Karlsruher Institut für Technologie

PUNCH 4NFDI

PUNCH 2.0 preparation meeting - Compute Work Package

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Compute in PUNCH 2.0

- Global picture
- Main deliverables
- Collaboration with Work Packages and Use Cases
- Involved institutions and FTEs

What we aim to provide

- **Federated Distributed Heterogeneous Compute Cloud**
  - Support HTC resources, single-node parallelism and distributed framework
  - Ease access to HPC resources for large-scale multi-node parallelism
  - Support local data access through site-specific storage systems
  - Support and extend entry points - user interfaces
  - Support data and software management
  - Support scalable and reproducible software deployment

Main deliverables

- **Extend computing infrastructure**
- **Ease access to computing resources**
- **Support data management**
- **Support software management**
- **Support software deployment**

Extend computing infrastructure

- **Support HTC and Cloud resources**
- **Ease access to HPC resources using PUNCH AAI**
  - Support Use Cases requiring large-scale multi-node parallelism
- **Support distributed frameworks** - Dask
- **Support local data access through site-specific storage systems** - S3, parallel file systems
  - Mapping to local user account
- **Better exploit and extend our GPU resources**
  - Image processing - in astronomy - better served by GPUs

Ease access to computing resources

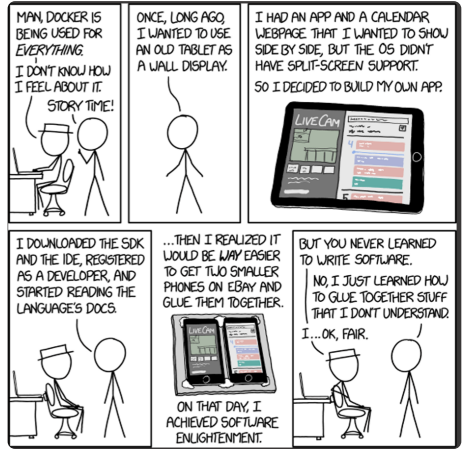
- **Extend and diversify our entry points**
  - Login nodes
  - JupyterHub
  - REANA
  - Grid Compute Element

Support data management

- **Support online storage**
  - To store, share and synchronise data between different machines
  - Mounted on login node if needed
- **Automate transfer to and from storage resources**

Support software management

- **Software management missing in PUNCH**
  - Prevent respect of FAIR principles
  - Showstopper for deployment and scalibility
  - Showstopper for builidng DRP
- **Overview of the LOFAR software and how to use it**
  Frits Sweijen - Durham University - LOFAR Data School 2024
- **LOFAR supports containerisation and versioning**
- **PUNCH should support software management as well**



Support software deployment

- **Dedicated container registry with automated CI/CD workflow**
- **Reproducible software deployment based on CVMFS**
- **Ensure scalable distribution of software across computing sites**

Collaboration

- **With the various Use Cases**
- **With the section "Common Infrastructure"**
  - IAM4NFDI
  - Software4NFDI
  - Jupyter4NFDI
- **With the DRP and SDP communities - workflows, analysis tools**
- **With the EESSI project - European Environment for Scientific Software Installations**

Involved institutions and FTEs

- **Current institutions having expressed their interest: 4 FTEs in total**
  - KIT: 1 FTE
  - FZJ: 0.5 FTE
  - TLS: 1 FTE
  - Göttingen: 0.5 FTE
  - DZA: 1 FTE
- **External partners to access HPC resources**
  - National High-Performance Computing Centres - NHR

Discussion

- **Distribution of tasks and commitments**
- **Start discussing early to identify priorities**
  - With the different Use Cases
  - With the DRP and SDP communities
  - With the section Common Infrastructure
- **Funding and distribution of tasks should be flexible**
  - Adpat to the needs of the consortium