

DAta from PHoton and Neutron Experiments

> DAPHNE 4NFDI

Bridget Murphy CAU - Kiel Christian-Albrechts-Universität zu Kiel

Bring together

...

- Universities
- Research institutions
- KFS-Committee for Synchrotron Research

4NED

- KFN-Committee for Neutron Research
- Large-scale photon and neutron facilities
- Wider community









Task Area Leaders: **Anton Barty** TA3, TA6 (DESY, **Speaker**) **Bridget Murphy** TA1 (CAU, **Speaker**) **Astrid Schneidewind** TA4, TA5 (FZJ, **Dep. Speaker**)

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to make the growing volume of valuable measured data FAIR for the DAPHNE4NFDI community, for the whole NFDI and the scientific community.

These key objectives will be achieved within DAPHNE:

Reuse data by:

- 1. Collection of (meta)data
- 2. Curated repository databases of data and metadata
- 3. Curated repository of managed software
- 4. Education and training in research data management
- 5. Connection to other NFDI consortia, national and international organisations



DAPHNE4NFDI

DAPHNE4NFDI - DAta from PHoton and Neutron Experiments

Collect TA1: Managing Data Production Store TA2: (Meta)data Repositories & Catalogues Hindable Accessible Interoperable

eusable



Managing metadata collection

Enabling re-use and repeatability of results, ideally searchable

- Specification of metadata standards (whitepaper)
- Electronic log books (ELN) at facilities/labs (whitepaper)
- Link to Sample Persistent Identifier IGSN
- Automatic capture of: instrument, sample environment

Collect

- and sample data @experiment
- Data format (Nexus, OpenPMD)



ExPaNDS ontologies

Document Control Information Settings Value

Settings	value
Document Identifier:	D3.2
Project Title:	ExPaNDS ontologies
Work Package:	WP3

https://zenodo.org/record/4806026#.YUh-kOdCRno



Community data repositories

A place to find published data - and in some cases the ability to reprocess data

Store

- Specification of metadata standards
- Sample description and sample PID
- Repository for processed and analysed data
- **Reference** data bases running at facilities and UNIs
- Public MetaData catalogue
 - https://public-data.desy.de









Raw-Data / Internal-Data / Public-Data Catalogues



Infrastructure for data and software re-use

Community data analysis software and data mining strategies including machine learning

Beamline (file-)system

Automated

exctraction

Sample change or realignment

terated curveffiting

refnx

Data

acquisition

Deep Lerning

package

mlreflect

Maxwell Cluster – Core filesystem

- Curate and deploy analysis software on cloud like infrastructures
- Shared Gitlab
- Automatise data analysis chains
- Adoption of common data models e.g. by using NeXus



eamline P08

L. Pithan et al. J. Synchrotron Rad. 30 (2023) 1064, L. Petersdorf et al. in prep.

XRR scan set

quick

slow

Notice

problems?

Use Cases – DAPHNE as a Role Model and Educator

Reusable powder refinement **Neutron TOF diffraction** FZJ – MLZ – ESS - RWTH

Energy and battery materials, catalysis Tomography TUM – MLZ – BAM – Hereon – HZB - KIT

Biological systems Diffraction (small and wide angle) Spectroscopy FAU– Uni Tübingen – EMBL - Uni Kiel

Correlated electron systems **Spectroscopy** KIT - FZJ - MLZ

> **Catalysis and materials High energy x-ray diffraction** HZDR – Uni Kiel - DESY

Amorphous materials for catalysis x-ray absorption spectroscopy KIT – TUB – Uni **Wuppertal**

Soft matter and liquid interfaces x-ray reflectivity Uni Kiel – Uni Tübingen

Biomaterials x-ray imaging LMU – Uni Göttingen

Dynamics Correlation spectroscopy - XPCS **Uni Siegen - EuXFEL**

Magnetic structures Ultrafast / Magnetic x-ray scattering DESY – Uni Siegen

Chemical systems x-ray emission spectra, **RIXS etc. KIT – ESRF - DESY**

X-ray Reflectivity DAPHNE4NFDI Use Case





NFDI Consortium



Nationale Forschungsdateninfrastruktur (NFDI) e.V.

Nationale Forschungsdaten Infrastruktur



nfoi Nationale Forschungsdaten Infrastruktur

Dissemination and outreach

The NFDI consortium as a role model and educator

Dissemination

- Project results within and outside DAPHNE4NFDI
- FAIR data concepts
- Broad synchrotron and neutron techniques with data related tasks
- Interaction with facilities and beamlines

Outreach

- Communication platform in the DAPHNE4NDI community
- Via KFS and KFN, ENSA and ESUO, ErUM-data, NFDI e.V
- Conferences
- Homepage, communication to the public



Integration into international research community

- DAPHNE4NFDI worldwide network
 > 30.000 synchrotron and neutron users
- European user organizations
- European Open Science: PaNOSC and ExPaNDS, OSCARS







ESUO/ENSA/DAPHNE4NFDI meeting

ESUO and ENSA with DAPHNE4NFDI held a European Data policy at PSI November 13th – 15th 2023

- Photon and neutron community white paper on the importance of FAIR and Open data principles
- Describe how users and facilities can work to provide open science.







DAPHNE: Bridget Murphy Christian Gutt, Astrid Schneidewind, Ullrich Pietsch,
ENSA: Henrik Ronnow, Lambert van Eijck, A.S,
ESUO: Cormac Mc Guinness, Bridget Murphy
ExPaNDS: Andrew Goetz

In discussion with ENSA and ESUO national delegates now in review



Sustainability within NFDI beyond initial DFG funding

Facilities: A unique anchor for Daphne and NFDI Science domains

A large and diverse research community

ANEDI

Integration

Daphne data infrastructure will be closely integrated with facilities, ensuring continued impact long after NFDI is over.

Continued operation of services

Operation of services and maintenance will be provided by the facilities after funding is over.

Career development

Ongoing positions, including long term, within facility computing groups sustain Daphne after initial funding.

Education

A culture of data curation and scientific software development will be embedded in University courses for students and future generations

Leading by example

Power user groups act as role models leading the community in entrenching best practices

Bridget Murphy, CAU, Kiel

DAPHNE4NFDI.de



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Thank you!