

The PUNCH4NFDI Consortium

Particles, Universe, NuClei and Hadrons for the NFDI

Kilian Schwarz

DESY

PUNCH GM Meeting - TA6, 07.07.2025



Work Package 1 (M. Zacharias & K. Schwarz)

D-TA6-WP1-1 (Noticeboard) (01/22)

- Being installed at DESY to go public
- To be connected to helpdesk

D-TA6-WP1-2 (physics.tools) (01/23)

- Exchange platform for information on archives, data management software, hubs)
- See specific slides WP4

D-TA6-WP1-3 (communication with NFDI) (continuous)

- Synergies on cross-cutting topics to be discussed with NFDI initiatives
- Important point: https://intra.punch4nfdi.de/?md=/docs/NFDI/sections.md
 Fill this page, when you take part in NFDI section (working groups, etc) meetings

D-TA6-WP1-3 (communication with NFDI) (continuous)

• Important point: https://intra.punch4nfdi.de/?md=/docs/NFDI/sections.md
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Common Infrastructures

List of Working Groups and members

Working Group ♦	Email 💠	General topics	PUNCH member
Overall Architecture	Sign-up		
Data Integration	Sign-up		A. Montanari, J. Künsemöller
Data Management Planning	<u>Sign-up</u>		H. Enke
Data Science & Al	Sign-up		A. Mohamed, N. Suvvi Neelakant
Data Transformation	Sign-up		C. Wissing, N. Suvvi Neelakantaia
Electronic Lab Notebooks	<u>Sign-up</u>		
Identity & Access Management	<u>Sign-up</u>		K.Schwarz
Infrastructure and Data Security	Sign-up		
Long-term Archiving	Sign-up		J. Chodak
Multi-Cloud	<u>Sign-up</u>	concept	K. Schwarz, C. Wissing, H. Enke Neelakantaiah, J. Künsemöller
Persistent Identifier	Sign-up		
Research Software Engineering	<u>Sign-up</u>	Marketplaces, JupyterHubs,etc	H. Enke, M. Zacharias, M. Blank

Metadata

List of Working Groups and members

Working Group	\$	Email	\$	General topics	♦	PUNCH members	\$	Meeting minutes	\$	Hot Topic	\$	Next meeting	\$
Cookbooks, Guidance and Best Practices		Sign-up											
Knowledge Graphs		Sign-up								B4N project approved			
Ontology Harmonization		Sign-up											
Research software metadata		Sign-up				C. Schmidt, O. Kaczmare	ek						
Search and Harvesting		Sign-up				M. Castro Neves							
Terminology Services		Sign-up											
TF Metadata						V. Tokareva							

23.02.24 12:00

For the next 1+ years in PUNCH 1.0:

D-TA6-WP1-4 (services and tools) (continous)

- Further development of physics.tools and noticeboard
- PUNCH connection to Base service <u>nfdi.software</u>
- Services and tools will be made available to the NFDI

D-TA6-WP1-5 (continuation of D-3) (continuation)

- Deepen ties with other NFDI consortia/sections/Base services
- Continue advertising PUNCH4NFDI at meetings (DPG, AG, etc.)
- start showing actual products and services
- PUNCH Lunches

Work Package 2 (K. Schwarz & D. Mallmann)

- D-TA6-WP2-1
 - Prototype PUNCH AAI (31 Mar 2022): done
 - Basic PUNCH AAI (31 Dec 2023): Unity dev requests #1, #2, #3
 - Extended PUNCH AAI (30 Sep 2026)
- D-TA6-WP2-2
 - Coordination with NFDI, national, international stake holders
 - Draft design (31 Dec 2022): done, published
 - Complete design (31 Dec 2024): done, published
- D-TA6-WP2-3
 - PUNCH AAI group management
 - Prototype (31 Dec 2022): done
 - Revised version (31 Dec 2024): in progress
 - Full group management (30 Sep 2026)

- AAI requirements described in
 - https://results.punch4nfdi.de/?md=/docs/Documents/AAI/aairequirements.md
 - These requirements are being implemented in the PUNCH AAI
 - Status of Development requests to Unity
 - Request 1: "Group information in tokens"
 - Implemented by Unity even before we made an official request
 - Detailed testing in PUNCH still in progress
 - Request 2: "Claim filtering" (only selected groups in tokens)
 - Implemented and tested
 - Detailed testing of workflows in PUNCH still in progress
 - Request 3: "Granular permissions"
 - In progress
 - In extended AAI meeting on June 04 decided for:
 - External policy service "behind" AAI with door for "token exchange with trusted client" to be kept open
 - · Current options: Unity performs call directly or Unity launches external script being discussed also with FZJ
 - · This request is completely supported by HIFIS
 - Additional: Indico access rights can be controlled via groups in PUNCH AAI
 - Currently being tested in the context of HIFIS

Work Package 3 (S Wagner & H. Hessling)

- D-TA6-WP3-1 (31 Jul 2022)
 - Reference guide on publishing data: living document
- D-TA6-WP3-2 (31 Dec 2022)
 - Reference guide for publishing software: living document
- D-TA6-WP3-3 (31 Dec 2023)
 - (Dynamic) Metadata frameworks for PUNCH-SDP: declared finished
 - Document (10 pages) by Tim Oelkers
 - To be followed up in PUNCH2.0 via DZA
- D-TA6-WP3-4 (31 Mar 2024)
 - Effelsberg data: data need to be converted, ongoing
 - Updated completion date: 31 Dec 2025
- D-TA6-WP3-5 (31 Dec 2024)
 - Converter for FITS/ROOT formats: done, being published
- D-TA6-WP3-6 (31 Dec 2025)
 - Metadata extensions: on track

D-TA6-WP3-3

- Highlights
- Tim Oelkers, "Overview of petabyte-scale metadata storage methods and frameworks" (10 p, 2023)
- Basis for future developments: SKAO project "Rucio-IVOA Metadata Integrations" (https://gitlab.com/ska-telescope/src/ska-rucio-ivoa-integration)

D-TA6-WP3-4

- Update
- Conversion is ongoing. However, converted data need to be recalibrated, which is a demanding task and cannot be realized within PUNCH 1.0 (reduced funding)

D-TA6-WP3-5

- Highlight: a Root to FITS conversion is realized, which makes it possible to link astroparticle data with astronomical data.
- The conversion is a prototype solution. Optimization potential for further development into a plug & play solution.

D-TA6-WP3-6

- Highlight: concept developed. Implementation would, in particular, allow linking of multi-frequency data via "extended metadata".

Work Package 4 (G. Duckeck)

- D-TA6-WP4-1: survey of PUNCH tools
 - Initial overview (31 Jul 2022): done, being published
 - Final list (30 Jun 2026)
- D-TA6-WP4-2 (30 Jan 2023)
 - Reference repository with CI: done, being published
- D-TA6-WP4-4 (30 Jun 2026)
 - Data analysis examples
- D-TA6-WP4-5 (30 Jul 2023)
 - Software platform: done, merged with Physics tool

Work Package 4 & 1

New developments in physics.tools, a search engine for software referenced in publications.

Also part of the **Base4NFDI** proposal, in the **nfdi.software** group.

- The service is now on a server in Heidelberg University (here)
- The software database, containing software extracted from papers on arxiv
 - For now testing the deployed website with a subset of the paper database
 - Moved citations of issues/branches/discussions/etc. in GitHub repositories
 that were appearing in the old version of the website to the citation of the main GitHub repo.
- The search engine:
 - Polished output of the standard version: now ordered by GitHub repo star counts, showing the repo description and the main programming language
 - Working on the Al-assisted version (i.e., that understands keywords): will use a fuzzy-match algorithm
 - with an embedding language model (w/ ollama and nomic-embed-text)
- Working on the feature Add your software
- Working on a Flask API to sync the database to the research software directory in nfdi.software



Work Package 4 & 1

Future development in physics.tools, a search engine for software referenced in publications.

- Currently, only our team in Heidelberg University is working on this
- By the end of September 2025, we shall be able to:
 - Complete the database
 - Extend the engine output with other providers (i.e. Zenodo), but also private websites that are cited in the papers
 - Finalize the Al-assisted search engine
 - Make it possible for users to ask to add software
 - Finalize the Flask API for the synchronization with nfdi.software
- For the future after then:
 - Automatize the harvesting of arxiv papers to compile the database, and the index for the Al model
 - Define cronjobs for the Flask API and the synchronization
 - Possible new features, which partially depend on what is included in the Integration phase in nfdi.software



Work Package 5 (S. Wozniewski & H. Enke)

- D-TA6-WP5-2 (30 Sep 2022)
 - Dynamic disk cache: done and published
- D-TA6-WP5-3 (30 Dec 2025)
 - · Memory based computing
- D-TA6-WP5-4 (31 Dec 2025)
 - Interfaces to supercomputer, GPU, GoeGrid
- D-TA6-WP5-5 (31 Dec 2024)
 - COBalD/TARDIS: done, being published
- D-TA6-WP5-6 (30 Sep 2022)
 - MultiCloud resources: done, being published
- D-TA6-WP5-7 (30 Sep 2026)
 - Standard analysis software in JupyterHub
- D-TA6-WP5-8 (31 Dec 2023)
 - Services via API: → changed to continuous
- D-TA6-WP5-10 (30 Jun 2024)
 - FTS and Rucio: in progress

5 deliverables left to be completed till end of PUNCH (1):

• D-TA6-WP5-3 (due Dec 2025):

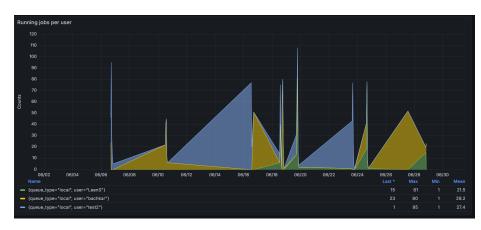
Gen-Z consortium was developing an open standard for memory-based computing, being explored and offered in this WP as a solution, in particular for astronomy use cases in the CASA framework. Gen-Z was replaced by Intel CXL (Compute Express Link), which requires some porting of CASA (ongoing).

Worked on by: HTW Berlin

 D-TA6-WP5-4 (due Dec 2025): PUNCH4NFDI EXPLORE service offering compute resources (hosted at Uni Göttingen) for LHC open data analysis – service is active
 Currently offered via own registration website and login – sorting out obstacles with PUNCH AAI ongoing

Worked on by: Baida A.

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- As of now, a total of **3,965 HTCondor clusters** have been submitted for ATLAS Open Datasets processing on **EXPLORE**.
- Each cluster contained between **9 and 29 individual jobs**, depending on the performed analysis.
- This results in an estimated total of **35,685 to 114,985 jobs** executed.
- These jobs were designed to process discrete samples in parallel, enabling scalable and efficient use of available compute resources

Public Access to CERN Open Data via GoeGrid — EXPLORE



Aim:

Provide public access to GoeGrid resources for CERN Open Data analysis, available since Q4 2024 (TA6-WP5-4).

Service Status:

Operational since November 2024, fully optimized after alpha/beta testing with 12 users and HEP Masterclass students.

Target Users:

- Students (school and university level)
- Citizen scientists and hobbyists
- · Independent and external theorists

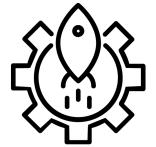
Access & Authentication:

- Email-based registration with SSH key login; no third-party authentication required.
- Under/over-18 flag and parental consent required for minors.
- Consent to Terms of Use mandatory.
- Account lifetime is 3 months, after which the user data is deleted.

Resources & Support:

- Dedicated compute resources via University of Göttingen
- Tutorials for HZZ, TTbar, and Hyy ATLAS Data analyses, including job execution and data visualization. Additional tutorials planned!
- Materials hosted publicly on <u>PUNCH GitLab repository</u>

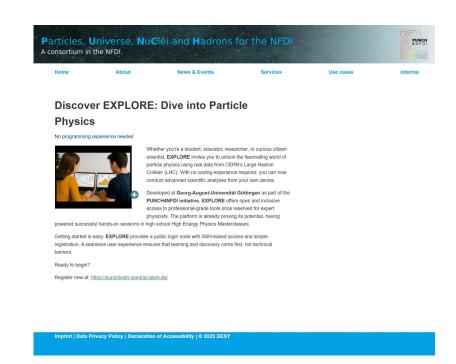


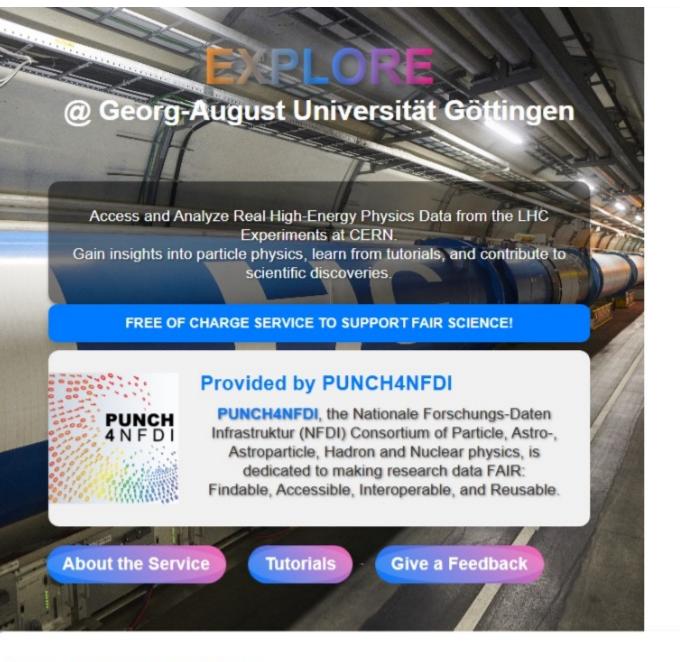


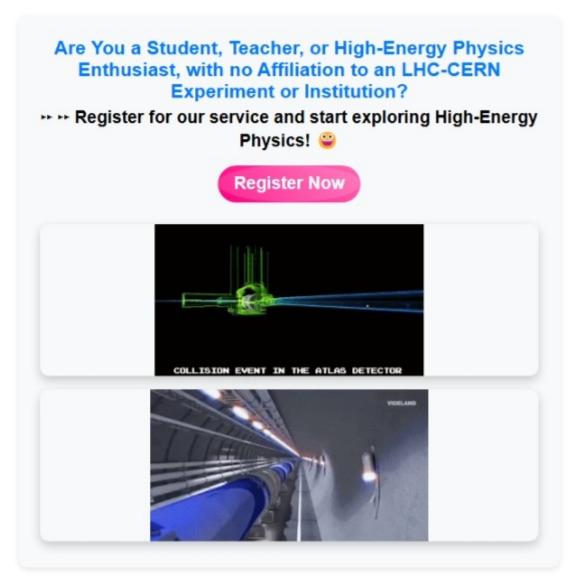
- Promoted on the PUNCH website and featured in the NFDI newsletter (May 2025).
- Scheduled presentation at <u>CoRDI 2025 in Aachen 26-28</u>
 <u>August:</u>

"EXPLORE: A Scalable Infrastructure for LHC Open Data Analysis and FAIR Data Provisioning" (Track: RDM Infrastructures).

- Considering integrating AAI for EXPLORE to boost user uptake, but modifications to the AAI are needed before use; growing the base of regular users remains a key challenge.
- We encourage community members to help advertise the service and invite potential users to register and explore the platform at: <u>EXPLORE Registration</u>.
- •PUNCHLunch planned in September 2025, reserve the date











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D-TA6-WP5-7 (due Sep 2026):

Integration of standard analysis software and newly developed tools into the JupyterHub platform at University of Münster via use case specific notebook images. Currently upgrade of the JupyterHub-Cluster. Service and images have already been used for classes of the PUNCH Young Academy, in particular.

Worked on by: Michael W.

D-TA6-WP5-8 (due Sep 2026 / continous):

Discussion of AUPs and related policies and identification of corresponding texts (for services accessed centrally via the PUNCH-AAI)

Worked on by: WP5/interested people, Harry E. & Sebastian W. as WP-Leads, resource providers

- D-TA6-WP5-10 (due June 2024)
 - Rucio and FTS instances in place
 - Configuration to a large extent in place
 - Extensive testing still do be done
 - Worked on by: TA6/TA2: K. Schwarz, C. Wissing

TA6 related delivery reports

Deliverable reports

- •D-TA2-WP2-1, D-TA2-WP2-4: Demonstrator for a federated compute infrastructure
- •D-TA5-WP1-1: Report on impact of on-line filtering on discovery potential
- •D-TA5-WP2-1: Curation & metadata schemes for Dynamic Filtering
- •<u>D-TA5-WP2-2: Strategy concept for identifying highly complex (multi-parametric)</u> <u>signals in huge data streams</u>
- •D-TA5-WP3-1: Specifying the concept of a Dynamic Archive
- •D-TA6-WP1-2 and D-TA6-WP4-5: physics.tools
- •D-TA6-WP1-3: Synergies on cross-cutting topics within NFDI
- •D-TA6-WP5-2: Dynamic disk caching for opportunistic resources
- •D-TA7-WP1-2: Establishment of the PUNCH4NFDI Young Academy
- •D-TA7-WP1-4: Critical Review of the Measures Developed and Development of a Feedback System to Guide Education and Training

Acknowledgements

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