The PUNCH4NFDI Consortium

# Particles, Universe, NuClei and Hadrons for the NFDI

Thomas Schörner (DESY) AG Meeting, Bremen, 15 September 2022





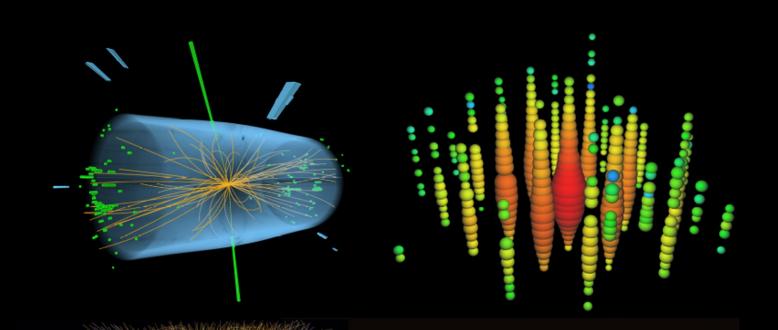
Gemeinsame Wissenschaftskonferenz GWK

# DEG Deutsche Forschungsgemeinschaft

# See also DFG.de/nfdi and nfdi.de

# Nationale Forschungsdateninfrastruktur (NFDI)

- Sustainable utilisation of research data
- Establishment of FAIR data management
- Connection to European and international efforts (like EOSC)
- Bottom-up approach of (30) independent consortia
- 5 (+5) year funding;
   85 MEUR / year





# Particles, Universe, NuClei and Hadrons for the NFDI (42 partners, 10k scientists, support from KET, KAT, KHuK, RdS)

The prime goal of PUNCH4NFDI is the setup of a federated and "FAIR" science data platform, offering the infrastructures and interfaces necessary for the access to and use of data and computing resources of the involved communities and beyond.

# Who We Are

### Universities, Helmholtz, Max Planck, Leibniz



#### **PUNCH** data are diverse

- in size and rate
- in complexity and purpose
- in abstraction level

#### **PUNCH4NFDI** expertise

- Big data and open data
- Data irreversibility and reduction
- Harnessing heterogenous resources
- Highly collaborative globally distributed data management

# FAIR@GSI Online data 30 EB

FAIR@GSI Physics 300 PB BBPB generation and the second second

worldwide

3,000PB (3EB)

rvey

ta 90

Low

420EB

**HL-LHC** 

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<sup>/</sup> Challenges

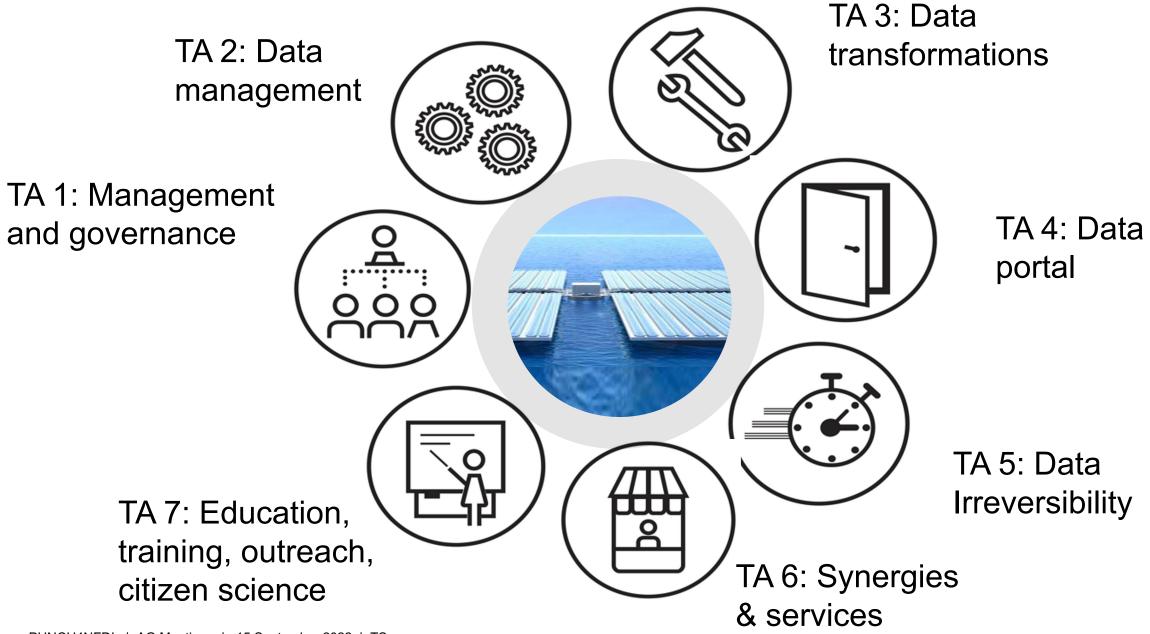
- FAIRification: data & workflows
- "big data" and "open data"

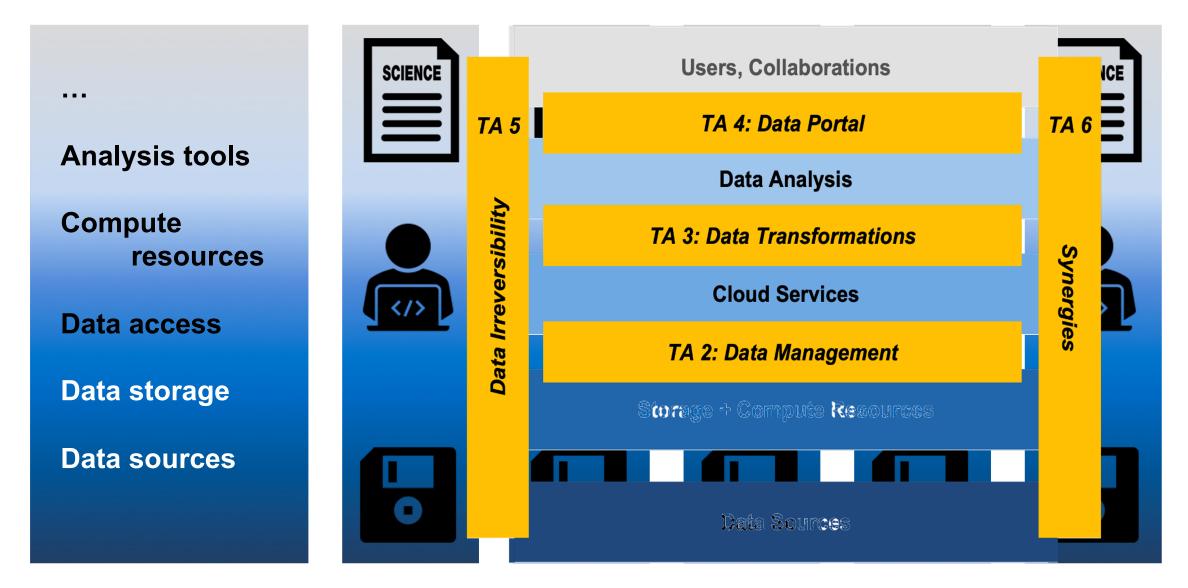
4EB

SKA1 mid archive

- Irreversibility challenge and data loss
- heterogeneous data & infrastructures
- transfer of knowledge

# **Task Areas**

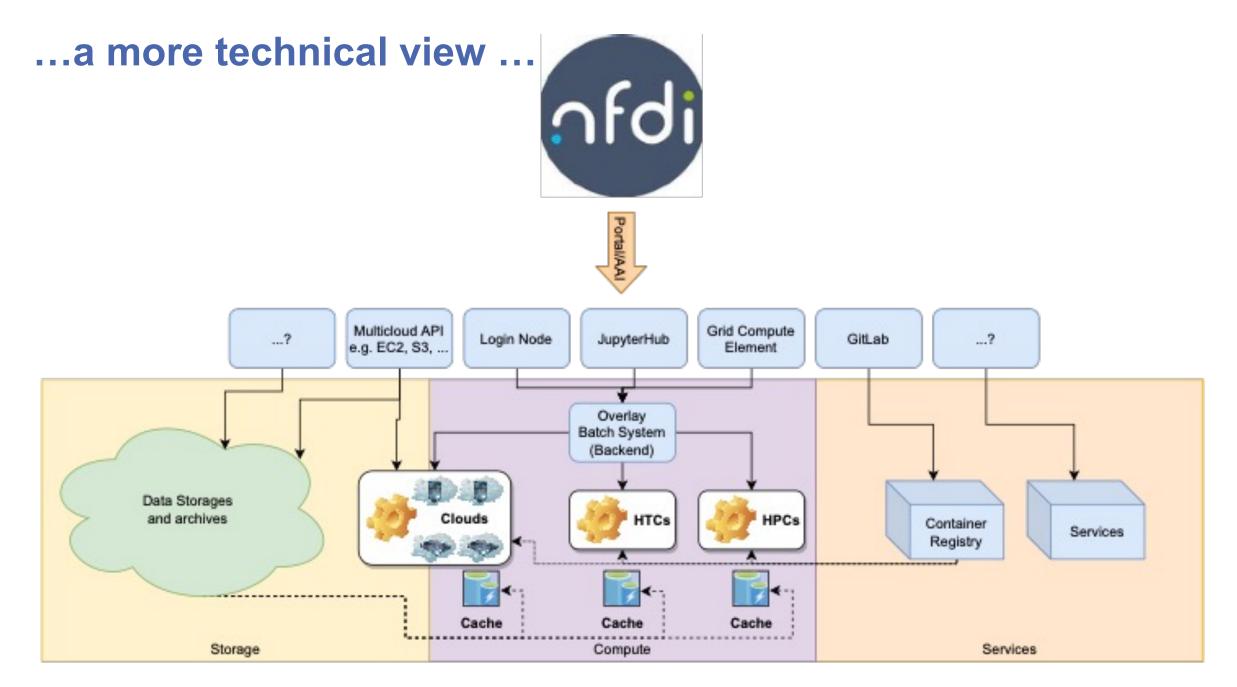




Flexibility, efficiency, scalability:

data volumes, number of users and analyses, heterogeneous resources; data combinations







# **The PUNCH4NFDI Marketplace**

Addressing fundamental problems of daily work

## Scientists want software or tutorials



A platform for collecting & managing requests:

- Users create requests
- Users search and comment requests
- Users vote for requests  $\rightarrow$  impact?
- Advantage for PUNCH4NFDI:
- No need to develop  $\rightarrow$  use existing resources
- No need to host anything  $\rightarrow$  cheap and easy
- Content can be generated from now now!

# inefficient:

- lots of manpower in the scientific community
- but also lots of parallel development

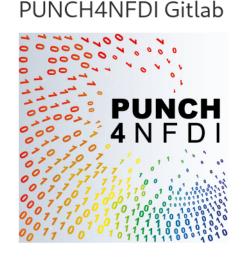
## instead:

coordinate creation of desired software/tutorials

| UNCH4NFDI<br>Questions Unanswered Tags Users Ask a<br>Iarketplace   | Question                          | *  |
|---|-----------------------------------|--|
| Recent questions and answers  |                                   | 8  |
| how do we bring Compute4Punch into service level ?<br>asked Jan 7 in Software by Kilian Schwarz   @ 3 views   | <ul> <li>▲ O O answers</li> </ul> | Search   |
| software services   |                                   | Welcome to PUNCH4NFDI<br>Marketplace, where you can ask                  |
| fast compression of 8 bit MeerKAT/SKA data         asked Dec 15, 2021 in Software by landessternwarte (180 points)   @ 3 views         library       compression         c       c++         radio data   | ↑ +1<br>∨ vote 0<br>answers       | questions and receive answers<br>from other members of the<br>community. |
| How to download Meerkat data?<br>asked Nov 22, 2021 in Tutorials by landessternwarte (180 points)   @ 1 view<br>data meerkat  | <ul> <li>○ 0 o answers</li> </ul> | All categories Software  |
| How to analyze HESS data with gammapy?         asked Nov 19, 2021 in Tutorials by landessternwarte (180 points)   @ 2 views         tutorial       data analysis       hess       gamma-ray       gammapy | ↑ +1<br>♥ vote O<br>answers       | Recent questions and answers   |
| Help get things started by <b>asking a question</b> .   |                                   |  |

# Gitlab in PUNCH4NFDI (1)

#### A multi-purpose application



#### Use the PUNCH4NFDI AAI !

| If your institution is not member / registered with<br>DFN-AAI or any other AAI |        |        |  |  |
|---|--------|--------|--|--|
| PUNCH4NFDI AAI can accommodate identification from<br>your account on           |        |        |  |  |
| ORCID   | GitHub | Google |  |  |

# Please read the Registration Instructions for the PUNCH4NFDI AAI:

https://www.punch4nfdi.de/sites/sites\_custom/site\_punc h4nfdi/content/el17438/el42359/el49152/PUNCH-AAIregistration.pdf

| Password     |          |            |
|--------------|----------|------------|
| Remember me  | Forgot y | our passwo |
|              | Sign in  |            |
|              |          |            |
| Sign in with |          |            |

## Understands OAUTH2 ( $\rightarrow$ talks with AAI)

Carries another communication tool: *Mattermost* 

### Major purposes:

- code management for software with versioning, branching, releases (tagging)
- support testing and code integration for distributed teams

#### Combined with **continuous integration (CI)**, this allows to build and manage containerised software installations

- Built-in capabilities for container registries
- Built-in registry for packages (various code languages: python, java ... )

# Combines with e.g. workflow engine REANA

# Gitlab in PUNCH4NFDI (2) PUNCH4NFDI intranet

| PUNCH4NFDI Intranet documentation  |          |    |            | (                  | edit page on gitlab |  |
|--|----------|----|------------|--------------------|---------------------|--|
| Particles, Universe,<br>NuClei and Hadrons<br>for the NFDI   |          |    |            |                    | PUNCH<br>4 N F D I  |  |
| Home Consortium NFDI TA2 TA3 TA4 TA5 TA6 TA7 Marketplace   |          | _  |            |                    |                     |  |
| Overview   |          |    |            | search (shift+f to | focus)              |  |
| The task areas of the PUNCH4NFDI consortium.   |          |    |            |                    |                     |  |
| TA 2: Data<br>management<br>TA 1: Management<br>and governance   | ₩        |    | ≡ Me       |                    |                     |  |
| TA 5: Data   | <u> </u> | 1  | 0          | Projects           |                     |  |
| TA 7: Education,<br>training, outreach,<br>citizen science   | 0        | Pr | 80         | Groups             |                     |  |
| a services   | Ē        | Re | $\bigcirc$ | Milestone          | 5                   |  |
| EScience@AIP Leibniz Institute for Astrophysics, An der Sternwarte 16, 14482 Potsdam, Germany, Tel: +49-331-7499-0 | រោ       | M  | X          | Snippets           |                     |  |
|  | B        | CI | U          | Activity           |                     |  |
|  | Φ        | Se |            |                    |                     |  |

Gitlab 'webhook' capability using md files; combined with web server application (built on Caddy software)

#### Allows for:

- collective editing of intranet content
- implementing editorial hierarchy
- fulfills all requirements of a content managing system

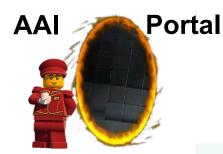
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|----------------------|---|--|---------------------------|
| Projects             | > | Q doc                                  | $\boldsymbol{\otimes}$    |
| Groups<br>Milestones | > | I intra- <b>doc</b> s-content<br>punch | itent $\Phi$              |
| Snippets             |   | I intra-docs<br>punch-dev              |                           |
| Activity             |   | I intra- <b>doc</b> s-rp<br>punch-dev  | 0 Tags 🗔 5<br>pr punch-de |

# **PUNCH4NFDI AAI**

Authentication & Authorisation Infrastructure

## Authentication: (step 1)

- should be possible via institution of PUNCH co-workers and users
- modern interface: OAUTH2 enables Identity-Providers (IdP)
  - home institution (DFN, CERN, ...)
  - ORCID
  - Google (and other Social accounts) to provide the verification of the identity (usually based on email )

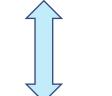


# Goal: single sign-on!

## Authorisation: (step 2)

- authenticated users get access to services
- access rights are connected by the account
  - groups
  - roles

are used to map (internally) account to access rigths



Infrastructure: Helmholtz-AAI

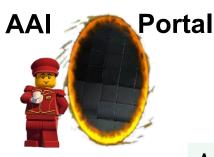
- Web interface for user
- Web interface for resource provider
- valid (web) services via API

# **PUNCH4NFDI AAI**

Authentication & Authorisation Infrastructure

Authentication: (step 1)

|  | Particles, Universe,<br>NuClei and Hadrons<br>for the NFDI<br>Assume was Mix |             |  |  |  |
|--|--|-------------|--|--|--|
|  | Login to PUNCH AAI user's home   |             |  |  |  |
|  | ORCI   |             |  |  |  |
| ou can log   | ; in using your institutional account or another account you have            | on the web. |  |  |  |
| Consorcio de Bibliotecas Universitarias de Galicia |  |             |  |  |  |
| CSŪC   | Consorcio de Servicios Universitarios de Catalunya                           |             |  |  |  |
|  | Consorcio para el disenyo, construccion y explotacion del                    |             |  |  |  |
|  | Consorcio para el Equipamiento y Explotación del Labora                      |             |  |  |  |
| (D)  | ORCID  |             |  |  |  |



### Authorisation: (step 2)

| PUNCH4NFDI Intranet documentation  | edit page on gitlab  |
|--|----------------------|
| Particles, Universe<br>NuClei and Hadr<br>for the NFDI   |                      |
| Home Consortium NEDI TA2 TA3 TA4   | TA5 TA6 TA7          |
| Marketplace Gitlab, Mattermost, Intrane<br>PUNCH   |                      |
| On 20.08.2021 an introductory session has been con<br>the <u>Ad Hoc team Collaborative Tools</u> | ducted, organised by |



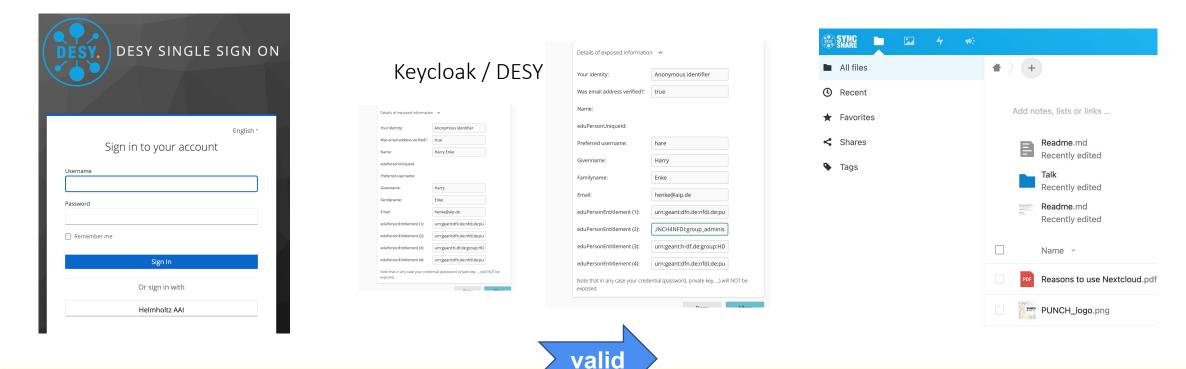
### Infrastructure: Helmholtz-AAI

- Web interface for user
- Web interface for resource provider
- valid (web) services via API

# **PUNCH4NFDI AAI**

Authentication & Authorisation Infrastructure

AuthenticatioAuthorisation info for another service with intermediate AAI instance



AAI

## Infrastructure: Helmholtz-AAI + DESY SSO

- Web interface for user
- Web interface for resource provider
- valid (web) services via API

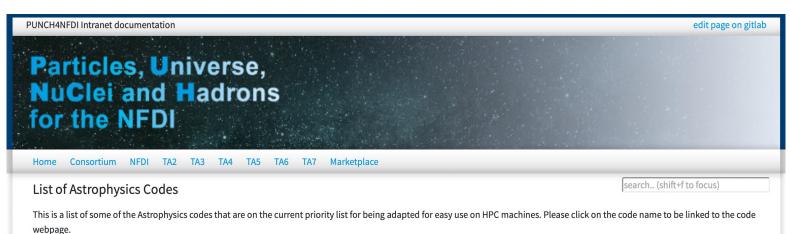
all co-workers, all users of resources resource provider register valid services (certificates, keys) draw information from AAI to provide (validated) services

Portal

# **The PUNCH4NFDI Portal**

... later entry point to the science data platform SDP

Also provided so far: collection & links of frequently used software for astro, HEP, lattice, ... in the PUNCH4NFDI intranet.



#### BHAC on gitlab.itp.uni-frankfurt.de

BHAC (the Black Hole Accretion Code) is a multidimensional general relativistic magnetohydrodynamics code based on the MPI-AMRVAC framework. BHAC solves the equations of ideal general relativistic magnetohydrodynamics in one, two or three dimensions on arbitrary stationary space-times, using an efficient block based approach.

#### • Bonsai on GitHub

Bonsai is a GPU gravitational [Barnes-Hut]-tree code. There also exists a version for SPH application.

#### • <u>CASA</u>

CASA, the Common Astronomy Software Applications package, is the primary data processing software for the Atacama Large Millimeter/submillimeter Array (ALMA) and NSF's Karl G. Jansky Very Large Array (VLA), and is frequently used also for other radio telescopes. The CASA software can process data from both single-dish and aperture-synthesis telescopes, and one of its core functionalities is to support the data reduction and imaging pipelines for ALMA, VLA and the VLA Sky Survey (VLASS).

#### CASTRO on <u>GitHub</u>

CASTRO is part of the AMReX suite of astrophysical hydrodynamics codes that collectively provide the simulation capabilities to model explosive astrophysical phenomena. Castro specializes in near-sonic and supersonic flows, where reactions can be an important driver of the dynamics. Radiation and magnetic contributions are supported. A lot of emphasis is placed on accurately coupling reactions and hydro, with a variety of time-stepping techniques available.

# Thank you!

## The PUNCH4NFDI Consortium

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