# The PUNCH4NFDI Consortium Newsletter Number 6

July 2023



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# 1. News and Highlights

The consortium elected Andreas Haungs (KIT) and Christiane Schneide (DESY) as new spokesperson and deputy, respectively, for the "Konsortium gemäß Satzung". We thank Thomas Schörner (DESY) and Susanne Pfalzner (FZJ), who held the positions until May 2023, for their commitment.

A series of workshops and in-person meetings took place in June 2023:

- a virtual Hands-on Workshop<sup>1</sup>, organised in part by members of Task Areas 2 and 3, for future ILDG users to learn about the current progress in modernising and re-activating ILDG;
- a SciTrace Hackathon<sup>2</sup> at AIP, organised in part by members of Task Area 4, to provide participants the opportunity to create SciTrace packages from their own workflows;
- a Workshop on Machine Learning and Data Processing on FPGAs<sup>3</sup> at DESY, jointly organised by members of Task Area 5 and XFEL, with a focus on experiment specific challenges and solutions; the first in-person meeting of the PUNCH4NFDI Executive Board at University Bielefeld.

From 12-14 June 2023, the "**Joint ECFA - NuPECC - APPEC**" (JENA) Computing workshop took place in Bologna, Italy<sup>4</sup>. The meeting was designed to address the need, felt by the three scientific communities and the European funding agencies alike, for discussions on the strategy for and implementation of European federated computing infrastructures, and it was the starting point for a working group process towards a white paper on the subject.

Thomas Schörner was invited to present a view on FAIR and open data management and its requirements in Europe, and discussed this also in view of the PUNCH4NFDI perspective. In fact, the NFDI structures established in Germany were very well received by the international workshop participants. As one outcome of the event, a closer collaboration between PUNCH4NFDI on the one hand side and the European ESCAPE collaboration on the other hand, in particular in the fields of the software data bases, data lakes, the science data platform, and workflows, is planned.

The **PUNCH Young Academy** programme has started in 2023. First, the One-to-one Mentoring Service was initialised. The mentor-mentee tandems operate for one year. Second, a two-day Software Development Training<sup>5</sup> was conducted by A. Sciarra, University Frankfurt.

Further workshops for young scientist are planned alongside the **PUNCH4NFDI Annual Meeting** which will take place on 12 - 13 October in Munich.

In case you have news that you want to share with PUNCH4NFDI, don't hesitate to send a mail to *info@punch4nfdi.de*. You can access all newsletters on our web site<sup>6</sup>.

<sup>&</sup>lt;sup>1</sup> https://indico.desy.de/event/39311/

<sup>&</sup>lt;sup>2</sup> https://indico.desy.de/event/38873/

<sup>&</sup>lt;sup>3</sup> https://indico.desy.de/event/39436/

<sup>&</sup>lt;sup>4</sup> https://agenda.infn.it/event/34738/

<sup>&</sup>lt;sup>5</sup> https://indico.desy.de/event/39136/

<sup>&</sup>lt;sup>6</sup> <u>https://www.punch4nfdi.de/news\_amp\_events/newsletter/</u>

#### 2. NFDI and related topics

**Base4NFDI**: From the first round of applications the proposal IAM4NFDI<sup>7</sup> received funding for a 6-months initialisation phase.

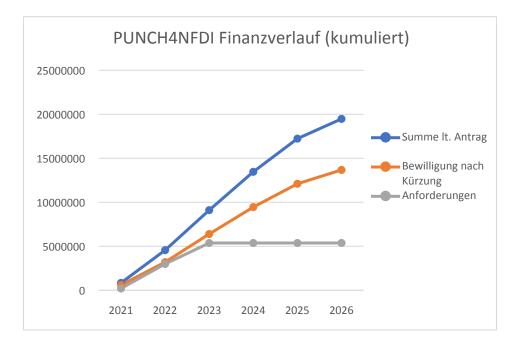
The second round of proposals was submitted in May 2023. This round comprised proposals for *Persistend Identifier Services* and *Terminology Services*. Both of these proposals were re-submitted after a revision. The Consortial Assembly of the NFDI has decided to fund both service applications for a one-year initialisation phase.

#### NFDI sections and task forces:

- A new section "Industry Engagement" has been established in March 2023. The section concept is available on Zenodo<sup>8</sup>.
- The Task Force Evaluation and Reporting has written a White Paper to formulate the handling of the goals of the NFDI, described in the Bund-Länder-Vereinbaung (BLV), during the evaluation of NFDI in 2024. The White Paper was accepted to serve as basis for the evaluation by the Consortial Assembly and will soon be published on Zenodo.

#### 3. Formal, legal and financial topics

The flow of funds has stabilised in 2023 – the demand was steady over the first three quarters. The cumulative spending profile of the consortium is shown in Figure 1.



*Figure 1: Spending profile of PUNCH4NFDI including Q4/2021 – Q3/2023. Blue - proposal; orange - DFG grant; orange - actual spending.* 

<sup>7</sup> https://www.nfdi-aai.de/

<sup>&</sup>lt;sup>8</sup> https://zenodo.org/record/7900079#.ZFT4nM7P02w

One Participant, Leibniz Institute for Solar Physics (KIS), was admitted as member in the PUNCH4NFDI "Konsortium gemäß Satzung".

On the level of Task Area leaders we report the change in Task Area 4 from Philip Bechtle (U Bonn) to Achim Geiser (DESY). Furthermore, we welcome several new work package leads: Nicola Malavasi (TA3.1 and TA3.4, LMU), Cornelius Grunewald (TA3.1, TU Dortmund), Victoria Tokareva (TA4.2, KIT) and Michael Zacharias (TA6.1, U Heidelberg).

# 4. Status of the consortium

#### Reporting in PUNCH4NFDI

The input to the quarterly reports, as decided by the PUNCH4NFDI Executive Board, will be reduced to a short update on the deliverables and information on TA members. Further information, for example on publications and published services, will be compiled on a yearly bases. This changes will come into effect by the third quarter (Q3/2023).

#### New people

New people who contribute to the work programme of PUNCH4NFDI are our most valuable asset! In this category of the newsletter, we try to give short introductions of newcomers to the consortium – welcome to everybody!



**Daniel Küttel (U Regensburg, TA2, 3 and 4)**: I am a scientific staff member at Regensburg University and working there on my PhD project in lattice QCD. For PUNCH4NFDI, I participate in TA2.1, TA3.2, and TA4.2. Furthermore, I contribute to the ILDG/LDG middleware

development. Contact: <u>daniel.knuettel@physik.uni-regensburg.de</u>

Ashraf Mohamed (DESY, TA5): I am Ashraf from Egypt, where I obtained my B.Sc. in Physics and Electronics in 2012. Afterwards, I obtained my M.Sc. in Theoretical Particle Physics with a focus on dark matter searches in 2017. Few years later, in 2021, I got my Ph.D. from RWTH Aachen University while working at DESY. I focused on supersymmetric dark matter data analysis using cutting-edge machine learning methods and detector hardware work. After my Ph.D. I have taken up a position to work as a "machine learning scientist" at the lastminute.com group. I joined PUNCH4NFDI TA5 to work on ultra-fast (real-time)

for particle tracking. Contact: <u>ashraf.mohamed@desy.de</u>





**Ding-Ze Hu (DESY, TA4):** I studied Applied Computer Science (Angewandte Informatik, M.Sc.) at Georg-August-Universität Göttingen. During the study and the Master Thesis, I mainly focused on data engineering, databases and software development. I started working at the DESY library in Hamburg in April 2023. I am part of the TA4 in PUNCH4NFDI, which is mainly for implementing and developing metadata schema for the scientific data in this project. Contact: ding-ze.hu@desy.de

Joschka Birk (UHH, TA3): I'm a PhD student at the University of Hamburg researching new machine learning methods for particle physics applications.

I obtained my Bachelor's and Master's degree at the University of Freiburg, where I was working on machine learning methods for top quark physics and flavour tagging improvements within the ATLAS experiment. I am interested in particle physics, machine learning and have a passion for tools like Docker containers which improve reproducibility in science.





**Michael Hübner (U Bonn, TA2 and 4):** I studied physics in Bonn and received my PhD in 2022 working on measurements of the Higgs to tau lepton decays and related tasks in the ATLAS collaboration. Afterwards, I joined the High Performance Computing and Analytics Lab in Bonn where I mainly worked within the HPC.NRW consortium. Among other things, I helped paving the way towards a common software stack across multiple HPC sites. In April 2023, I joined the IT department of the physics institute in Bonn and at the same time the PUNCH4NFDI consortium. I plan to contribute to TA2 and TA4, trying to bring together use cases and different elements of the envisioned workflow pipelines.

**Reza Salkhordeh (U Mainz, TA2):** I am a postdoctoral researcher at the Johannes Gutenberg-Universität Mainz since Nov. 2018. I received my B.Sc. from Ferdowsi University of Mashhad in 2011, M.Sc and Ph.D. from Sharif University of Technology (SUT) in 2013 and 2018, respectively. During my Ph.D., I mentored four M.Sc. and six B.Sc theses. My Ph.D. thesis is titled "Optimization of Operating System to Employ Emerging Memory Technologies". I was a member of PPoPP'18 artifact evaluation committee and a reviewer for Elsevier Microprocessors and Microsystems (2016) and Transactions on Computer-Aided Design of Integrated Circuits and Systems



(2018). I was a member of Iran's National Elites Foundation. My research interests are storage systems design, solid-state drives, non-volatile memories, operating systems design, and caching architectures. Contact: <u>rsalkhor@uni-mainz.de</u>



Simon Thiele (U Bonn, TA2): I am a PhD student at the University of Bonn, working in Data Analysis for the ATLAS experiment, specifically on using machine learning for analyzing multi-tau final states of diboson events. did my Bachelor's Degree at the University of Münster and my Master's at the University of Bonn. For PUNCH I am working in TA2 on using XRootD for storage solutions.

Contact: <u>simon.thiele@uni-bonn.de</u>

# 5. Upcoming events and excitements

- 12 14 September 2023, 1st Conference on Research Data Infrastructure<sup>9</sup>, • organized by NFDI in cooperation with KIT, in Karlsruhe
- Organised by the PUNCH Young Academy, **Tools & Services Training**<sup>10</sup> will • take place as hybrid event in Munich and online on 11 October 2023
- PUNCH4NFDI Annual Meeting<sup>11</sup>, 12 13 October 2023 in Munich, including • public sessions
- A complete list of PUNCHLunches can be found in the intranet and in Indico: https://indico.desy.de/category/743/ ). If you have suggestions for the seminar series – let us know at info@punch4nfdi.de.
- For a complete list of TA and other working meetings, see the Indico category • https://indico.desy.de/category/741/

# 6. Recent talks, results, and publications

To be found at least partly on the web page, the results page<sup>12</sup> and in ZENODO (https://zenodo.org – just search for "PUNCH4NFDI" or – if you are interested in the broader scope - "NFDI").

- Gauge-equivariant neural networks as preconditioners in lattice QCD<sup>13</sup>
- Open data and open-source tools throughout research data life cycle: KCDC • example<sup>14</sup>
- Overview of petabyte-scale metadata storage methods and frameworks<sup>15</sup>
- (Thoughts on) Requirements on FAIR Data Management<sup>16</sup>

<sup>&</sup>lt;sup>9</sup> https://www.nfdi.de/cordi-2023/

<sup>&</sup>lt;sup>10</sup> https://indico.desy.de/event/40315/

<sup>&</sup>lt;sup>11</sup> https://indico.desy.de/event/38458/

<sup>&</sup>lt;sup>12</sup> https://results.punch4nfdi.de/

<sup>&</sup>lt;sup>13</sup> https://arxiv.org/abs/2302.05419

<sup>&</sup>lt;sup>14</sup> <u>https://zenodo.org/record/7937830</u>

<sup>&</sup>lt;sup>15</sup> <u>https://results.punch4nfdi.de/?md=/docs/Documents/metadata-overview.md</u>

<sup>&</sup>lt;sup>16</sup> https://zenodo.org/record/8037379