The PUNCH4NFDI Consortium

Particles, Universe, NuClei and Hadrons for the NFDI

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





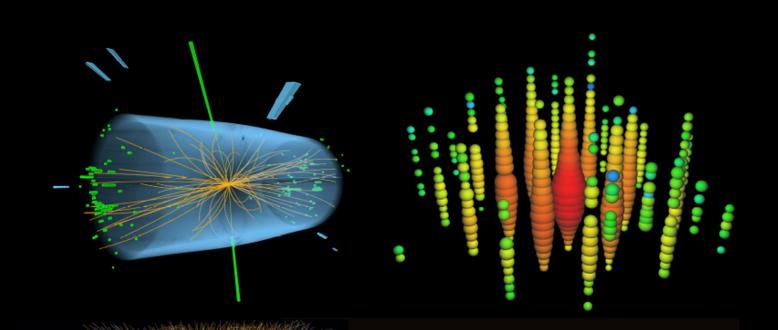
Gemeinsame Wissenschaftskonferenz GWK

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)

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Low

420EB

HL-LHC

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[/] Challenges

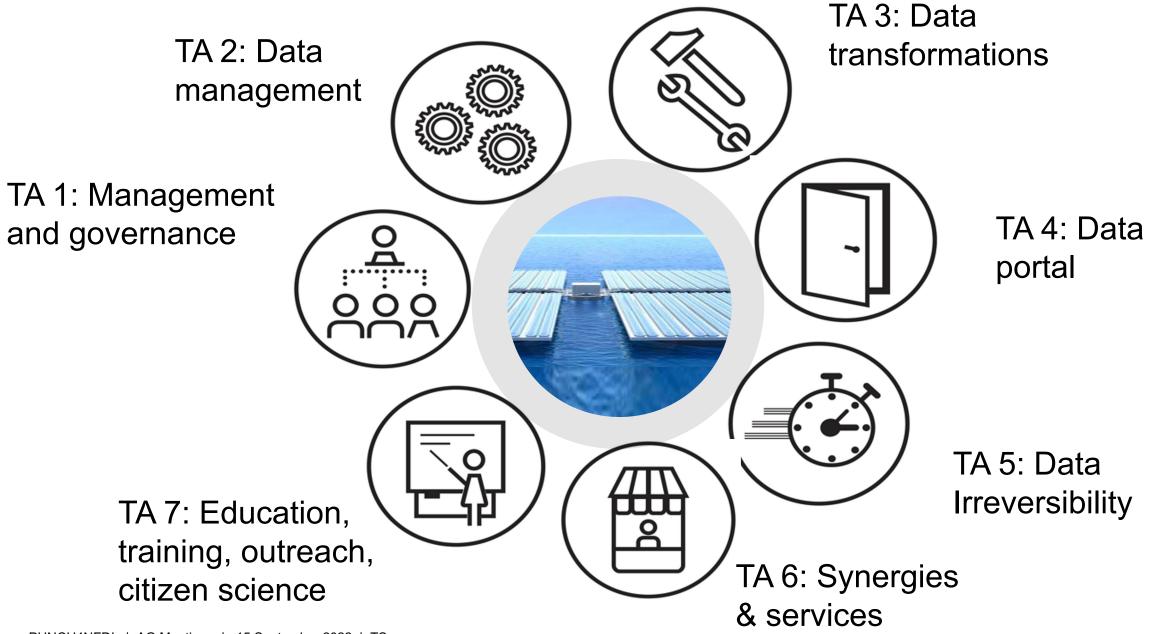
- FAIRification: data & workflows
- "big data" and "open data"

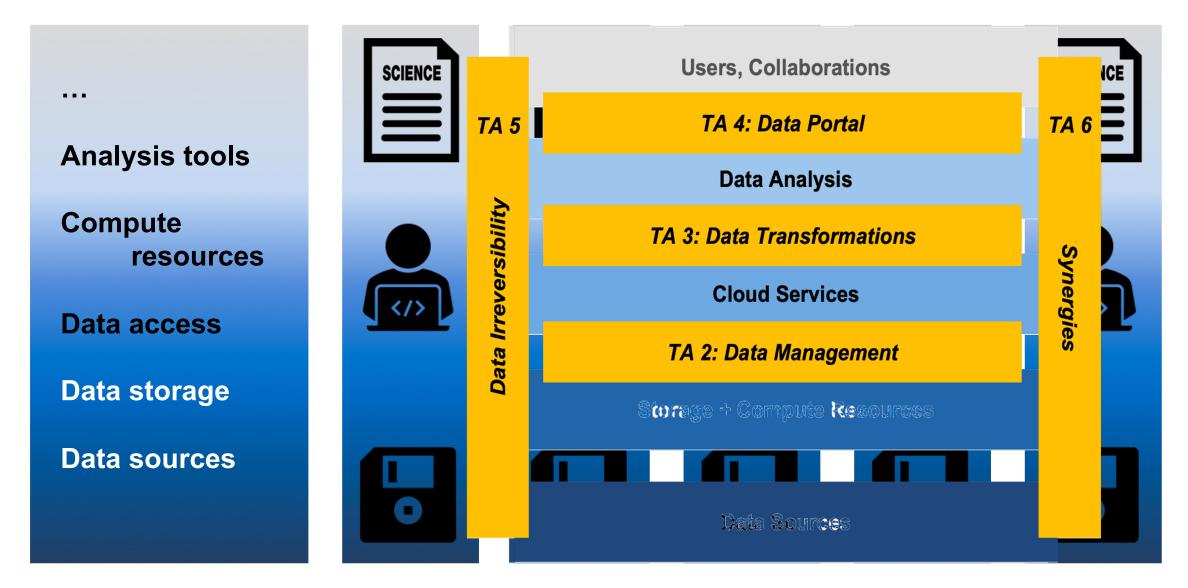
4EB

SKA1 mid archive

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

Task Areas

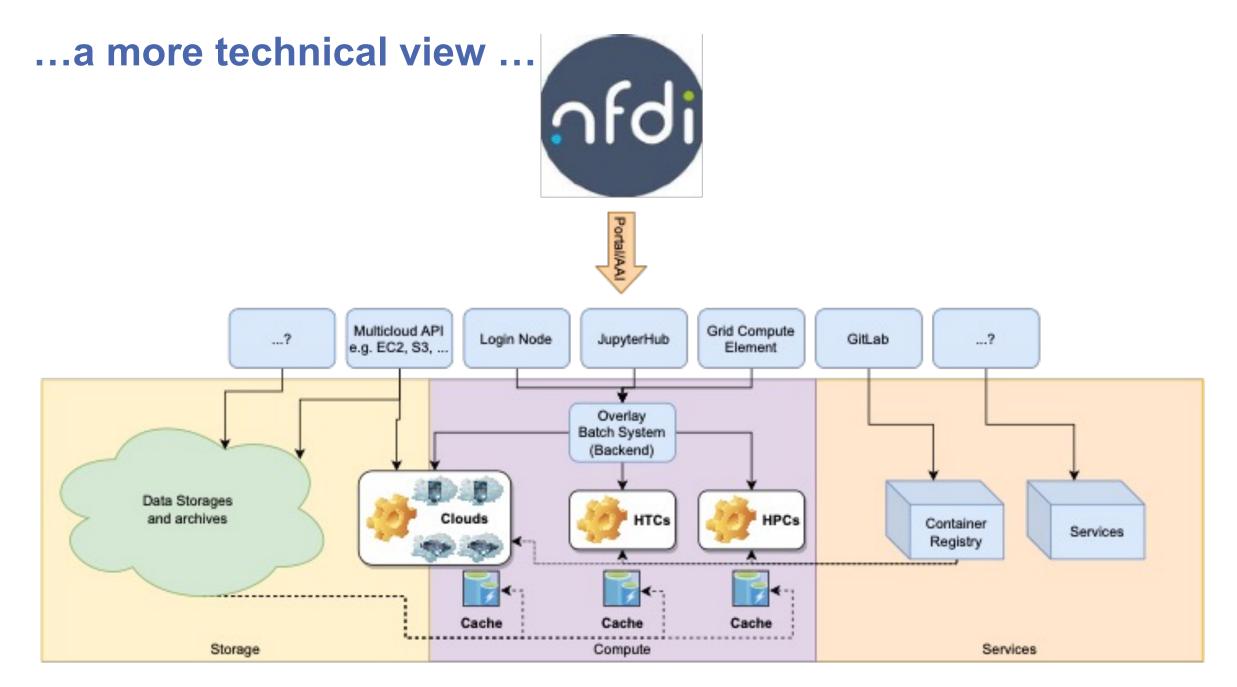




Flexibility, efficiency, scalability:

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



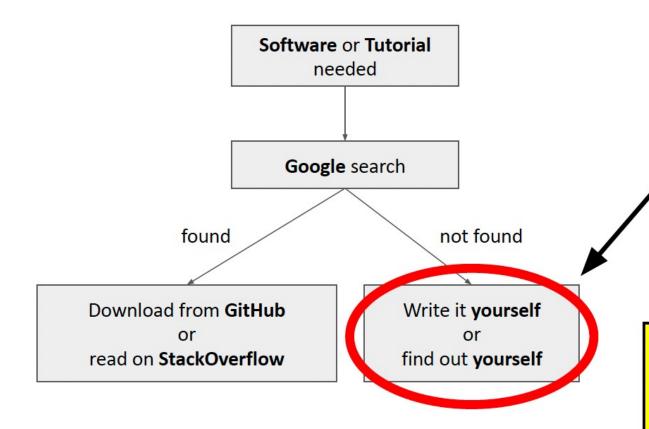




The PUNCH4NFDI Marketplace

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

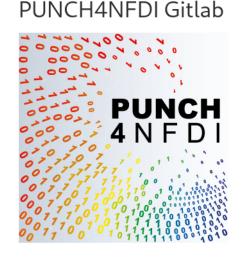
instead:

coordinate creation of desired software/tutorials

UNCH4NFDI Questions Unanswered Tags Users Ask a Iarketplace	Question	*
Recent questions and answers		8
how do we bring Compute4Punch into service level ? asked Jan 7 in Software by Kilian Schwarz @ 3 views	 ▲ O O answers 	Search
software services		Welcome to PUNCH4NFDI 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 ∨ vote 0 answers	questions and receive answers from other members of the community.
How to download Meerkat data? asked Nov 22, 2021 in Tutorials by landessternwarte (180 points) @ 1 view data meerkat	 ○ 0 o answers 	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 ♥ vote O answers	Recent questions and answers
Help get things started by asking a question .		

Gitlab in PUNCH4NFDI (1)

A multi-purpose application



Use the PUNCH4NFDI AAI !

If your institution is not member / registered with DFN-AAI or any other AAI				
PUNCH4NFDI AAI can accommodate identification from 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, NuClei and Hadrons for the NFDI					PUNCH 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 management TA 1: Management and governance	₩		≡ Me			
TA 5: Data	<u> </u>	1	0	Projects		
TA 7: Education, training, outreach, citizen science	0	Pr	80	Groups		
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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

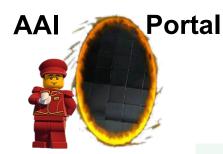
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Groups Milestones	>	I intra- doc s-content punch	itent Φ
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Activity		I intra- doc s-rp punch-dev	0 Tags 🗔 5 pr punch-de

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)

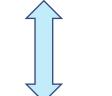


Goal: single sign-on!

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

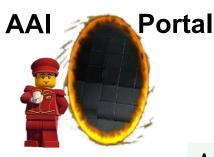
- Web interface for user
- Web interface for resource provider
- valid (web) services via API

PUNCH4NFDI AAI

Authentication & Authorisation Infrastructure

Authentication: (step 1)

	Particles, Universe, NuClei and Hadrons for the NFDI 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 NuClei and Hadr for the NFDI	
Home Consortium NEDI TA2 TA3 TA4	TA5 TA6 TA7
Marketplace Gitlab, Mattermost, Intrane PUNCH	
On 20.08.2021 an introductory session has been con the <u>Ad Hoc team Collaborative Tools</u>	ducted, organised by



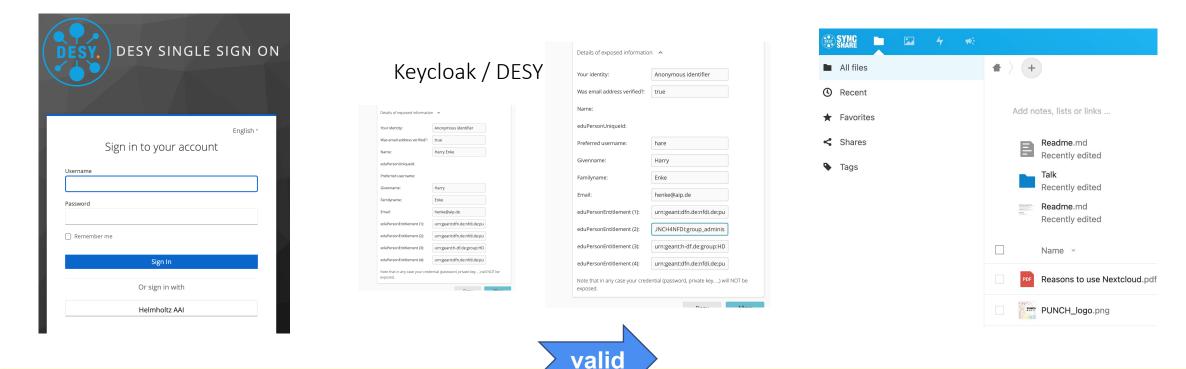
Infrastructure: Helmholtz-AAI

- 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

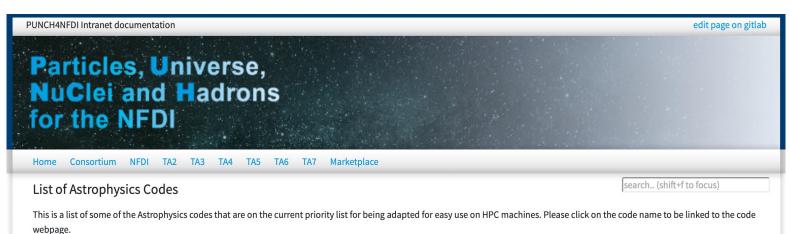
all co-workers, all users of resources resource provider register valid services (certificates, keys) draw information from AAI to provide (validated) services

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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