## 1 Binding Letter of Intent

as Advance Notification of a Full Renewal Proposal



This is the **binding Letter of Intent** of the PUNCH4NFDI Consortium (required as advance notification for renewal proposals in 2025)

## 2 Formal Details

- Name of the consortium
   Particles, Universe, NuClei and Hadrons for the NFDI
- Acronym of the consortium
   PUNCH4NFDI
- Applicant institution
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- Spokesperson PD Dr. Thomas Schörner, thomas.schoerner@desy.de, DESY

# **Co-applicant institutions**

Institutions in bold are newly added as co-applicant institution in the second funding phase.

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- Rheinische Friedrich-Wilhelms-Universität Bonn (Bonn) Regina-Pacis-Weg 3, 53113 Bonn Prof. Dr. Dr. h.c. Michael Hoch
- Technische Universität München (TUM) Arcisstraße 21, 80333 München Prof. Dr. Thomas F. Hofmann
- Thüringer Landessternwarte Tautenburg (TLS) Sternwarte 5, 07778 Tautenburg Prof. Dr. Markus Roth
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#### **Co-spokespersons**

Names in bold highlight newly added co-spokespersons in the second funding phase.

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#### **Participant institutions**

Institutions in bold are newly added as participant institutions in the second funding phase.

- Bayerische Akademie der Wissenschaften, Leibniz-Rechenzentrum (LRZ), Garching
- CERN (CERN), Genf (CH)
- Deutsche Physikalische Gesellschaft (DPG), Bad Honnef
- Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen
- Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden
- Humboldt-Universität zu Berlin (Berlin), Berlin
- Institut für Sonnenphysik (KIS), Freiburg
- · Johannes Gutenberg-Universität Mainz (Mainz), Mainz
- Max Planck Computing and Data Facility (MPCDF), Garching
- Max-Planck-Institut für Astrophysik (MPA), Garching
- Max-Planck-Institut für Radioastronomie (MPIfR), Bonn
- Technische Informationsbibliothek (TIB), Hannover
- Technische Universität Darmstadt (Darmstadt), Darmstadt
- Technische Universität Dortmund (Dortmund), Dortmund
- Universität Bochum (Bochum), Bochum

- Universität Freiburg (Freiburg), Freiburg
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- Universität Münster (Münster), Münster
- Universität Regensburg (Regensburg), Regensburg
- Universität Siegen (Siegen), Siegen
- Universität zu Köln (Köln), Köln
- Verein für datenintensive Radioastronomie e.V. (VdR), Bonn

## 3 Objectives, Work Programme and Research Environment in the Second Funding Period

### Main review boards

- Fachkollegium 3.24 Teilchen, Kerne und Felder
- Fachkollegium 3.25 Astrophysik und Astronomie

Further associated review boards:

- Fachkollegium 3.23 Optik, Quantenoptik und Physik der Atome, Moleküle und Plasmen
- Fachkollegium 4.43 Informatik

## Main Objectives and Task Areas

PUNCH4NFDI is the NFDI consortium of particle, astroparticle, astro-, hadron and nuclear physics. It covers a substantial fraction of **curiosity-driven basic research in physics**, and in particular of data-intense physics **at large research facilities**. Much of the work of the consortium is embedded in international collaborations and cooperations, which often precludes solely national "island" solutions. The PUNCH<sup>1</sup> community has always been at the forefront of technological developments. In particular, it is an avid pursuer and early adopter of the FAIR principles and a leading force concerning the "big data" and "open data" aspects of scientific data management.

In its first funding period, the particular focus of the PUNCH4NFDI Consortium was on achieving a deeper understanding of the requirements of the diverse involved communities, on laying technical foundations in terms of federated infrastructures, on a data and service platform and hub, as well as on establishing concepts for data and metadata management. In the second funding period of PUNCH4NFDI, hereafter referred to as PUNCH-2.0, the consortium will build on this foundation and achieve **six main objectives** O1-O6 (see figure 1):

<sup>&</sup>lt;sup>1</sup>"PUNCH" is the acronym for "Particles, Universe, NuClei and Hadrons".

- O1) further development and continuous adaption of the technological basis for PUNCH4NFDI federated infrastructures and development of sustainable operating models for them;
- O2) derivation of sustainable services suited for the PUNCH communities and for easy transfer to other domains in the framework of the NFDI sections and the Base4NFDI initiative;
- O3) full establishment of the Science Data Platform as user interface to open and FAIR data, digital research products, workflows, and science tools;
- O4) implementation of a set of complementary and generic use cases that allow easy customisation by a large user community with a standardised set of metadata;
- O5) education and training of the PUNCH communities and beyond on the FAIR and open science possibilities offered by PUNCH4NFDI and NFDI tools and services;
- O6) contributions to the overall development of the NFDI architecture, including solutions to the question of sustainability; fostering of national and international connections.



Figure 1: Main objectives of "PUNCH-2.0" and their connection to the foreseen task areas.

To achieve these objectives, PUNCH-2.0 foresees work in the following task areas:

**Task area 1 "Technical Foundations"** develops and operates the technical components necessary for the implementation of PUNCH4NFDI use cases and services, namely storage facilities and (meta)data catalogues (work package 1.2), computing facilities and accounting tools (work package 1.3), REANA as workflow execution environment, registries for software and containers with executables (work package 1.4). The TA also features the overall "Technical Coordination" (work package 1.1) that orchestrates the interplay among the technical components.

**Task area 2 "Science Exploitation**" connects the technical foundation of TA 1 with the central elements of the envisaged Science Data Platform. Of particular importance are the registry of digital research products and the organisation of access to and use of standard community tools

for data exploitation, data management, and resource allocation (work package 2.1). In addition, the task area implements a number of use cases (work packages 2.2–2.7) and leaves room for future use cases that will become the focus in later project stages. These use cases will showcase different model usages of the PUNCH4NFDI infrastructure and have been selected to cover a variety of topics.

**Task area 3** "Service Management and Outreach" covers – on the one hand – the training and education aspects as well as the definition, implementation and communication of FAIR open science practices in the PUNCH communities (all in work package 3.2). The TA also organises the contacts to and relations with PUNCH4NFDI stakeholders like the NFDI and its sections, Base4NFDI, other consortia, EU science clusters like ESCAPE, EOSC, ErUM-Data, and others (work package 3.3). At its core, in work package 3.1, the TA is responsible for the identification, finalisation and promotion of PUNCH4NFDI services to the PUNCH communities and beyond.

**Task area 4 "Project Management and Governance"** is responsible for the management of the entire project, the internal governance, the legal and financial administration of the project, and the user communication in the sense of web page design and maintenance, slide and document template setup, maintenance of social media channels, design of outreach material, and other related tasks.

Compared to the first funding period, PUNCH-2.0 will adapt its **governance structure** such that the focus will gradually move from the creation of technical solutions to the derivation and support of sustainable services and to their distribution in the user community. A new task area structure will support this process.

## **PUNCH4NFDI Infrastructures**

PUNCH-2.0 will build on the work and results of the consortium in its first funding period. This also includes tools and services developed and deployed so far that form an important ingredient of the work programme of task areas TA 1 and TA 2.

The already established **federated compute and storage infrastructures** of the consortium, **Compute4PUNCH** and **Storage4PUNCH**, integrate heterogeneous resources provided by some of the consortium's co-applicant and participant institutions (DESY, FZJ, KIT, LMU, LRZ, Münster, GSI, etc.). The technology is largely based on tools developed in the high-energy physics community for the world-wide LHC computing grid (WLCG). The software for jobs on Compute4PUNCH can be provided via the CERN Virtual Machine File System (CVMFS) – an open-source software package maintained by CERN with international contributors. Reproducible jobs are deployed via REANA, using the consortium's registries for software and containers and their preparation by GitLab using CI/CD (hosted by AIP).

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Digital research products (DRPs) are central for the PUNCH4NFDI approach to FAIR and open data and workflows. The **registry for digital research products** (RPR) is, therefore, a major objective of the first funding period of PUNCH4NFDI. The database and web interface are currently hosted at AIP.

In addition, the consortium provides a **metadata and file catalogue with an access management system**. The technology is based on the International Lattice Data Grid (ILDG) but was rebuilt by PUNCH4NFDI during the first funding period. Two instances of the system are currently provided by the consortium (at Universität Bielefeld and DESY Zeuthen).

In terms of **authentication and authorisation infrastructures** (AAI), PUNCH4NFDI builds on the Unity AAI based Helmholtz ID. To accommodate new requirements, the consortium has developed new tools and features, such as the MyToken service that seamlessly extends the lifetime of the OpenID connect access tokens for use in prolonged complex workflows across the PUNCH4NFDI infrastructure.

The PUNCH4NFDI Consortium has set up a slew of **collaborative tools** in order to organise the shared work, including an Indico section for meeting organisation, a chat platform via Mattermost, a GitLab instance for code management (at AIP), and a shared cloud environment based on Nextcloud (at DESY).

A **helpdesk system** has been deployed to offer user support for general questions concerning the PUNCH4NFDI Consortium, for questions regarding the usage of our services and tools, as well as for questions regarding training and education.

## Interfaces to NFDI

The PUNCH4NFDI Consortium is embedded in the structures of the NFDI and participates in a number of specific activities. There are also dedicated, specialised cooperations with other consortia, of which a few examples are listed below.

PUNCH4NFDI and **NFDI4DataScience** are exploring the use of shared infrastructures and tools for artificial intelligence (in particular LLM) solutions in physics. Planned joint efforts are i) the collaborative development of pipelines for crawling, indexing, and constructing semantic vector databases; ii) metadata extraction and domain-specific knowledge base construction to support cross-community data management and reuse; iii) standardization of collected data to improve interoperability and usability for assistant agents.

Together with **DAPHNE4NFDI**, PUNCH4NFDI is exploring joint solutions in the field of common infrastructures, in particular with respect to storage resources and (meta)data catalogues, and workflow organisation. This connection arises naturally because of an overlap in participating institutions and the organisation of the research at large research infrastructures. Joint suggestions

for base service proposals are foreseen e.g. for federated infrastructures.

Together with the consortia DAPHNE4NFDI, FAIRmat, MaRDI, NFDI-MatWerk, NFDI4Cat, and NFDI4Chem, the PUNCH4NFDI Consortium is collaborating in the "**Physical Sciences in NFDI**" **initiative**, which unites experts on a broad spectrum of topics in physics, chemistry, mathematics and informatics. In workshops and talks, "Physical Sciences in NFDI" invites leading scientists to showcase good (data) practices to an international, interdisciplinary audience and foster discussions on various topics around research data management. In addition, the initiative contributes to discussions on data management in university curricula in the physical sciences, and on other topics. We will continue to enhance this activity in the second funding period.

The Technical University of Darmstadt, together with Universitäts- und Landesbibliothek Darmstadt, is exploring the potential of the COSCINE tool, developed in the context of **NFDI4ING together with other consortia**, for research data management in physics. Together, Technical University of Darmstadt and PUNCH4NFDI will in particular work on metadata schemata with the AIMS part of COSCINE and the PUNCH4NFDI platform.

PUNCH4NFDI members are involved in a number of NFDI sections and working groups, most notably in the section on "Common Infrastructures", and less e.g. in "Metadata". From this work, contributions to so far two successful **Base4NFDI base service projects** arose – IAM4NFDI and nfdi.software.

## 4 International and National Networking

A large share of PUNCH research is taking place at **international facilities** (e.g. CERN, ESO), under the guidance of **international institutions** (e.g. ESA), and in **large international collaborations**: The PUNCH sciences and the technical solutions developed in them are by definition international or even global. Consequently, PUNCH research is in many places guided by **international roadmaps and strategies** (ICFA, European Strategy for Particle Physics, APPEC, Astronet, US decadal roadmaps, etc.). It follows naturally that in PUNCH sciences there are many discipline-specific international data initiatives (e.g. WLCG, IVOA, ILDG, ESCAPE) and important standardisation working groups (e.g. IVOA, ICFA Data Lifecycle Panel). Members of the PUNCH4NFDI Consortium participate in many of these activities and often shape them. In this way, the **alignment of the work** of PUNCH4NFDI **with international research needs** (in terms of data management solutions and federated data infrastructures) is ensured.

A more formal international collaboration has been defined, in summer 2024, by a common **letter of intent with ESCAPE**, the European Science Cluster of Astronomy & Particle Physics ESFRI Research Infrastructures. ESCAPE and PUNCH4NFDI share the goal of enhancing open science practices in fundamental physics research. Synergies are expected at the level of strategy discussions and tool & service implementation (e.g. analysis facilities, software data bases, federated infrastructures). ESCAPE is also the consortium's discipline-specific connection to the EOSC.

The consortium's strong international perspective is, at the same time, a **challenge and a blessing**: a blessing – because PUNCH4NFDI developments are backed by decade-long experience with solutions scaled to many thousands of users; a challenge – because of natural tensions between the various national and international structures and boundary conditions. It is one of the tasks of PUNCH4NFDI to turn these tensions into **profitable and viable solutions**.

PUNCH4NFDI is **backed by the elected community representations** KET, KAT, KHuK, and the Council of German Observatories (RdS). With increasing numbers of implemented use cases and roled-out services, the connection to the represented communities will substantially be strengthened, with benefits for science and for the dynamics of PUNCH4NFDI developments. Dedicated **boards within the PUNCH4NFDI governance** ensure direct exchange with and engagement of the community: i) the international Scientific Advisory Board oversees the entire consortium and its general directions; ii) the User Committee, appointed by KET, KAT, KHuK, and RdS, represents user needs across sub-disciplines; iii) the Infrastructure and Resource Board aligns consortium work with the capacities of major infrastructure and data providers.

PUNCH4NFDI partner institutions are involved in five of the recently newly established or extended **DFG clusters of excellence**, which will help to leverage the work of the PUNCH4NFDI Consortium and to further foster the user community.