The PUNCH4NFDI Consortium

Particles, Universe, NuClei and Hadrons for the NFDI

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



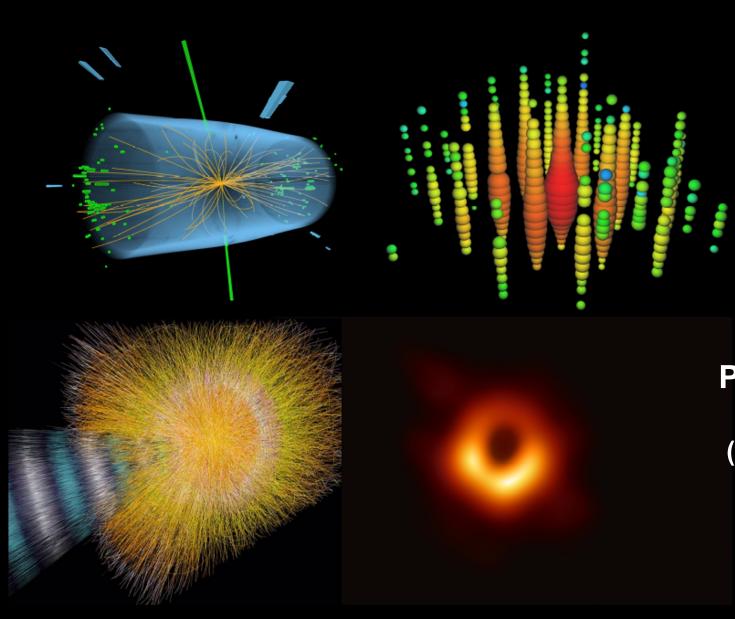




Nationale Forschungsdateninfrastruktur (NFDI)

- 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

See also DFG.de/nfdi and nfdi.de





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



















































































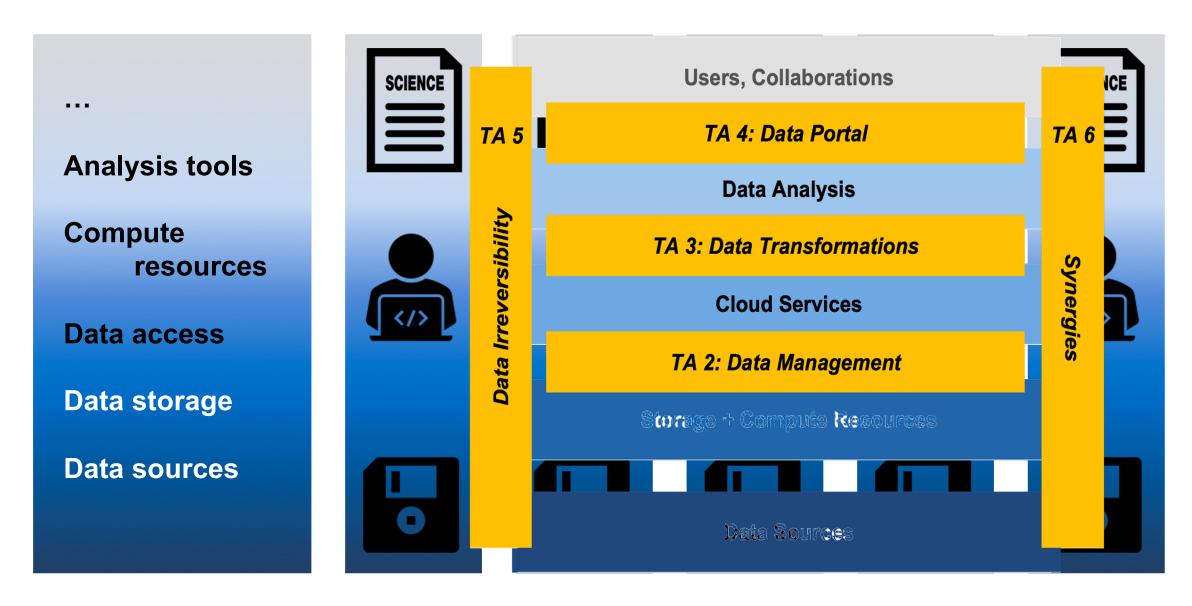






Task Areas

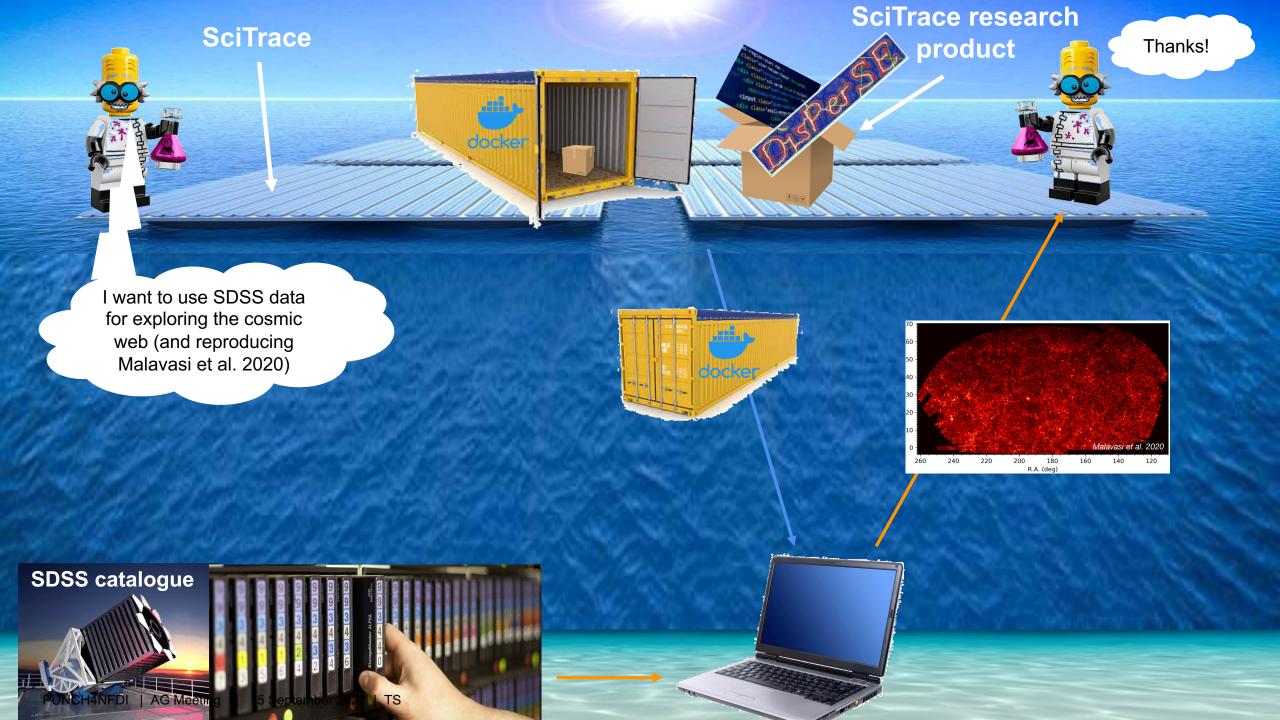
TA 3: Data TA 2: Data transformations management TA 1: Management TA 4: Data and governance portal TA 5: Data **Irreversibility** TA 7: Education, training, outreach, TA 6: Synergies citizen science & services



Flexibility, efficiency, scalability: data volumes, number of users and analyses, heterogeneous resources; data combinations



...a more technical view ... nfdi Multicloud API **Grid Compute** ...? Login Node JupyterHub GitLab e.g. EC2, S3, ... Element Overlay Batch System (Backend) Data Storages and archives Clouds **HPCs HTCs** Container Services Registry Cache Cache Cache Storage Compute Services



The PUNCH4NFDI Marketplace

Addressing fundamental problems of daily work

Scientists want software or tutorials

Software or Tutorial needed Google search not found found Download from GitHub Write it yourself or read on StackOverflow find out **yourself** A platform for collecting & managing requests:

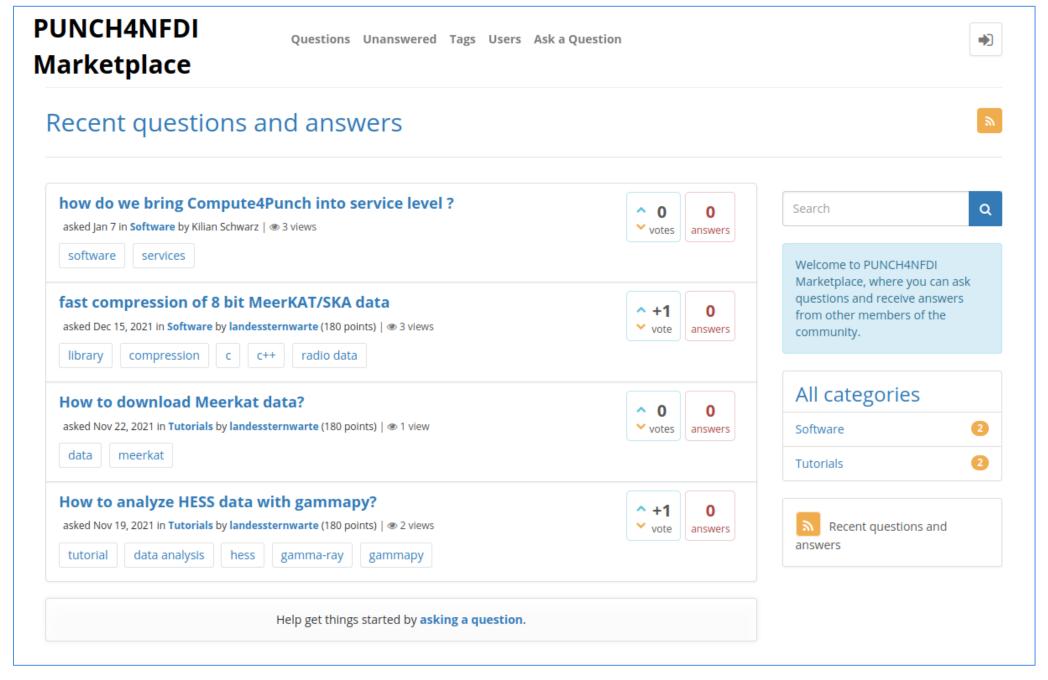
- Users create requests
- Users search and comment requests
- Users vote for requests → impact?
 Advantage for PUNCH4NFDI:
- No need to develop → use existing resources
- No need to host anything → cheap and easy
- Content can be generated from now now!

inefficient:

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

instead:

coordinate creation of desired software/tutorials



Gitlab in PUNCH4NFDI (1)

A multi-purpose application

PUNCH4NFDI Gitlab

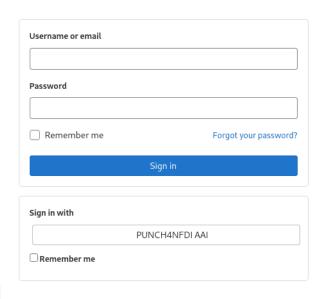


Use the PUNCH4NFDI AAI!

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/ell7438/el42359/el49152/PUNCH-AAIregistration.pdf



Understands OAUTH2 (→ 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

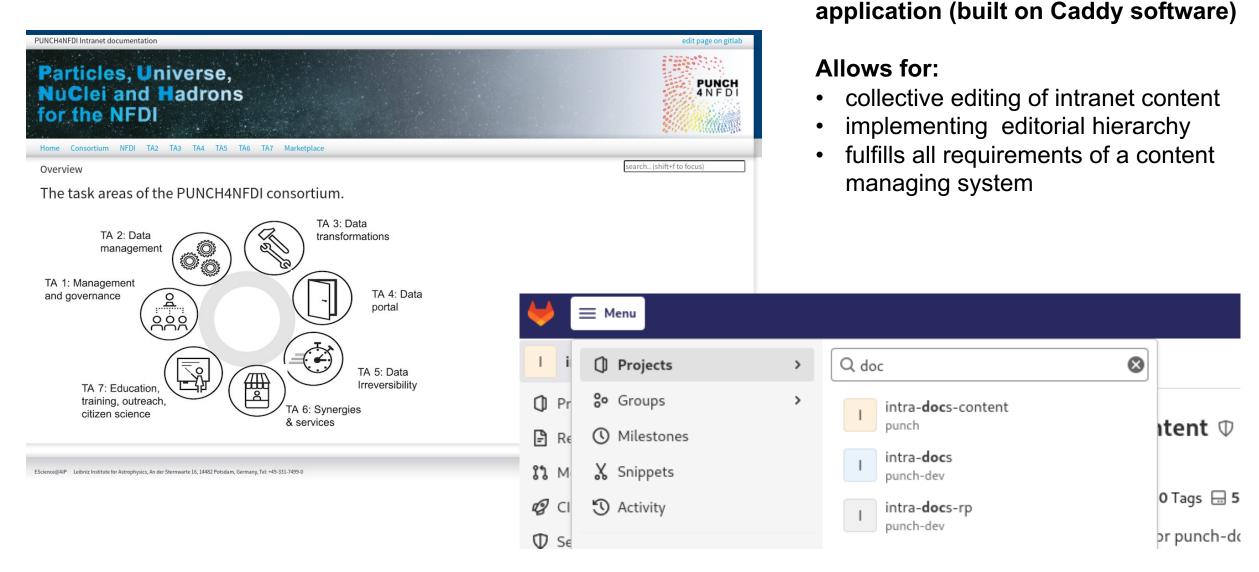
Combined with **continuous integration (CI)**, this allows to build and manage containerised software installations

- 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



Gitlab 'webhook' capability using md

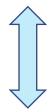
files; combined with web server

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)



Infrastructure: Helmholtz-AAI

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





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



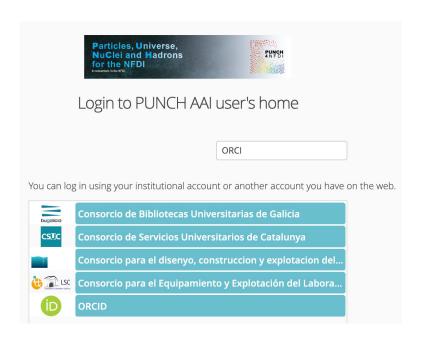


all co-workers, all users of resources resource provider register valid services (certificates, keys) draw information from AAI to provide (validated) services

PUNCH4NFDI AAI

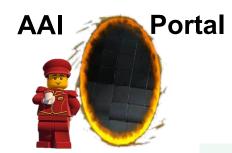
Authentication & Authorisation Infrastructure

Authentication: (step 1)



Infrastructure: Helmholtz-AAI

- Web interface for user
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Authorisation: (step 2)





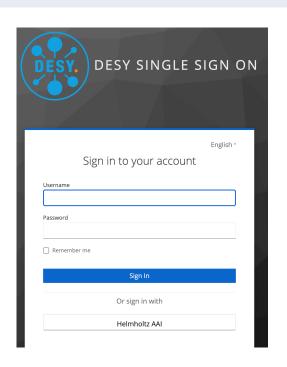
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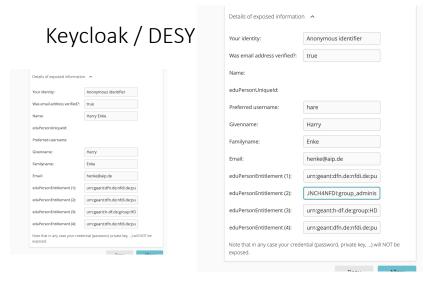
PUNCH4NFDI AAI

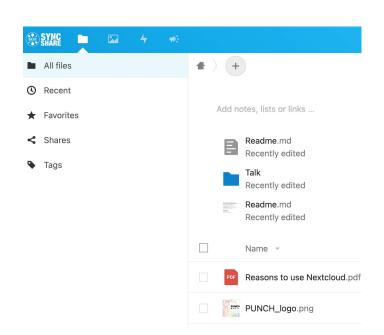
Authentication & Authorisation Infrastructure



Authenticatio Authorisation info for another service with intermediate AAI instance

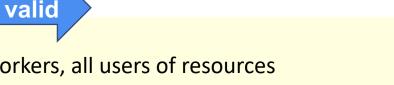






Infrastructure: Helmholtz-AAI + DESY SSO

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

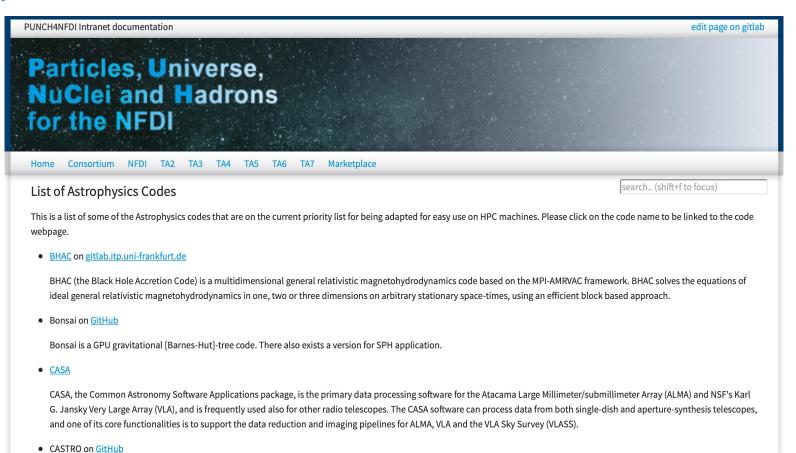


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The PUNCH4NFDI Portal

... 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.



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

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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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