehensive overview of the experiment we have integrated time-resolved XPCS analysis into the EuXFEL metadata preview tool DAMNIT [4].

(4) X-ray absorption spectroscopy: A curated reference database is being developed to save beamtime and increase analysis efficiency. The database has been created for XANES/EXAFS in the first phase [5] and will be extended to XES.

References

[1] A. Barty *et al.*, Zenodo, 2023, DAPHNE4NFDI - Consortium Proposal, https://doi.org/10.5281/zenodo.8040606
[2] L. Pithan, *et al.*, J. Synchrotron Rad. 30 (2023) 1064.
[3] A. Hinderhofer *et al.*, J. Appl. Cryst. 56 (2023) 3.
[4] https://damnit.readthedocs.io (accessed 2024-04-06)
[5] A. Gaur, *et al.*, Proc Conf Res Data Infrastr 1 (2023), https://doi.org/10.52825/cordi.v1i.258

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I plan to submit also conference proceedings

Yes

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