# NFDI 2020

## Template for Submission of Letters of Intent

### 1 Binding letter of intent as advance notification or non-binding letter of intent

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| ☒ | Binding letter of intent (required as advance notification for proposals in 2020) |
| ☐ | Non-binding letter of intent (anticipated submission in 2021) |

### 2 Formal details

Planned name of the consortium:

Data from Photon and Neutron Instruments for NFDI

Acronym of the planned consortium:

DAPHNE4NFDI

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## 3 Objectives, work program and research environment

### 3.1 Research area of the proposed consortium:

21 (Biology), 22 (Medicine), 23 (Agriculture, Forestry and Vet. Med.), 31 (Chemistry), 32 (Physics), 34 (Geosciences), 42 (Thermal Engineering/ Process Engineering) and 43 (Materials Science and Engineering)

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

DAPHNE4NFDI centers on data challenges resulting from the high data rates and volumes facing users of large scale analytical facilities, and the even greater challenge of making that data FAIR for the wider community of tens of thousands of researchers across diverse fields who may not themselves be facility users but nevertheless make use of valuable data and results from X-ray and neutron as a part of their research.

Publicly funded X-ray and neutron facilities provide scientists with access to cutting edge state of the art analytical instrumentation to further their research across a broad range of scientific disciplines from medicine to physics, biology, chemistry, engineering, materials science and cultural heritage. Access to instrumentation is heavily oversubscribed and as a result only a fraction of access requests can be granted, typically through a peer review process. Importantly, the measured data is valuable not only to the individual researchers granted beamtime but also to the wider scientific community who rely on the results of such measurements. With increasing requests but limited access to facilities there is a pressing need for the ability to reuse valuable data measured by others. A major challenge is making this data FAIR so that the scientific community beyond individual research groups lucky enough to be granted time on instruments can make use of the measured data. This is necessary in order to not only make published results repeatable from the raw data, but also to enable new discoveries using data measured in past experiments performed by others.

An additional challenge is the sheer volume of data involved. Individual experiments can produce up to millions of files and in some cases over 700TB data per week. The community of active users performs thousands of individual experiments at central facilities each year across many disciplines using a range of techniques and a diverse set of instrumentation. Indeed the community is currently witnessing a fundamental change in both the amount of recorded data and the corresponding data rates triggered by the increase of brightness of the sources themselves (X-ray free-electron laser, high brightness storage rings and new neutron facilities) and by the rapid increase of size and speed of modern detectors. Research in the X-ray and neutron communities is therefore experiencing new challenges in terms of data processing, storing and management previously known only from experiments in areas such as high-energy physics. To be successful, this transition requires an investment in efficient research data management for the community. This is the challenge addressed by DAPHNE4NFDI.

DAPHNE4NFDI brings together the X-ray and neutron science community with the large-scale research facilities to advance the state of data management and data reuse in the community. Representing not only the needs of users employing X-ray and neutron techniques, but also the community of scientists beyond active users who directly or indirectly make use of data collected at these facilities, DAPHNE4NFDI supports scientists working in condensed matter science, chemistry, structural biology, material sciences, engineering, medicine and other fields who rely directly or indirectly on data from facilities for parts of their work. This breadth of impact of DAPHNE4NFDI arises because X-ray and neutron data contains diverse information about condensed matter such as information about crystalline structures, electronic and magnetic properties, dynamic properties, x-ray and neutron images etc. The community of beneficiaries numbers in the multiple tens of thousands.

The interaction and connection between users and facilities is a key element of DAPHNE4NFDI, since implementing data management requires a joint and coherent approach with the facilities

acting as data custodians and the user communities acting as data curators. Practical outcomes for the user community will be achieved by working closely with the large user facilities which generate data and increasingly provide storage and cloud computing for users. Solutions and tools generated in DAPHNE4NFDI will be provided to the user community to manage data from lab-based X-ray sources and the institutionally run X-ray sources (DELTA, KARA) as well.

The core of DAPHNE4NFDI is focused on technical task areas:

- Managing data during experiments:
  This aim is to capture sample metadata and record the experiment protocol and information in a cross-compatible electronic logbook integrated into the instruments at the facilities. To achieve this aim standardisation of data formats is also promoted.
- Finding and reusing data:
  DAPHNE4NFDI will deliver a standardised metadata database to allow locating and interpreting data. The advent of big data analyses necessitates that the catalogue is not only searchable by humans but also machine readable. We will also establish machine-readable reference databases in areas where they are currently still missing for key analysis (e.g. XANES, XES).
- Storing and analysing data:
  Data collected at x-ray and neutron facilities are typically subjected to software intensive data reduction and analysis. DAPHNE4NFDI will make tools developed by ‘power user’ groups available to all users, including remote data analysis and re-analysis, making saved data available to and analysable by the wider science community beyond facility users.

Technical tasks are supported by the following task areas:

- Communication, cooperation with other NFDI consortia and international partners:
  DAPHNE4NFDI aims to define common data policies, workflows and standardized best practices for a broad variety of scientific communities across biology, condensed matter physics, physics, chemistry, geology, medicine, and material sciences which are connected through the common use of similar X-ray and neutron methods and data schemes. DAPHNE4NFDI will work with other NFDI consortia as well as integrate into European user organizations such as ESUO / ENSA and the consortia of facilities such as LEAPS and LENS.
- Dissemination and outreach, communication with user communities:
  The task further aims to coordinate and foster communication among the user communities and after successful determination of tools with users on the outreach and dissemination of data management related topics (workshops, schools, etc.). This includes not only educating the community in the FAIR data principles, but also propagating data management topics into university curricula e.g. through lectures and courses and aims at communication with existing and planned excellence clusters, collaboration research centres etc..

DAPHNE4NFDI will play a central role in the digital transformation of data from X-ray and neutron facilities, facilitating the making of measured data FAIR for the broad and vast science community of researchers who make use of results and data in their research.

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

**Hardware and hosting:**

Data storage and part of the analysis for DAPHNE4NFDI will be handled in-house at the facilities. This represents a substantial in-kind contribution, particularly with regard to expertise and know-how. PETRA III and Eu-XFEL take advantage of the DESY computer centre, which is connected to and draws experience from the field of particle physics through operation of a Tier-2 centre within the WLCG for HEP. This infrastructure provides fast disk storage for online analysis, backed by tape storage of data for long term archiving. Remote analysis and data download portals are available through shared resources. Standard data formats and containers such as NeXus help simplify data handling. At MLZ, data storage and archives are currently operated locally in collaboration with the Leibniz Supercomputing Center (LRZ) which can also provide long term tape storage. DAPHNE4NFDI will build on top of this infrastructure and extend the architecture towards cloud and remote computing models in line with the goals of the European Open Science Cloud (EOSC) and associated European projects Photon and Neutron Open Science Cloud (PaNOSC) and EOSC Photon and Neutron Data Services (ExPaNDS).

**Software development services:**

DAPHNE4NFDI is backed by scientific computing software development expertise from scientific computing groups at the facilities and their existing cooperation (PaNOSC, ExPaNDS) who will guide the progress of software development within DAPHNE4NFDI. For example, DESY plays a leading role in professionally developing the software package dCache for data storage management management (see dCache.org) including modern, industry-like methods of quality assurance, release management and support, but is still searching for a database solution which exists at the other facilities (HZB, HZDR, ILL, ESRF, ESS - mainly ICAT, sciCAT). These procedures will be adopted by and used within DAPHNE4NFDI with code peer review, continuous integration-deployment-testing cycles, time-based-releasing and formation of teams responsible for programming and release processes. The highly advanced instrument control software NICOS - also adopted by ESS, PSI - provides excellent conditions for automatic capture of the instrument and sample metadata in a modular manner (well related to the different needs of different subcommunities). At HZB, the connection to Helmholtz Metadata Collaboration (HMC) will strengthen synergies. A significant portion of the in-kind contribution from facilities such as DESY, MLZ, EMBL and HZB is provided in the form of software development expertise. The main goal of DAPHNE4NFDI is working closely with end users to develop solutions that match their work flows and provide solutions that match their needs, with rapid prototype turnaround followed by thorough testing before facility wide deployment. This will be done in a first step in small teams by Use Cases and extended to all facilities after.

**Established standards and data formats**:

Data captured by area detectors is commonly but not exclusively stored in HDF5 format. The Hierarchical Data Format (HDF) itself is a de facto standard for storing binary data and is used by various scientific communities and companies. The NeXus standard is commonly used and is a subset of HDF5 with well defined, experiment-specific metadata schemata, but does not capture all metadata yet. DAPHNE4NFDI will use services and tools from the Physikalische Technische Bundesanstalt (PTB) to ensure data quality, comparability and proper data standards. DAPHNE4NFDI will utilize library tools, services and knowledge (such as ORCID, DOI, interlinking, semantic annotation etc.) from the TIB for incorporating professional library aspects into the consortium.

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

Interfaces and overlap to other consortia have been discussed in a pre-NFDI workshop in Berlin on May 6 2019 with FAIRMAT, NFDI4CHEM, NFDI4ING and MATWERK and later with NFDI4CAT. Together we identified the scientific fields to be addressed by the different NFDI consortia, the structure of the potential user community and data producers, challenges and potential fields of synergies. A further meeting hosted by the DPG on June 10 2020 with interested consortia considered how best to represent physics in NFDI to maximise synergy and avoid duplication.

A detailed collaboration has been agreed with FAIRMAT. While the specific needs, tasks and challenges for both consortia in terms of data management are quite different we agreed to collaborate on the following tasks: 1. Define a science driven common pilot project to identify the needs and interfaces in terms of data structures, data exchange and metadata; 2. Organize a common workshop in 2021; 3. Define and develop translating software of the electronic logbooks to facilitate data exchange. We have also identified common tasks and topics with the consortia NFDI4CHEM, MATWERK, NFDI4ING. Here, we aim to collaborate on streamlining of metadata and e-logbook development. As characterization of data plays an important role in NFDI4CAT and NFDIMATWERK, X-ray and neutron operando data are relevant to both. Furthermore, both provide an excellent platform for interaction with industry and thus outreach. Development of data formats and for correlative techniques with joint workshops are planned.

Driven by the BMBF ErUM Data initiative the eight user communities organized in the research of the universe and matter (ErUM) field conceived a coordinated long-term action plan. The group devised a joint catalogue of measures to advance digital transformation between the X-ray/neutron science community, astrophysics, particle and hadron physics. In the field of data management, we clearly identified the need for science driven solutions adapting to the different community's needs. Despite the different science fields, we identified overlap and mutual interest in areas such as management of metadata, open data and handling large data sets. Here, the X-ray and neutron community would benefit from the experience and best-practice examples from the particle and astrophysics community via PUNCH4NFDI. Within the ErUM data process, a cross community platform "partnership for digitalization" has been proposed. This partnership would support collaboration also in terms of wider aspects of digitalization such as hardware, data analysis, outreach, web- interfaces etc. and strengthen the link between DAPHNE4NFDI and PUNCH4NFDI with cross-community actions in ErUM data.

DAPHNE4NFDI agreed to collaborate with the Deutsche Physikalische Gemeinschaft (DPG), TIB and PTB as partners in our consortia - all of whom are participants in the NFDI4PHYS consortium. These partners can contribute uniquely to DAPHNE4NFDI in outreach, library services and standardization and metrology services of X-ray and neutron data to benefit NFDI4PHYS, DAPHNE4NFDI and all NFDI. Discussions with NFDI4HEALTH highlighted collaboration opportunities on cross cutting topics including data security.

DAPHNE4NFDI will promote local interfaces to other consortia. Synergies can effectively promoted when consortia have active involvement in more than one consortium: in the case of DAPHNE4NFDI for example Kiel University (DAPHNE4NFDI, NFDI4Objects, NFDI4CHEM and FAIRmat in the first round), Karlsruhe Institute of Technology (e.g., DAPHNE4NFDI, NFDI4CHEM, NFDI4CAT, NFDI4Ing, NFDI4Phys, FAIRmat, Helmholtz-program "Information"), Siegen University(DAPHNE4NFDI, PUNCH4NFDI, NFDI4Phys). Here we plan internal meetings twice a year in order to develop a cohesive approach and cross links. For example in Kiel: curriculum development; a common approach to Metadata and a university internal policy on FAIR data handling.

## 4 Cross-cutting topics

Please identify cross-cutting topics that are relevant for your consortium and that need to be designed and developed by several or all NFDI consortia.

Online logbooks: DAPHNE4NFDI will contribute to the development of electronic logbooks with appropriate APIs for insertion of flexible instrument data alongside mapping of user and instrument metadata to collected data. This will be very useful across a range of fields.
Making data FAIR beyond single consortia: between scientifically related consortia and even more so between the disciplines is a considerable challenge that needs to be addressed by the whole NFDI. Interoperability, storage, archiving, definition and use of complex metadata structures beyond a single discipline need to be addressed across the NFDI.
Training, outreach and design of the NFDI: While the awareness of FAIR data is increasing, bringing topics of data management into university curricula is a considerable challenge which is directly linked to the long-standing success of the whole NFDI idea. In addition,, t he question of how to organize the interface areas of the consortia is highly relevant for DAPHNE4NFDI.
Storage and archiving of data, hardware: Hardware is not funded in the published framework of the NFDI. However, the question of where and how the data is stored, how to access, copy and work with the data in technical terms needs to be addressed by the whole NFDI.
Analysis of big data: This is not a topic within the current NFDI framework. Nevertheless, the large amounts of data that will be handled and provided by NFDI also implies that for many disciplines new ways of analyzing data (e.g. machine learning and others) will be required. The interface of the NFDI to other initiatives in Germany (e.g. ErUM Data, Artificial intelligence funding by BMBF, etc.) needs to be developed by NFDI as well.

We identified the following cross-cutting topics where our consortium could contribute to the overall NFDI.
Metadata and data management - outreach and dissemination into the broader scientific community and industry:The DAPHNE4NFDI partners come from a broad range of scientific fields in the natural sciences but still have well defined data as provided by the large scale facilities involved. Thus we see the potential to develop coherent standards for metadata, data management and best practice examples which are accepted and of interest for a diverse user community and to disseminate it into the broader context of NFDI. DAPHNE4NFDI has also considerable experience in handling and managing large data sets. DAPHNE4NFDI reaches into and is of interest for smaller university groups in a wide range of activities within the natural sciences. DAPHNE4NFDI also represents users from industry.
Helping to implement data policies/data structures by structuring of user communities: A large part of the NFDI is about communication. Communication between data users and data providers is needed for establishing e.g. data policies such as open data or defining metadata standards. DAPHNE4NFDI is well prepared to tackle this problem due to the structured user organization and the coherence of data-flow coming from a few large-scale data providers only. Here, DAPHNE4NFDI can contribute to the overall NFDI by best practice examples and successful workflows of defining data policies and organizing a larger community.
Implementation of FAIR principles on a European level: The German user organizations KFS/KFN active in DAPHNE4NFDI and the X-ray and neutron facilities are embedded in a larger European context with well-organized structures. User organizations with democratically elected representatives comprise over 30.000 users organized in the European user organizations (ESUO/ENSA). DAPHNE4NFDI has close ties to ESUO/ENSA and LEAPS/LENS

and is thus ideally suited to actively participate in European initiatives such as e.g. PANOSC or EXPANDS. Solving FAIR and challenges such as metadata creation and curation on a European level is a realistic goal for the X-ray and neutron community. We therefore envision that DAPHNE4NFDI can contribute considerably to the international/European aspect of the whole NFDI.

Education/training:The aspect of education and training of future scientists and generating awareness for data management matters is of considerable importance for DAPHNE4NFDI. Bringing these topics into university curricula in the natural sciences is a considerable challenge. Here, DAPHNE4NFDI will start from KFS and KFN, with the help of both the DPG and other organizations (DBG, DECHEMA, etc.) but also by cooperation with universities and data science schools, establish courses at universities. Our broad user community in combination with the science driven needs of the DAPHNE4NFDI user groups will help to generate enough (science driven) interest for advancing university curricula.