

DAta from PHoton and Neutron Experiments – DAPHNE4NFDI – Annual Meeting 2023

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Data from PHoton and Neutron Experiments – DAPHNE4NFDI – Annual Meeting 2023

From April 3rd to 5th 2023, more than 90 participants of the DAPHNE4NFDI consortium met on the DESY campus in Hamburg. Overall, 25 different German and European institutions were represented on-site, with users across diverse communities including physics, chemistry, biology and engineering, linked by a common interest in synchrotron radiation- and neutron-based advanced techniques at large-scale facilities. DAPHNE4NFDI is a DFG-funded consortium working on “Data from PHoton and Neutron Experiments” (www.daphne4nfdi.de, [1]) in the context of the German national science data infrastructure initiative NFDI.

DAPHNE4NFDI

The DAPHNE4NFDI consortium engages directly with the German large-scale facilities and their user communities via direct involvement of the Committee for Research with Synchrotron Radiation (KFS, Komitee Forschung mit Synchrotronstrahlung) and the Committee for Research with Neutrons (KFN, Komitee Forschung mit Neutronen). The goal of the consortium is the development towards FAIRer workflows at large-scale facilities, for example by introduction of federated data and software catalogues for photon and neutron experiments, in a joint effort of both German university research groups and operators of large-scale facilities towards FAIR large-scale infrastructures data. The consortium is funded by the German Research Foundation (DFG), within the framework of the National Research Data Infrastructure (NFDI) and it is a joint effort of both German university research groups and operators of large-scale facilities. The outcomes of DAPHNE4NFDI are relevant to similar facilities worldwide.

The meeting

The meeting consisted of lively exchanges on topics centered around the management of the large and complex multi-modal data sets now produced at our large-scale facilities. This includes the use of data catalogues to track data from creation to publication, and ultimately make data openly accessible alongside publications. Related to this is the introduction of integrated electronic logbooks, unique sample identifiers which match user workflows so that essential information about the samples is collected alongside and synchronized with the experimental data. A software ecosystem is also being developed whereby research groups can deploy their software on facility infrastructure for use by other researchers—including workflow documentation so that analysis is repeatable and all software in the analysis chain is properly cited. The overarching goal is to improve data management infrastructure so as to shorten the

time between measurement and publication for all users.

The meeting opened on April 3rd with a DAPHNE4NFDI-focussed session in which the members engaged in passionate exchange of ideas and thoughts during parallel round table discussions on selected wide-interest topics (e.g., use cases, metadata and related ontologies, vocabularies and schemata, electronic lab notebooks - ELNs, RDM in wider initiatives) (Figure 1). The main points of discussion were later shared in the plenum, to foster further interest and debate and facilitate exchanges during the first poster session, in front of about 40 contributions presenting among others ELNs, RDM concepts, metadata pipelines, AI and real-time data processing tools.

The first day of the meeting was concluded by a captivating public lecture by Andrea Thorn (University of Hamburg), entitled “The Coronavirus Structural Task Force: Open Data

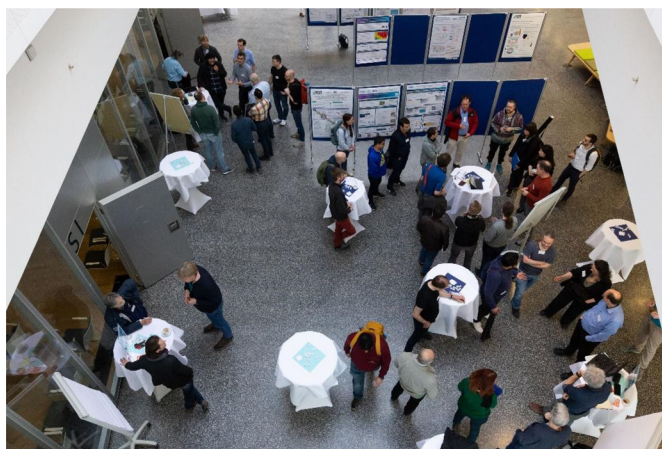


Figure 1: DAPHNE4NFDI members discussing during the “round table” session. © Svenja Hövelmann (CAU Kiel/DESY).

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in Structural Biology.” The importance and impact of large-scale facilities research was perfectly highlighted in the lecture by narrating the race against time towards the structural elucidation of the SARS-CoV-19 virus, one of the biggest and more urgent challenges of recent times. The critical role of open and FAIR data was evidenced in an impressive manner by the possibility of avoiding errors in the literature already at an early stage through access to preliminary data and intensive dialogue with responsible groups.

The DAPHNE4NFDI members meeting continued in the morning of the second day, with parallel sessions covering aspects like metadata, deep learning, data analysis software and online platforms for the training of young scientists. The parallel sessions were aimed as further discussion opportunities to address the main challenges and possible approaches to tackle them. The members of the consortium, for example, agreed on its role in generating momentum for the broader community to investigate and adopt new standards for workflows/software and standardized open data, coupling scientific knowledge with bet-

ter software practices and improved data management (Figure 2).

In the afternoon of day 2, the open part of the meeting for all interested users started with the general presentation of the consortium to the wider audience by Bridget Murphy (CAU Kiel).

Several different impressive recent developments in machine learning, autonomous experiments, and data concepts in Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Dresden-Rossendorf (HZDR) and European X-Ray Free-Electron Laser (EuXFEL) were presented, followed by presentations on similar European initiatives, like ExPaNDS [2]. As an example, Linus Pithan (DESY, formerly University of Tübingen) presented a tool based on neural networks for the online fit of X-ray reflectivity data, without the need for user software to be directly installed in the beamline environment. European actions were also discussed in the presentation by Paul Millar (DESY) on OSCARS proposals, intended to consolidate and widen the results that were previously achieved already in ExPaNDS and PaNOSC. This complemented also an earlier impressive talk by Oliver Knodel

on the online training platform, the pan-training.eu portal [2, 3].

Evidence was also given to the interplay between the DAPHNE4NFDI community and the ErUM-Data (Exploration of the Universe and Matter), a hub providing teaching activities in the field of digitization [4]. Questions arising from the presentation of Dirk Lützenkirchen-Hecht (Bergische Universität Wuppertal) were: how to stimulate the participation of communities in the workshops and schools organized by the ErUM-Data-Hub and how to promote the interest for such kind of activities in general.

The third day of the meeting was opened by a warm welcome of Edgar Weckert, Director of Photon Science at DESY, highlighting the recent developments and future perspectives at the Hamburg-based facility that will interconnect with the DAPHNE4NFDI consortium. The meeting in Hamburg highlighted the strong exchange between the large-scale facilities within DAPHNE4NFDI and their user community about research data management, e.g. as outlined in a talk by Moritz Hannemann (FZ Jülich/MLZ) with an overview on the data management concept at MLZ. Further contri-



Figure 2: Participants following a contribution. © Svenja Hövelmann (CAU Kiel/DESY).



Figure 3: Participants of the DAPHNE4NFDI Annual Meeting 2023 in the foyer of the CFEL building of the DESY campus. © Svenja Hövelmann (CAU Kiel/DESY).

butions presented included the efforts towards the creation of a reference database for X-ray absorption spectra (Sebastian Paripsa, Bergische Universität Wuppertal), and discussed the challenges and solutions to implement FAIR workflows for equipment running at university laboratories (Jonas Graetz, FAU Erlangen-Nürnberg) (Figure 3).

Overall, the meeting fostered very fruitful and constructive discussions and stimulated the

exchange of ideas among scientists with different approaches to common problems, leading to new inputs and concepts for excellent science.

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Disclosure statement

No potential conflict of interest was reported by the authors. ■

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