

## **DAPHNE4NFDI**

### Letter of Intent for Renewal Proposals in 2025

**18.06.2025**

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**1. Binding letter of intent as advance notification of a full renewal proposal**

x	Binding letter of intent (required as advance notification for renewal proposals in 2025)
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## 2. Formal details

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- Acronym of the consortium  
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### 3. Objectives, work program and research environment in the second funding period

- Research area of the proposed consortium

- 2.11 Basic Research in Biology and Medicine
- 3.12 Chemical Solid State and Surface Research
- 3.13 Physical Chemistry
- 3.16 Polymer Research
- 3.17 Theoretical Chemistry
- 3.21 Condensed Matter Physics
- 3.22 Statistical Physics, Nonlinear Dynamics, Complex Systems, Soft and Fluid Matter, Biological Physics
- 3.23 Optics, Quantum Optics, Physics of Atoms, Molecules and Plasmas
- 3.44 Mineralogy, Petrology and Geochemistry
- 4.21 Process Engineering, Technical Chemistry
- 4.32 Materials Science

- Concise summary of the consortium's main objectives and task areas:

The main goal of DAta from PHoton and Neutron Experiments for NFDI (DAPHNE4NFDI)<sup>2</sup> is to increase FAIRness of data for the Photon and Neutron (PaN) user community to support scientific knowledge gain from their valuable data. Further aims are to improve the reusability of data, e.g. through provision of annotated training data sets for machine learning based analysis tools. The science our user communities is carried out at large-scale research facilities (LSFs) in which user groups, following a competitive peer review process, perform specialized experiments at the LSF, often complemented with data from their home laboratory. This common point of access provides DAPHNE4NFDI a unique opportunity to inform, provide services, promote, and distribute tools for research data management (RDM), and to implement the FAIR data principles in the community.

Within the first funding period, demonstrator data pipelines and databases have been established and their functionality validated. One of the main target areas for the continuation proposal will be the transfer of the demonstrators into standard operation. Moreover, increasing adoption of FAIR data practices is fostered, e.g. through expansion of the public databases to more use cases, the formulation of community-agreed quality control criteria, and the coordination with other NFDI consortia towards OneNFDI. Beyond the national scene, DAPHNE4NFDI is contributing to both the national German NFDI, and the PaN topical node of the European Open Science Cloud (EOSC).

To achieve its aims, DAPHNE4NFDI is organized in six different task areas (TAs) along RDM-related topics. **TA1:** Managing Data Production is dedicated to metadata standardization and collection during experiment, subsequent data processing, and analysis. TA1 will also explore emerging techniques based on large language models (LLM) for metadata extraction. The measures will cover (i) electronic laboratory notebooks and automated metadata capture, their interoperability and deployment at the instruments for metadata collection; (ii) metadata specification and schemata of sample description and experiment conduction as well as of data processing and analysis steps; and (iii) further development and roll-out of standardized data

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<sup>2</sup> Barty, A. et al. 2023 DOI: 10.5281/zenodo.8040605

formats, such as NeXus and data streams. **TA2:** (Meta)data Repositories and Catalogues focuses on findability and accessibility of data through metadata catalogues and open data repositories, with the aim to establish interconnected datasets and catalogues that adhere to FAIR principles across neutron and synchrotron radiation sources, universities, and research institutions within DAPHNE4NFDI and beyond. Measures include (i) the expansion of open data and reference data catalogues to foster adoption from a wider community; (ii) establishing quality control procedures for metadata catalogues and reference data repositories; and (iii) catalogue integration to facilitate interoperability with the NFDI and EOSC. This includes integration with ongoing ontology developments within NFDI and the consolidation of a PaN data model to access data via common interfaces in collaboration with the EOSC community. **TA3:** Infrastructure for Data and Software Reuse will focus on providing FAIR scientific software and analysis tools alongside the associated data. Software provision, application, and skills development are achieved through: (i) the finalization and deployment of mature, FAIR-compliant software developed that is made available through a central repository. Robustness and reproducibility will be supported through quality control measures such as testing, Continuous Integration/Continuous Deployment (CI/CD), and code review; (ii) the application of workflow and analysis tools across scientific use cases, including the integration of machine learning techniques for experiment control and data analysis; and (iii) the training and upskilling of developers through workshops, documentation sprints, and secondments, aimed at promoting standardized coding practices and ensuring long-term software quality.

In addition to the technical task areas, the work program entails two communication and outreach task areas reflecting the coordination needs for a community driven effort, both across the PaN community in the national and international context as well as the wider NFDI. **TA4** focuses on Dissemination and Outreach inside and outside the consortium, across the different scientific communities. Dissemination within the consortium will be achieved via annual meetings, talks at Collaborative Research Centers (CRCs) and user meetings, as well as scientific conferences. TA4 will continue the training and education efforts, e.g. through the implementation of data management topics into university curricula, such as the established “Ringvorlesung” on X-ray/neutron techniques combined with data concepts or schools implementing workshops on FAIR principles. Extending the PaN Training Catalogue and e-learning platforms, we aim to provide lecture material to universities and other institutions. The External Communication and Policy Task Area, **TA5**, coordinates with the needs and requirements of the community in the wider national and international context; such as DAPHNE4NFDI’s engagement with EOSC through the national NFDI and the topical PaN node. TA5 also serves as DAPHNE4NFDI’s central point of contact for cross-consortia collaboration within the NFDI and for coordination with Base4NFDI services towards OneNFDI. The overall coordination of DAPHNE4NFDI and management and coordination of the financial and organizational aspects of the consortium is executed within **TA6**. Across the task areas, the following companies will contribute to DAPHNE4NFDI: Rudolf Schneider, HUBER Diffraktionstechnik GmbH & Co. KG, Bernd Hinrichsen, Momentum Transfer, Julian Schmehr, X-Spectrum GmbH, Peter Gaal, TX Products UG, Stefan Brandstetter, Dectris Ltd., Vanhoyland Geert, Bruker AXS GmbH

Orthogonally to the task areas we have use cases that demonstrate and validate the developed RDM tools and services for different scientific applications. These use cases serve as testbeds, which provide feedback and support the iterative developments within the task areas. They include the full spectrum of RDM workflows: Capturing rich and structured metadata (TA1);

making data findable and accessible via metadata catalogues (TA2); ensuring reusability through user-friendly access to the necessary software tools (TA3); promoting RDM awareness and adoption within the scientific community (TA4); and establishing the required frameworks through national and international coordination (TA5).

- Brief description of the proposed use of existing infrastructures, tools and services that are essential in order to fulfil the planned consortium's objectives

The consortium primarily builds on existing infrastructures operated by large-scale research facilities (LSFs) as part of their mandate to provide services to users, as well as computing centers at universities and research institutes. As such, the goals of DAPHNE4NFDI are closely aligned with those of the infrastructure providers. DAPHNE4NFDI benefits from significant in-kind contributions from its partners, enabling the development and deployment of services through LSF infrastructure, ultimately making them available as regular user services. Specifically, in the area of electronic laboratory notebooks (ELNs), several systems are already in use across participating sites; including ICAT+ - ELN, MLZ - ELN, SciLog, snip, and others. These tools require further integration into the respective facility infrastructures.

For metadata catalogues, the consortium primarily uses two systems: ICAT and SciCat. In both cases, the large-scale facilities (LSFs) within the consortium are actively involved in their development, working in collaboration with other European PaN facilities to ensure alignment and compatibility. Within TA3, the provision of analysis software depends largely on the storage and computing capabilities of the infrastructure providers. These services are run using a modern software stack that includes Kubernetes and message queue systems for communication and workload management. All tools and services developed are based on free and open-source software, supporting sustainability and reuse.

In areas of overlap with other NFDI consortia, such as NOMAD (FAIRmat) or electronic lab notebooks like Chemotion and LabIMotion (NFDI4Chem), further progress will be followed closely and the uptake into DAPHNE4NFDI depends on the developments within those respective consortia.

Most of the services supporting the internal organization of the consortium are currently provided through HIFIS. These include platforms such as Nextcloud, Mattermost, the Indico conference management system, and GitLab (Helmholtz Codebase). A key infrastructure component for DAPHNE4NFDI is the Helmholtz ID, an authentication and authorization system that operates in coordination with IAM4NFDI.

The open data demonstrators developed during the first funding period are hosted on the HIFIS infrastructure operated by the Helmholtz Association, as well as on AWS cloud storage. In the continuation proposal, we plan to expand these public databases and establish reference data repositories, building on the instances currently deployed on HIFIS. As an external dependency, we rely on IGSN and DataCite for DOI minting for data and sample registration. Additionally, DAPHNE4NFDI is preparing the necessary foundations for integrating its metadata catalogues into EOSC, which is expected to evolve in parallel with the runtime of this consortium.

- Interfaces to other NFDI consortia: brief description of existing agreements for collaboration and/or plans for future collaboration

To achieve **OneNFDI**, DAPHNE4NFDI actively collaborates with all NFDI consortia, in particular with FAIRmat, MaRDI, NFDI-MatWerk, NFDI4Cat, NFDI4Chem, NFDI4ING and PUNCH4NFDI and with Base4NFDI. DAPHNE4NFDI is a co-organizer of Physical Sciences in NFDI collaboration<sup>3</sup>. Together with FAIRmat, MaRDI, NFDI-MatWerk, NFDI4Cat, NFDI4Chem and PUNCH4NFDI, we organize workshops and colloquia to showcase good (data) practices to an international, interdisciplinary audience; and foster discussions on various topics around research data management in the broad spectrum of topics in physics, chemistry, mathematics and informatics. Due to the scientific method-oriented focus of our consortium and the existing synergies with the consortia NFDI4Cat, NFDI4Chem, and FAIRmat, we aim to constantly address interfaces and continue to exchange on topics such as metadata standards and electronic laboratory notebooks. DAPHNE4NFDI and PUNCH4NFDI collaborate closely through the BMBF-funded ErUM-Data initiative with shared members and joint discussions on research data management, large-scale infrastructure needs, and persistent identifiers. DESY, serving as the applicant institution for both consortia, facilitates this collaboration through monthly meetings focused on strategic coordination, and shared IT resources. DAPHNE4NFDI members are actively involved in all five NFDI sections and several working groups, including institutional voting. The consortium contributed to the Base4NFDI proposal<sup>4</sup>, participated in the PID4NFDI submission, and became the second-largest user of Helmholtz Federated IT Services (HIFIS) in 2022, making Helmholtz AAI a key IAM4NFDI use case.

Building on the foundations already established within our consortium, DAPHNE4NFDI will increase its engagement in the cross-cutting topics of (meta)data standards and PIDs, also in connection with Base4NFDI services. As base services like TS4NFDI, KGI4NFDI, and IAM4NFDI mature; DAPHNE4NFDI will explore collaborations to support metadata accessibility and their integration into future "data spaces". Together with PUNCH4NFDI, DAPHNE4NFDI will work on synergies related to catalogues. Within the cooperation with FAIRmat, the NOMAD catalogue and ELN for laboratory experiments are already in use by PaN users and within DAPHNE4NFDI use cases; including work on interfaces to the SciCat catalogue system. These activities will be expanded in a joint use case. Similarly, samples prepared by various chemical routes are used at PaN facilities, and the links between the Chemotion/LabIMotion and PaN repositories are being established. Further seeds for collaboration are the catalysis use case with NFDI4Cat and the high energy (magnetoelectric sensors) use case with MatWerk.

#### 4. International and national networking

DAPHNE4NFDI represents more than 7,000 registered facility users in Germany who conduct around 3,000 experiments annually at large scale facilities (LSFs) worldwide, publish roughly 3,000 papers (with an average of nine authors per paper), and generate currently more than 50 PB of data each year. Importantly, through the involvement of the Committees Research with Synchrotron Radiation (KFS<sup>5</sup>) and Research with Neutrons (KFN<sup>6</sup>), virtually all neutron and

<sup>3</sup> National Research Data Infrastructure (NFDI) e.V. 2021c.

<sup>4</sup> Bernard, L. et al. 2022.

<sup>5</sup> KFS *Komitee Forschung mit Synchrotronstrahlung*

<sup>6</sup> KFN *Komitee Forschung mit Neutronen*

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synchrotron users in Germany are connected to this proposal. Communication and networking are well established via annual user meetings, conferences, and workshops. We plan to continue and further expand these successful efforts in the second funding period.

DAPHNE4NFDI has successfully brought together academic research groups from universities with LSFs and their associated computing infrastructures. As a result, the consortium has established close cooperation with Helmholtz AI, the Helmholtz Metadata Collaboration (HMC), and HIFIS. These collaborations will be further strengthened and expanded in the second funding period, with a particular focus on integrating and aligning developments from Base4NFDI with Helmholtz Incubator activities.

The fields of photon and neutron sciences are inherently international, with user groups conducting experiments at LSFs worldwide. DAPHNE4NFDI builds on established international, facility-driven collaborations and EU-funded initiatives such as OSCARS<sup>7</sup> and EOSC<sup>8</sup> nodes. The ongoing engagement with organizations such as ESUO<sup>9</sup>, ENSA<sup>10</sup>, LEAPS<sup>11</sup> and LENS<sup>12</sup>, and ensures the continuous international embedding. DAPHNE4NFDI contributed significantly to the RDM policy development at facilities, and became a selected PaNOSC node in the first wave of the EOSC Federation build-up phase. DAPHNE4NFDI will continue to shape and adopt common RDM solutions in international collaborations — such as the SciCat<sup>13</sup> and ICAT<sup>14</sup> metadata catalogue collaborations or through the engagement in the Research Data Alliance (RDA); to ensure high efficiency, interoperability and sustainability of the RDM measures.

DAPHNE4NFDI will continue to serve on international boards such as the NeXus common data format as well as on international scientific advisory bodies such as the ESRF council, and the Scientific Advisory Committees (SAC) of the LSFs ESRF, SINQ (PSI) and MAX IV and the Ada Lovelace Centre (ALC, STFC) Steering Committee.

DAPHNE4NFDI will continue to have an established International Advisory Board (IAB). Its strong foundation within the scientific user community, its connection to the Helmholtz Association and to LSF at the national and international level makes DAPHNE4NFDI a key player to provide FAIR data, supporting excellent scientific outcomes in the PaN research fields.

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<sup>7</sup> OSCARS *Open Science Clusters' Action for Research & Society*

<sup>8</sup> EOSC *European Open Science Cloud*

<sup>9</sup> ESUO *European Synchrotron and Free Electron Laser User Organisation*

<sup>10</sup> ENSA *European Neutron Scattering Association*

<sup>11</sup> LEAPS *League of European Accelerator-based Photon Sources*

<sup>12</sup> LENS *League of Advanced European Neutron Sources*

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