Karlsruher Institut für Technologie

Latest Developments of the PUNCH4NFDI Compute and Storage Infrastructures

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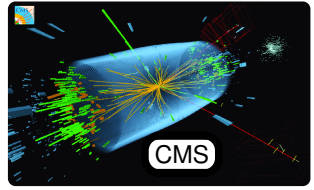
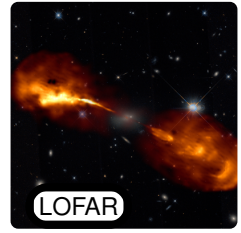
What is PUNCH4NFDI?

Consortium within the **NFDI** - National Research Data Infrastructure in Germany

Particles, **U**niverse, **N**u**C**lei and **H**adrons for the **NFDI**



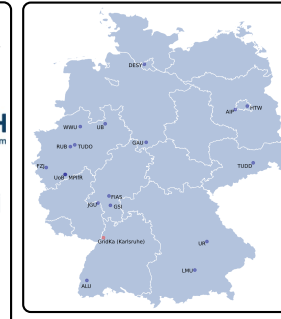


- From elementary particles to large scale structures
- **Similar challenges** with large data volume
- **Different expertise** in dealing with it

Setup a **federated** and **FAIR** science data platform

- Provide **infrastructures** to process and store **data**
  → Latest news about storage, compute and AAI
- Provide **data portal** to build and re(use) **research products**
  → Integration into analysis platform REANA

PUNCH4NFDI communities

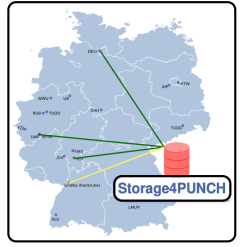


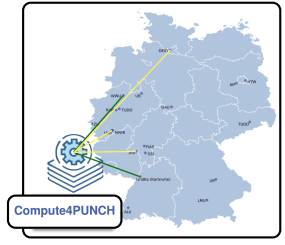
Institutions committed to providing compute and storage resources

Universities and research centers throughout Germany

Infrastructure pillars

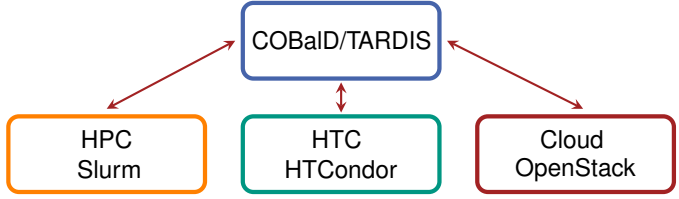
- PUNCH4NFDI has to cope with increasing amount of data and compute need
- Integrate available **storage** resources into a federated storage platform
  → **Storage4PUNCH** (Bonn, DESY, GSI, KIT)
- Federate available **compute** resources
  → **Compute4PUNCH** (Göttingen, LMU, LRZ Cloud, KIT, WWU)
- Provide **transparent access** to these resources
  → **Single entry point**
- **Secure** access to these resources
  → **Token-based Authentication**





Compute4PUNCH key ingredients

- Heterogenous compute resources with different schedulers, architectures, operating systems
- Aggregate resources in a single **Overlay Batch System** based on **HTCondor**
- Provision resources to the OBS using **COBalD/TARDIS meta-scheduler**
  $\rightarrow$ Single federated pool with dynamic extension on a user-demand basis
- **TARDIS** integrates available resources into OBS
- **COBalD** does balancing, job to resource matching, ensures effective usage

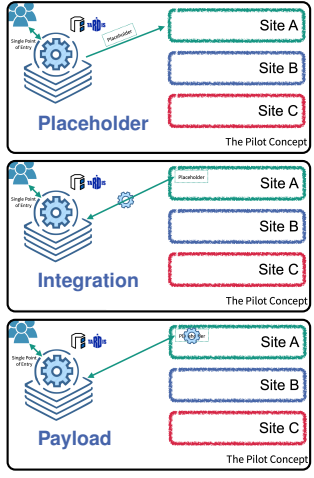


Resource provisioning and payload assignment

- Placeholder job - a drone - is submitted to the site
- Drone allocates and integrates resource into the OBS and provides a specific environment via a container
- Payload pulled from the OBS and assigned to the resource

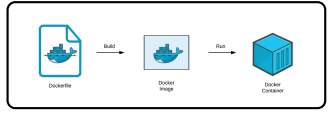
User interacts with the OBS through a single entry point:

- Login node - provided
- JupyterHub - expected soon
- OIDC token-based authentication

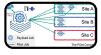


Typical analysis workflow

- Containerise analysis software
- Make it available in PUNCH4NFDI container registry
- Distribution via the CVMFS file system



- Job submission from login node 

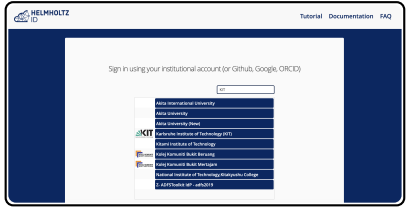
- HTCondor worker node started 

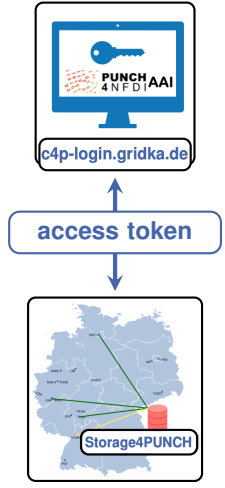
- Job executed with container retrieved from CVMFS

```
[root@c4p-login ~]# ls /cvmfs/unpacked.cern.ch/gitlab-p4n.aip.de\:5005/compute4punch/container-stacks/
caracal_container:latest          htcondor-wn:latest          simulation-wn:latest        wltg-wn:latest
caracal_container_new_stimela:latest  lincwn:latest          snakemake_arcane:latest
h4leptons:latest                  lqcd_analysis:latest        snakemake-wn:latest
```

Storage4PUNCH

- Endpoint at DESY and KIT using dCache
- Endpoints at Bonn and GSI using XRootD
- WebDav/XRootD as transfer protocol
- **Token-based access using Helmholtz AAI**





- Register once to Helmholtz AAI provider
- Once registered - access token generated with oidc-agent
- Storage4PUNCH accessed from login node

Access token

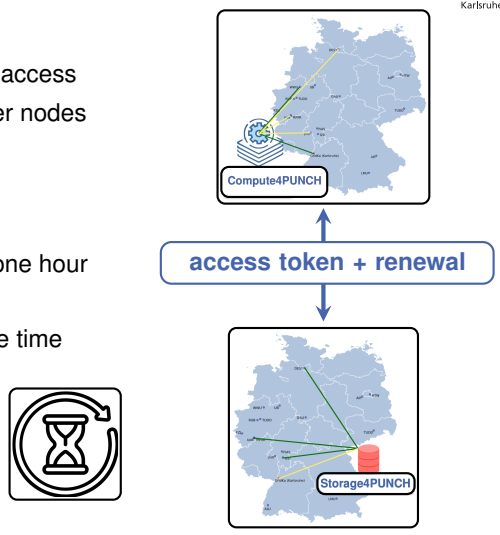
- Helmholtz AAI access tokens are mandatory to access Storage4PUNCH from Compute4PUNCH worker nodes

→ Have to be **inserted** in the HTCondor job

- Access tokens have a limited life time of about one hour

→ Have to be **renewed** for jobs exceeding their life time

→ **Need a mechanism to renew access tokens on-the-fly on the worker nodes**



Access token management

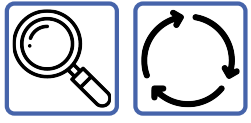
HTCondor provides a **Credential daemon (Credd)**

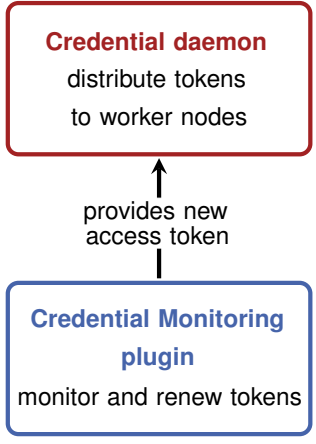
- **Agnostic** to type of tokens
- Responsible for their **distribution**

This daemon relies on **Credential Monitoring plugins (CredMon)**

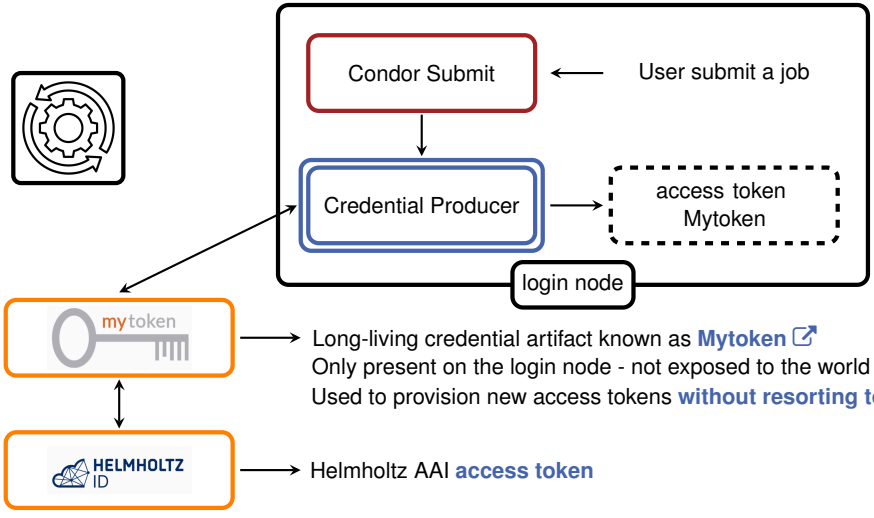
- **Specific** to type of tokens
- Responsible for their **monitoring** and **renewal**

→ **Specific CredMon plugin to monitor and renew Helmholtz AAI access tokens**

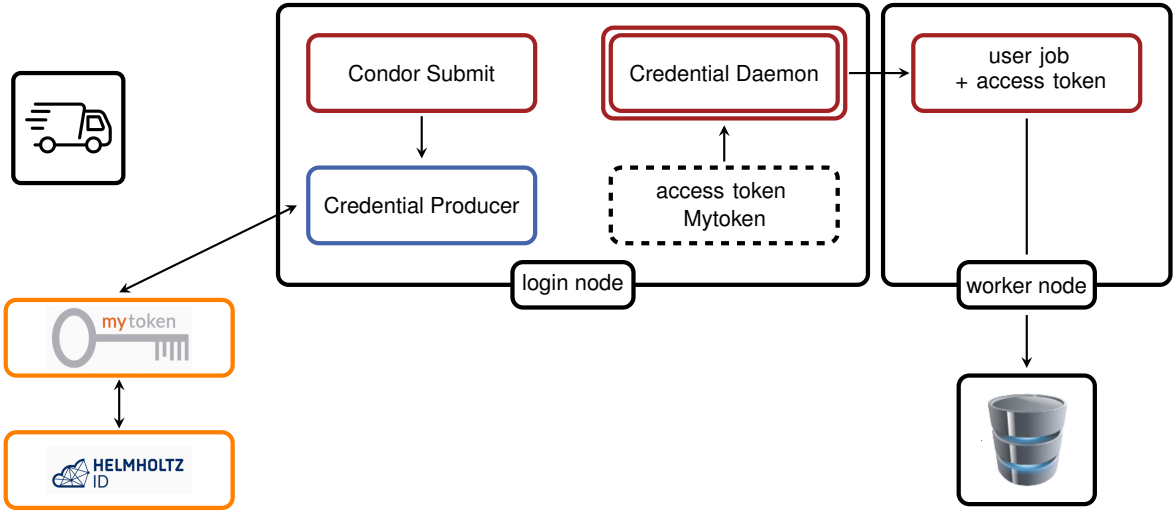




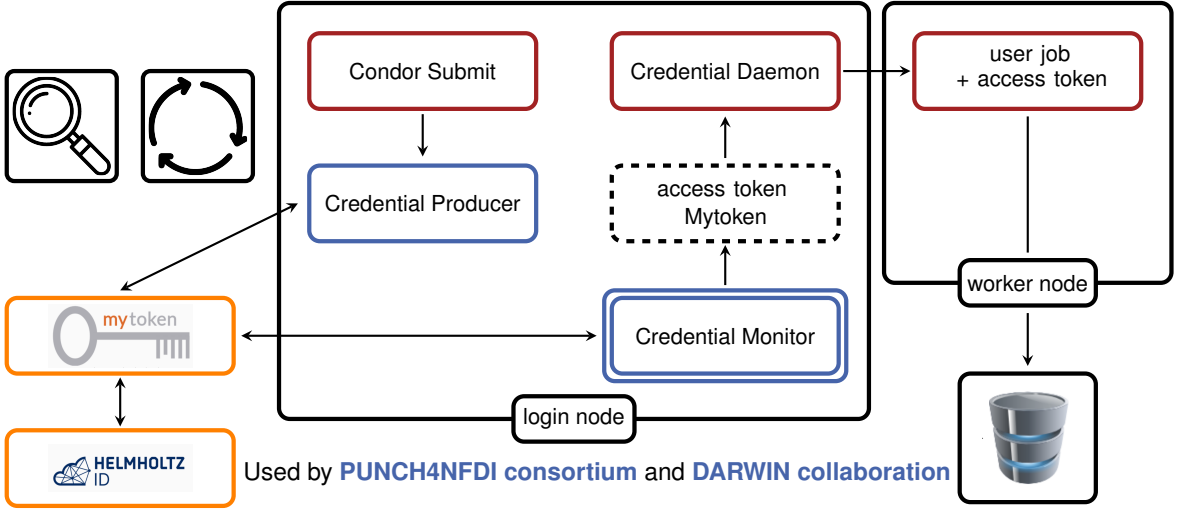
Production


Condor Submit
User submit a job
Credential Producer
access token
Mytoken
login node
mytoken
Long-living credential artifact known as Mytoken
Only present on the login node - not exposed to the world
Used to provision new access tokens without resorting to the user
HELMHOLTZ ID
Helmholtz AAI access token

Distribution



Monitoring and Renewal



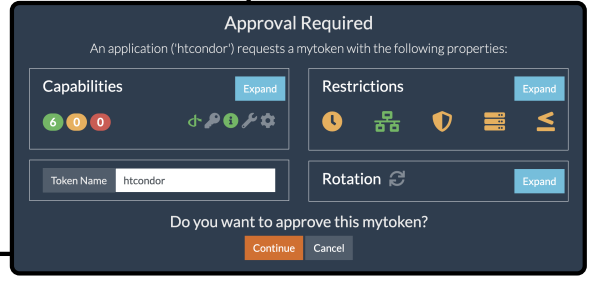
Job configuration

```
executable = analysis.sh
use_oauth_services = helmholtz  → Only need to specify AAI prodiver
should_transfer_files = YES
output_destination =
helmholtz+https://dcache-desy-webdav.desy.de:2880//pnfs/desy.de/punch/analysis
output = logs/$(machine).$(cluster).$(process).out
error = logs/$(machine).$(cluster).$(process).err
log = logs/$(machine).cluster.log
request_cpus = 1
request_memory = 256
+SINGULARITY_JOB_CONTAINER = "analysis:latest"
queue 1
```

Job submission

```
condor_submit analysis.jdl
Submitting job(s)
Hello benoit_roland!  You are going to submit your HTCondor jobs.
No credential has been found!
Please visit the following url in order to generate your credential:
https://mytoken.data.kit.edu/c/XWSdsgNC
Starting polling and waiting for your approval...
Your credential has been successfully created!
Its remaining life time is 6 d 23 h 58 m 46 s.
1 job(s) submitted to cluster 1142
```

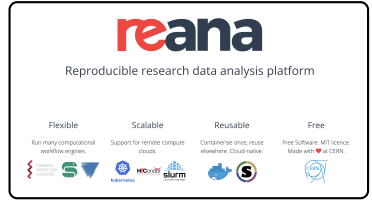
→ **Visit specified URL and approve Mytoken**



REANA overview

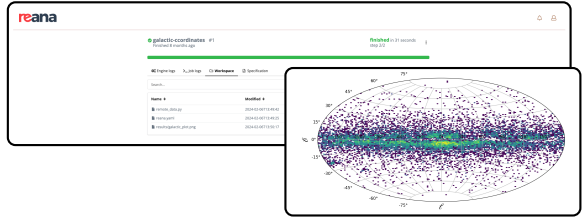
PUNCH4NFDI Data Portal → Single entry point to Research Products

- Data, metadata, software
- Workflow description and history
- Results and publication



Reproducible research data analysis platform REANA → Build Reproducible Research Products

- Supports various computational workflow engines
- Container-based workflow
- User-friendly CLI client and GUI



PUNCH4NFDI REANA server hosted at AIP in Potsdam

Integration in REANA

Scalable compute model and several compute backends known as Job Controllers

- Responsible for job execution and management
- Available for HTCondor, Slurm and Kubernetes
- HTCondor compute backend based on Kerberos tickets

→ **Developed HTCondor Job Controller based on OIDC tokens**

- Produce and upload Mytoken credential to REANA server
- Upload from server to login node for job submission
- Execute and manage HTCondor job on Compute4PUNCH

Different steps fully automated

Job Controller in production and in REANA stable release soon

Summary

- Overview of Compute4PUNCH and Storage4PUNCH latest developments
- Implementation of access token management in HTCondor
- Used by PUNCH4NFDI consortium and DARWIN collaboration
  See presentation on the DARWIN infrastructure by Robin Hofsaess earlier this week
- Integration of Compute4PUNCH into REANA analysis platform

Thanks a lot for your attention!

References

- **FLATICON** - Free Icons and Stickers for your projects.
- Max Fischer, Eileen Kuehn, Manuel Giffels, Matthias Schnepf, Stefan Kroboth, Thorsten M., Oliver Freyermuth. **MatterMiners/cobald (0.14.0) 2023.**
- Manuel Giffels, Max Fischer, Alexander Haas, Stefan Kroboth, Matthias Schnepf, Eileen Kuehn, P. Schuhmacher, Rene Caspart, Florian von Cube, Peter Wienemann. **MatterMiners/tardis (0.8.2) 2024.**

- **CVMFS** - CERN Virtual Machine File System.
- **Mytoken** - Web service to provide OIDC access tokens to long-running compute jobs.
- **C4P-HTCondor** - HTCondor with OIDC access tokens monitoring.
- **REANA** - Reproducible research data analysis platform.
- **REANA Compute4PUNCH Job Controller** - HTCondor Job Controller with OIDC access tokens.

Job submission, production and monitoring

- Next job submission

```
condor_submit analysis.jdl
Submitting job(s)
Hello benoit_roland!  You are going to submit your HTCondor jobs.
A valid credential has been found with a remaining life time of 5 d 4 h 3 m 12 s.
1 job(s) submitted to cluster 1155.
```

- Mytoken standalone production also possible - allow automated job submission afterwards
- Monitoring also handles access token revocation
- User informed at submission time when Mytoken life time below 1 day