DAPHNE4NFDI TA1 Face to Face Workshop

ELNs and Metadata

From September 20 to 22nd, members of DAPHNE4NFDI Task Area 1, Managing Data Production, met in Frankfurt to discuss metadata fields, metadata schemes and electronic lab notebooks for instrument scientists. 25 people met in person, so this was an excellent opportunity to network and exchange views. Four people attended the event remotely, enabling to exchange opinions also from other projects, such as PaNOSC and ExPaNDS, facing similar tasks.

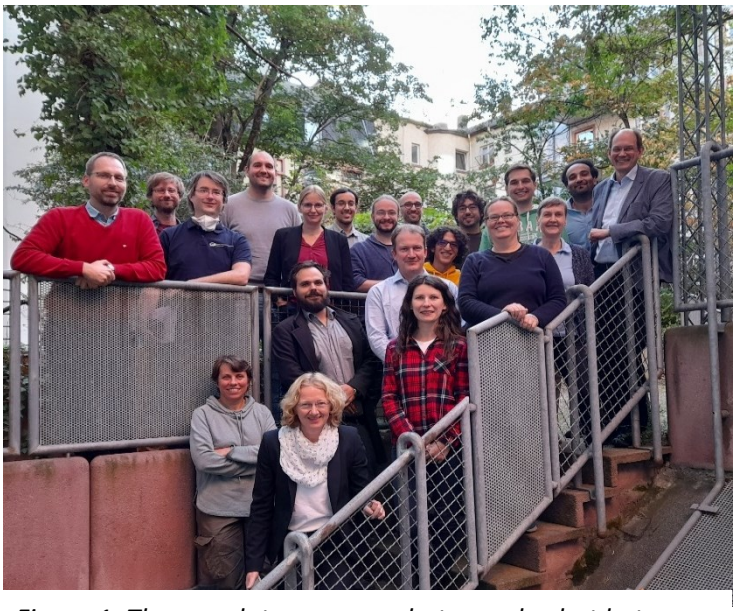

Figure 1: The mandatory group photograph, shot between inspiring sessions, showing exhausted but happy participants.

After a short introduction to the status of the project and FAIR data, electronic lab notebooks (ELNs) from users and facilities were presented. A number of participants also gave suggestions which metadata would be relevant for a specific application.

This introduction went well into Day 2, and after lunch, participants started to discuss which metadata and which ELN requirements are relevant for DAPHNE4NFDI users.

Besides a good overview on already established ELNs at some facilities, also general requirements for an ELN were discussed. It became soon quite clear that also the user's and instrument scientist's workflows are important to decide which metadata are useful. It also became apparent that Neutron- and Photon-users cover many different applications.

A pivotal question was, how data should be interconnected. A sample is usually prepared in the lab, it has been characterized by different measurements, and all this information must be connected with the measurement at the beamline.

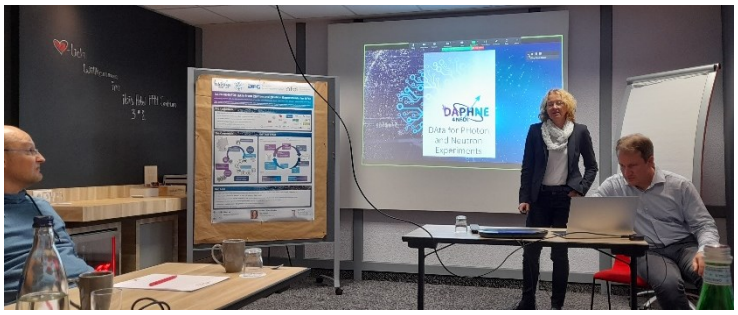

Figure 2: Live@the discussions of day 1.

Results of our discussions

Three main findings were the result of the discussions:

- a list of mandatory requirements for ELNs
- a list of relevant and optional metadata fields
- typical workflows and metadata schemes

Typical use cases, defined by specific institutions, were also streamlined and described in depth. However, further clarification of specific workflows is necessary. The team agreed that this is an iterative process that will continue throughout the project.

	Use Case	Method	Institution	DAPHNE tasks
1	**Biological Matter**	**X-ray imaging**	LMU München Univ. Göttingen	Data and metadata capture Re-use of data and software
2	**Dynamics Coherent Scattering XPCS**	**X-ray absorption spectroscopy (XANES/EXAFS)**	Univ. Siegen EuXFEL	Data and metadata capture
3	**Amorphous materials and catalysis**	**X-ray absorption spectroscopy (XANES/EXAFS)**	KIT TU Berlin Univ. Wuppertal	Catalogues, metadata specific., Data re-use, analysis software,
4	**Chemical systems**	**X-ray emission spectra, RIXS etc.**	KIT ESRF, DESY	Data catalogues, combination of theor./ experim. Data, RDB
5	**Dynamics in correlated electron systems**	**Inelastic X/N scattering**	KIT, FZ Jülich	Metadata specification, ELN
6	**Soft matter and liquid interfaces**	**X-ray reflectivity**	Univ. Kiel, Tübingen	Overall: data, metadata, ELN and software management
7	**Magnetic structures**	**Ultrafast / Magnetic x-ray scattering**	Univ. Siegen	Web-oriented access to FAIR analysis software and catalog
8	**Structure Refinement Accessible and reusable**	**Neutron powder refinement**	FZ Jülich, ESS Univ. Aachen	Web-oriented access to FAIR analysis software and catalog
9	**Engineering Materials, Catalysis, Battery Materials**	**Tomography with neutrons and photons**	TU München BAM, HZG, HZB	Overall: data, metadata, ELN and software management
10	**Proteins and Soft matter**	**Diffraction (small and wide angle) Spectroscopy**	Univ. Kiel, Erlangen Tübingen, EMBL	Metatdata specifications, analysis software, data catalogues
11	**Electrochemistry and - catalysis, particle acceleration**	**High-energy x-ray diffraction**	Univ. Kiel DESY, HZDR	Metadata specification, ELN, software catalogue

Figure 3: Overview of applications for Neutron- and Photon-users.

In sum, it had been a great opportunity to meet up and talk directly to each other. Specific outbreak groups will meet separately to further work on these findings.

If you are interested in joining DAPHNE4NFDI, please contact our coordinator:
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More info about DAPHNE4NFDI: https://www.daphne4nfdi.de/english/index.php