Nationale
Forschungsdateninfrastruktur
für disziplinäre und
transdisziplinäre Physik

NFDI4Phys

Letter of Intent 2021

6. August 2021

1 Binding letter of intent as advance notification of a full proposal

x	Binding letter of intent (required as advance notification for proposals in 2021)

2 Formal details

- Planned name of the consortium

Nationale Forschungsdateninfrastruktur
für disziplinäre und transdisziplinäre Physik

- Acronym of the planned consortium

NFDI4Phys

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3 Objectives, work programme and research environment

- Research area of the proposed consortium

NFDI4Phys serves a community representing nine domains of Physics, six of which follow the DPG's section structure, spanning with their topics a wide range of length scales from angstroms (atoms) to thousands of kilometers (societies). Two further application-oriented domains are independent and working on multiple length scales. These eight domains, together with the consortia DAPHNE4NFDI, FAIRmat, and PUNCH4NFDI cover all of disciplinary Physics. In contrast, our ninth domain Transdisciplinary Physics represents those fields where physicists work but are not rooted in the DPG. Most of these fields are transdisciplinary target disciplines of Physics. The nine domains

- Atoms and Molecules
- Optics and Photonics
- Cold Plasma
- Biological Physics
- Dynamics, Statistical Physics and Soft Matter
- Socioeconomic Physics

- Quantum Information and Artificial Intelligence
- Biomedical Physics

- Transdisciplinary Physics

are all conceptually linked by hierarchy of levels in nature as proposed by Philip W. Anderson in his seminal paper “More is different” [Anderson 1972]. Recently Erik Hoel in “When the map is better than the territory” [Hoel 2017] and George F. R. Ellis with “The Dynamical Emergence of Biology From Physics: Branching Causation via Biomolecules” [Ellis 2019] have enriched that idea with causal structure. On this base, we build a theoretical concept for minimally heterogeneous research data management (RDM) by observing universality classes of data structures within the framework of the philosophy of information. Domains and Task Areas establish paradigmatic use cases (UCs) which define our work program, covered by the following panels within the **DFG classification scheme**:

Disciplinary Physics fields

308 Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas
310 Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics

Transdisciplinary fields

201 Basic Research in Biology and Medicine
- **02** Biophysics
- **07** Bioinformatics and Theoretical Biology

108 Philosophy
- **02** Theoretical Philosophy

Concise summary of the planned consortium's main objectives and Task Areas

We target groups of all sizes, working with heterogeneous data types in Disciplinary and Transdisciplinary Physics, with a focus on servicing small laboratories. For all of them, RDM must become as simple as accessing the internet. For the latter, the internet protocol suite TCP/IP has standardized the communication of bitstreams, but the information within different streams is yet not self-explanatory. Currently, the best suggestion for a corresponding solution are FAIR digital objects (FDOs). Another overarching aspect is the Physics of Emergence which introduces hierarchical levels in nature. Physics has been practising transdisciplinary cooperation for at least three decades with other scientific disciplines at higher levels outside its traditional domain; not only in Biological Physics, which has already paradigmatically broadened the disciplinary canon of Physics, but also in newer domains such as Socio-Economic Systems. The core idea of Transdisciplinary Physics is to understand the complex structures of a particular discipline within its respective special jargon. Our aim is to foster genuinely New Physics overcoming disciplinary borders via an integrated RDM. In order to guarantee the benefit for the user community, the working program will be processed by joint project groups of RDM experts and pilot users, representing our use cases. Pivotal for this endeavor is an information-theoretic characterization of complexity. We will engage in a general discussion about the structure of information across the hierarchical levels of nature to help passing semantic borders, e.g. between phenomena like order (Physics) and function (Biology), from a data-driven perspective. NFDI4Phys manages the necessary FAIR data and tools within our Task Areas (TAs) as follows:

TA FAIR Laboratory

The key objective of this TA is to FAIRify local workflows of data generation and through that, ease administration and lookup during the daily work with data. The guiding idea is to design scientific RDM workflows on the local scale such that best practices for handling research data are easy to introduce and beneficial for the daily research work.

TA Metadata and Ontologies

This TA enables FAIR data management via digitized research documentation with interoperable metadata models. It defines domain standards aligned to general standards with the use cases provided by NFDI4Phys members. It sets up infrastructure components (terminology service, metadata catalog, knowledge graph for research contributions) and addresses the application of standards, quality-related metadata models, and metadata literacy with other TAs.

TA Federated Repositories

The key objective of this TA is to design federated repositories that allow seamless contextualizaton of all research objects and processes in a FAIR manner. FDOs pointing to devices, preparation or analysis steps will be registered in a searchable NFDI portal.

TA Quality Criteria and Standards

The documentation of data, metadata and software interfaces is essential for realizing FAIR data for Physics. In particular, there is a high demand for open binary formats that allow efficient access to large amounts of data. The elaboration of recommendations and the definition of best practices for data acquisition and processing will enable exemplary review systems for data and metadata, aided by semi-automated tools. The implementation of quality criteria for data and metadata will finally result in the deduction of norms and standards for specific use cases.

TA Evolving Infrastructure

Quantum Research Data Management addresses the feedback loops required between classical and quantum computers in a hybrid variational quantum simulation. FDOs are well suited for implementing Quantum RDM, as their modular architecture allows to adjust their low-level functionality while keeping the high level interfaces essentially unchanged.

Quantum Artifical Intelligence, especially quantum machine learning, which ranges from implementing algorithms in quantum computers to developing quantum neural networks, is already pursued by DFKI and DESY to tackle the huge amount of next generation data from the LHC at CERN.

Quantum Quality and Standards, i.e., quality assessment and curation of quantum data will need to account for the statistical representation of quantum states, which are destroyed upon readout of a quantum device. Standards have to be hardware-agnostic and flexible.

Computing resources for NFDI4Phys (storage capacity, resources for the access and metadata services, analysis tools) are provided by FZJ via the Jülich Supercomputing Centre.

TA Community Interactions

Data literacy comprises skills such as critical thinking, problem solving, computational thinking, data ethics, data citation, and data sharing. We will develop a comprehensive training and education program for different status groups, covering both interdisciplinary and domain-specific aspects. DPG and its Working Group Young DPG will be key partners and act as multipliers in a community building effort coordinated with other NFDI consortia as a cross-cutting topic contribution.

Surveys will be conducted remotely to evaluate our community's evolving needs in RDM, and inform our TAs. For instance, we query local labs in order to acquire an ontology of Physics via patching of these local instantiations of domain semantics.

Development of a Use Case Template for Physics is a central priority. It will deliver a canonical RDM workflow for all sub-disciplines. We choose Polarimetry as a well-established method, in order to start with a minimal, sufficient set of metadata and tools, and develop it further in regular communication with all other domains.

Domains and Interfaces cultivates contact with and between domains, and TAs within the consortium, and via our interfaces to other consortia. We are fostering our dual infrastructure encompassing technology and scientific discourses alike.

TA Governance

Governance provides the three essential pillars steering, monitoring, and communications.

Proposed use of existing infrastructure, tools and services

The first NFDI4Phys community survey, conducted in spring 2020, spotlights the patchy, heterogeneous state of digitization in Physics research in Germany. In many cases, the research is high-tech by nature, yet crucial documentation steps are often performed with pen and paper. Proprietary binary formats used by instruments inhibit interoperability and introduce system breaks. For want of widely accepted controlled vocabularies, terminology lacks consistency, impeding knowledge transfer across disciplines. In daily life, physicists overcome obstacles with technical skills, ingenuity, and a do-it-yourself spirit – as long as research is performed on local data by individuals or small groups. However, systemic solutions are necessary when discourse moves to public data and FAIRness, particularly in transdiciplinarity. This is why we approach FAIR data from two angles: community building on the one hand and a bottom-up process building bridges between small-scale technical solutions already in use on the other.

NFDI4Phys partners contribute to NFDI4Phys' infrastructure with a range of established services. They host and maintain technical RDM services that have defined data structures and workflows like storage routines and data transformations with respective inputs and outputs. These local solutions need to be integrated into an overall infrastructure. Examples are **CaosDB** of MPI DS for the Physics of Complex Systems, the **Cologne Database for Molecular Spectroscopy** used in the domains of Atoms and Molecules as well as Astrophysics, or **INPTDAT** for Plasma Technology. The **Open Research Knowledge Graph (ORKG)** is an infrastructure for the semantic description of research contributions. Local, technical solutions need to be connected on a (sub-)community level to allow FAIR data management within Trans-/Disciplinary Physics. A single point of access will be established based on existing open solutions like Dataverse, elabFTW, CaosDB, Omero, Git and many others. NFDI4Phys aims at service integration via standardized interfaces, allowing a shared space of research data that fosters FAIRness. Unambiguous metadata annotations are achievable by serving standardized terminology with a dedicated **Terminology Service** for NFDI4Phys. To enable the community to set up RDM for domain-specific needs, NFDI4Phys will also provide catalogs giving an overview of general and domain-specific resources, e.g. a **Metadata Standards Catalog** utilizing the open code base of the RDA Metadata Standards Catalog. Similar registries may be required for community resources like metadata extraction tools, converters or research software. Next to technical solutions, there are non-technical service structures established by the partners, e.g. educational programs like **DataTrain** offered for PhD candidates at the University of Bremen or **PID Services** (consultation, DOI registration). Non-technical solutions serve as models adaptable to the specific audience of NFDI4Phys or will be offered as is. Furthermore, the Jülich Supercomputing Centre provides **computing resources and access to its storage hierarchy**.

Interfaces to other funded or proposed NFDI consortia

We have some major* interfaces and several smaller collaborations defined by common use cases with other consortia.

NFDI4Bioimage* works with us on RDM of general image data. As images are an intrinsic data category of several of our domains, we are especially interested in canonical research workflows to unify processing. Imaging domains include Plasma Physics, Biological Physics, Biomedical Physics, and some sections of Transdisciplinary Physics. Further common interests are the handling of proprietary data (NMR Imaging) and security of patient data (Cancer DB).

NFDI-Neuro* shares with us RDM of network data for our domains Biological Physics, Socio-Economic Systems, and sections System Biology and Biological Categories of Transdisciplinary Physics. We are going to look for universal (meta)data formats. Our common focus on RDM of information processing ties in with our cross-cutting interest in the structure of information.

Text+* is providing expertise in Natural Language Processing, especially entity typing. Their expertise in language modelling ties in with our effort for a general data reader emphasizing the role of semantic information.

NFDI-MatWerk* shares our interest in process-driven structure formation in thermal non-equilibrium. This is a topic of general interest, e.g., for plasma-treated interfaces, motile cell fronts, and 3D printing solidification zones. We are going to look for universal (meta)data formats and processes.

NFDI4Datascience* collaborates closely with us on establishing FDOs as an integral part of our national research data infrastructure. Especially, we will work on a portal to an FDO repository and a project registry, enabling a crosswalk with linked data. In addition, we foresee cooperation on the ethics of digitization and AI (see the cross-cutting topic "Self Assessment").

NFDI4Ing We seek to establish cooperation with NFDI4Ing "archetypes" that describe workflows close to those in the NFDI4Phys community, in particular "Ellen" who works on numeric models with a wide variety of input disciplines, and "Doris" for high-performance measurements and computing.

DAPHNE4NFDI, FAIRmat, and PUNCH4NFDI* will cooperate with us on data literacy and an overall ontology of Physics in communication with the DPG and the American Physical Society.

DAPHNE4NFDI and PUNCH4NFDI share solutions for huge technical systems and collaborations which will augment our semi-scalable tools.

PUNCH4NFDI will cooperate with NFDI4Phys to develop storage infrastructure, AI methods, and tools for big-data analysis applicable to, e.g., socio-economic systems in NFDI4Phys.

FAIRmat has initiated some metadata work on devices in their field (like electron microscopes). We will cooperate, when building up our registries to achieve joint lookup solutions.

NFDI4Chem* and NFDI-MatWerk form a working group with 4Phys on open binary formats and format conversion. First prototypes for converters already exist, and will be amended based on the canonical workflows that will be found by TA FAIR Laboratory.

MarDI and PUNCH4NFDI are discussing a joint service for statistical analyses and non-Gaussian uncertainty distribution, to which NFDI4Phys is going to contribute.

NFDI4Biodiversity, NFDI4Health, KonsortSWD & Berd are important foci to be developped.

4 Cross-cutting topics

NFDI4Phys has signed and supports the “Leipzig Berlin Declaration”. Acknowledging the workshop report informed by the first nine funded consortia, we identify these cross-cutting topics (CCTs) as most relevant and offer significant contributions for other consortia:

Fair Digital Objects provide fitting **infrastructure, interoperability and interfaces** for NFDI consortia. By representing NFDI in the international FDO Forum, we contribute to the development of a **common vision and strategy** as well as **internationalization** efforts. Needs for FDO standardization will be layed out in a roadmap by DIN as the conduit to European, and international standardization, together with TÜV and the FDO Forum.

Standards and norms have yet to be recognized explicitly as a CCT. NFDI4Phys, with PTB, Germany’s national metrology institute as a co-applicant, is uniquely suited to liaison with quality infrastructure actors for new standards emerging from the NFDI. In particular, we seek harmonization for the “metrology roots” of research data, i.e. physical quantities, units of measurement, etc. This topic intersects with **policy advice and consultation.**

Quality management and assurance address similar issues from the user workflow viewpoint. Building on synergies with standardization efforts, responsibility and review systems for research data to be developed in NFDI4Phys are only two examples of potential contributions.

Metadata, terminologies, provenance will be addressed in a forming section of NFDI e.V. The lack of controlled vocabularies and machine-actionable terminologies for now severely stymies FAIR data in Physics. Key expressions shared by different fields with differing connotations and semantic content need to be addressed as a major problem in transdisciplinary research.

User-driven development is highly relevant for our community, which heavily relies on self-developed software. We are keenly interested furthering research software engineering.

Training and education are a prerequisite for success of the NFDI in general and for instigating **cultural change** in particular. Our focus on data literacy and respective interfaces with other (related) consortia demonstrate our growing engagement in RDM education.

Quantum RDM for generic use cases will be outlined in NFDI4Phys (see above). We suggest the establishment of a suitable format for cross-consortium collaboration. Synergies with corresponding groups on **Quantum AI** should be realized.

Structure of information is a pivotal topic for NFDI which we propose should be the subject for a NFDI section. Data need to be categorized according to their context. In addition to pure entropic information, they may carry function and semantic content which need to be handled separately. This is a central issue relevant for all disciplines, we are happy to take the lead.

Transdisciplinarity is a common vision, we share with Methods4NFDI and foster together.

Self-Assessment of the NFDI as an institution aiming at FAIR data is warranted to investigate the sustainability of solutions. Further, we need to ask what impact FAIR access to data will have on society. Could public FAIRness be unfair to single individuals? Should RDM really do all that what technology allows? Accordingly, we propose a NFDI section for technology assessment and philosophy of NFDI. We are fortunate to be guided on the history and ethics of science as well as on public awareness by two distinguished members of our board.