Leibniz-Institut für
Astrophysik Potsdam

Astrophysics in PUNCH communities

Common and different data management approaches

H. Enke | EURO-LABS | 27.02.2024

The PUNCH4NFDI Consortium

Particles, Universe, NuClei and Hadrons for the NFDI

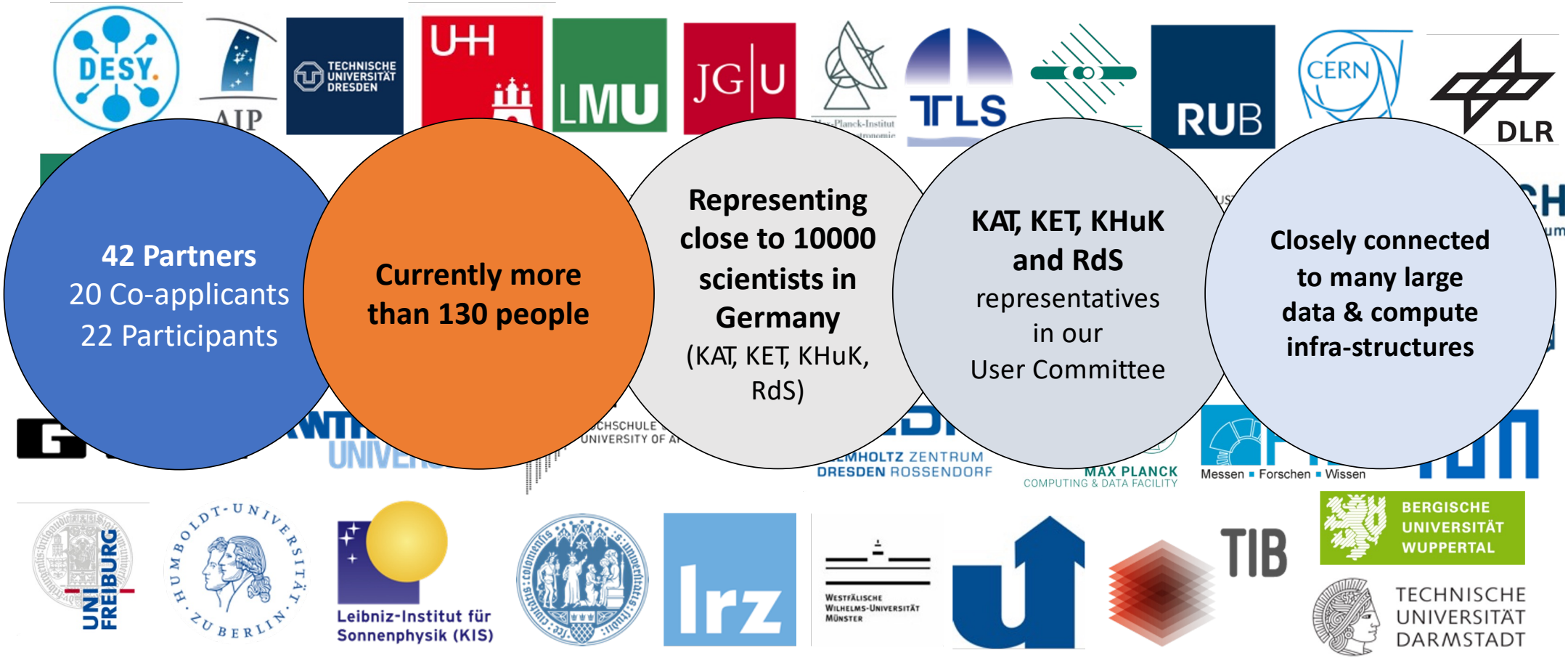
Harry Enke, TA4 AIP

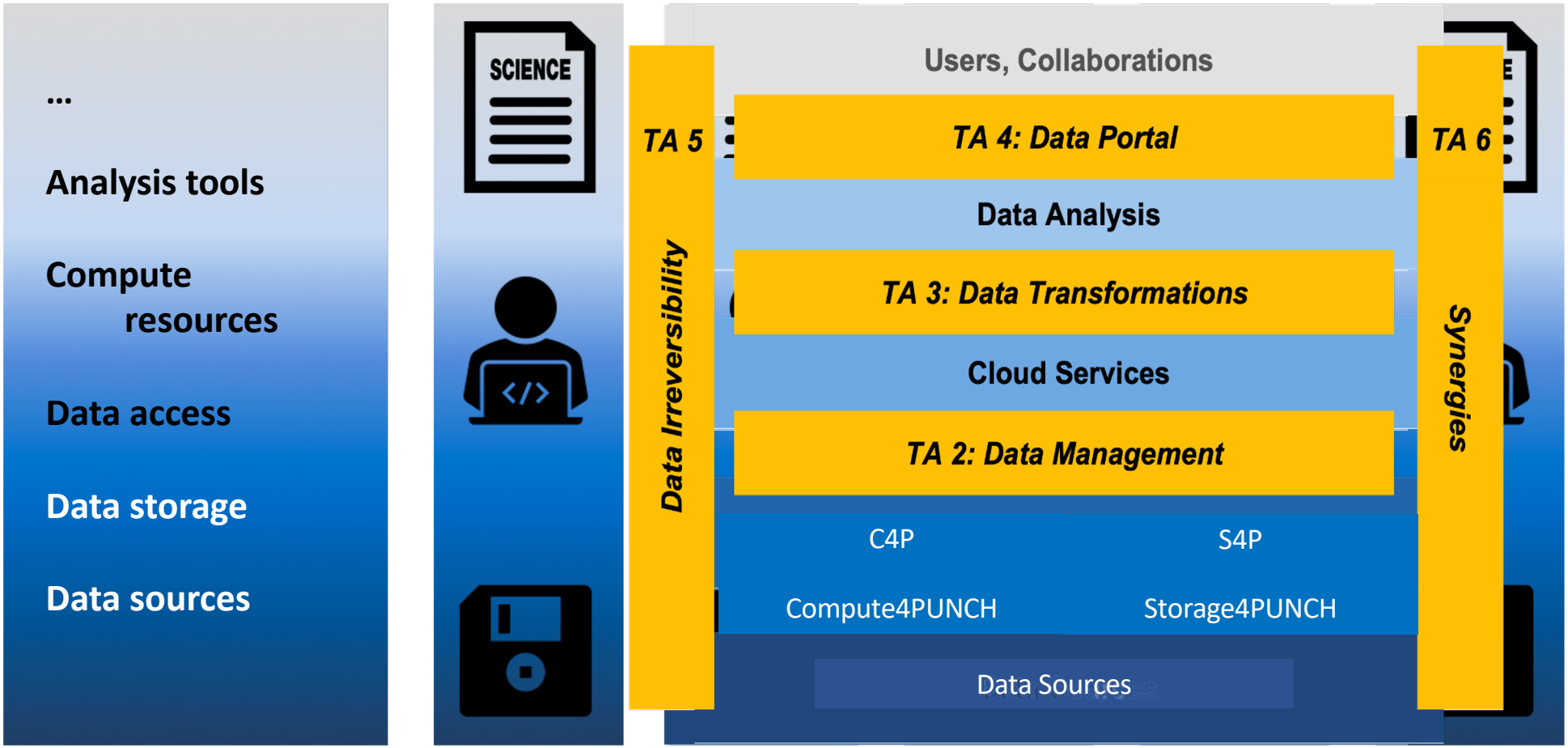
~~General Meeting, München, 12+13 October 2023~~

(EURO-LABS, brief detour)

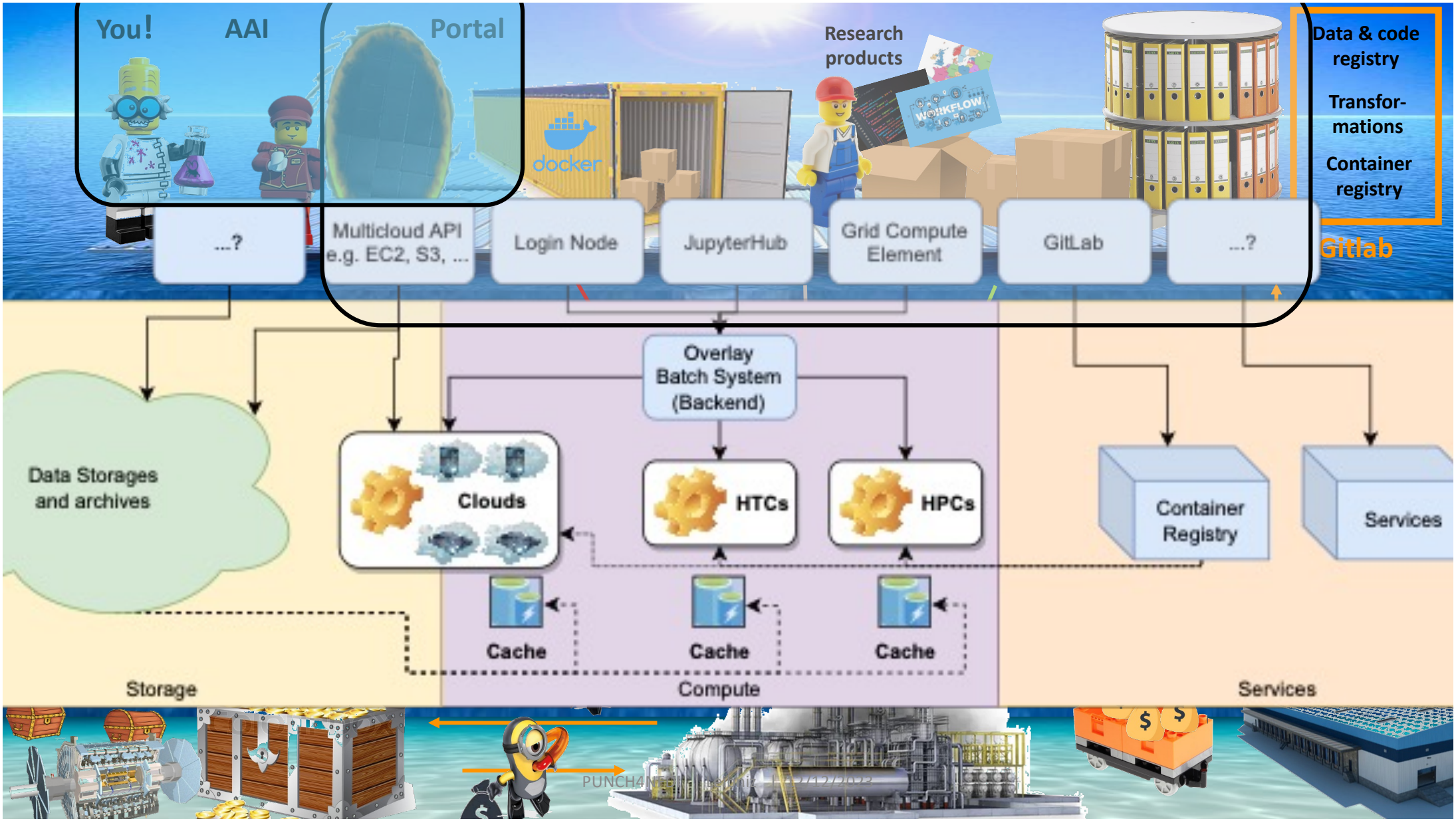
Who We Are

Universities, Helmholtz, Max Planck, Leibniz





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


You!
AAI
Portal
Research products
Data & code registry
Transfor-mations
Container registry
docker
WORKFLOW
...?
Multicloud API e.g. EC2, S3, ...
Login Node
JupyterHub
Grid Compute Element
GitLab
...?
Gitlab
Overlay Batch System (Backend)
Data Storages and archives
Clouds
HTCs
HPCs
Container Registry
Services
Cache
Cache
Cache
Storage
Compute
Services

Communicating Scientific Results

Collecting Data

Astronomy

Calendars, Tables of planetary movements and star constellations

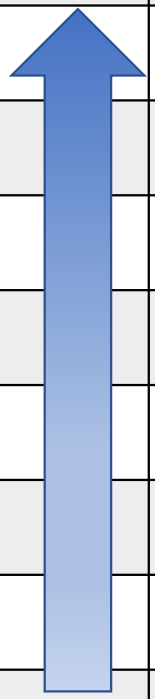
Babylonian astronomers developed arithmetical techniques for calculating astronomical phenomena;

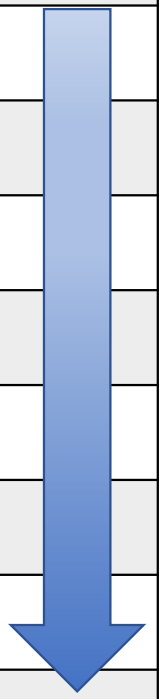
Hipparchus produced geometric models for calculating celestial motions.

Ptolemy claimed to have derived his geometrical models from selected astronomical observations by his predecessors spanning more than 800 years. (Almagest)

Data Storage: Capacity vs. Duration

Material	**Durability**	**Capacity** {assuming UTF8}
Clay & Stone	thousands of years	~ 200 char = ~800 Byte
Papyrus	100 .. N*1000 years	~ 500 char= ~2000Byte
Vellum	100.. 1000 years	~ 1000 char= ~4000 Byte
Paper {sheet} **Book**	50 ... N*100 years	~ 6000 char= ~24000Byte = ~24KB ~ 100 pages = ~2.4 MB
Floppy Disk **CD/DVD**	< 5 years < 7 years	~ 512 KB .. 1440 KB < 1 TB
Tape (LTO9)	10..15 years	~ 45 TB
Hard Disk	< 10 years	24.0++ TB
SSD	< 10 years	~ 218 TB





Astronomy - Data History

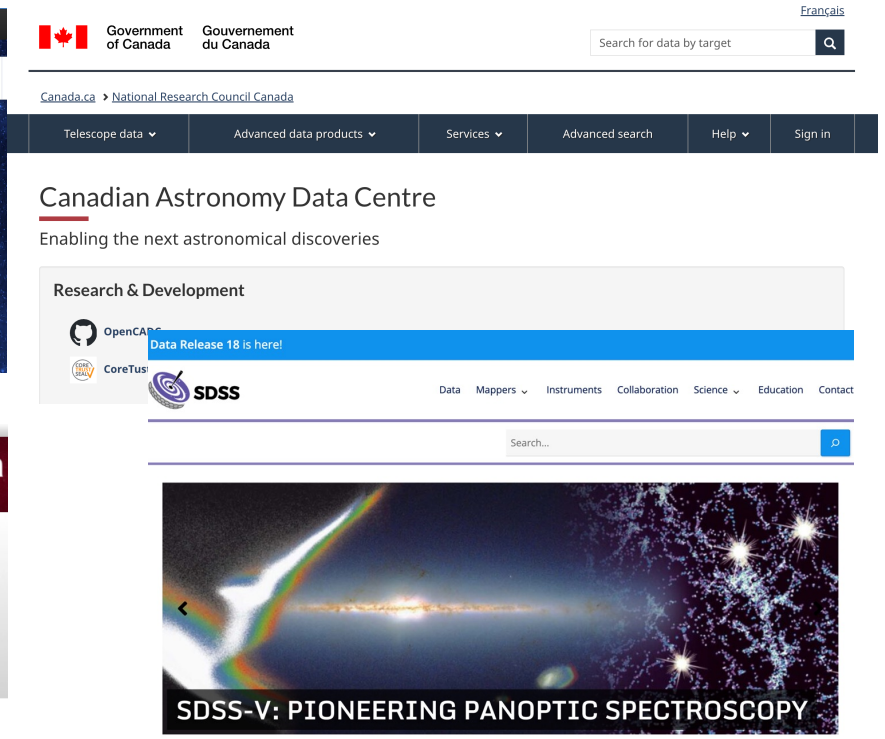
Important historical star tables

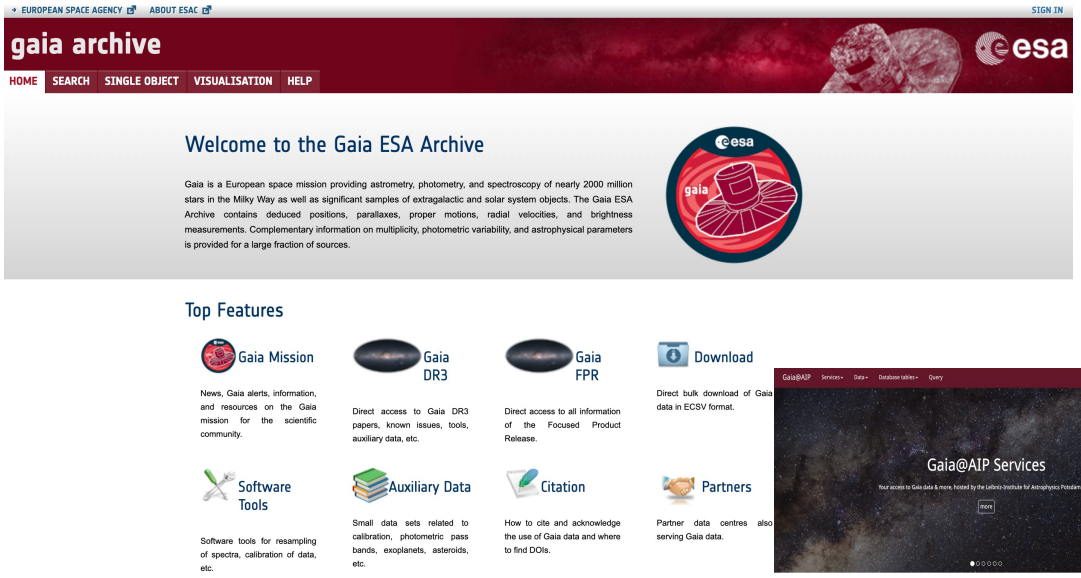
* ca **150**, *Almagest* – contains
  last known star table by Ptolemäus, **1028 Stars**
* **1627**, *Rudolphinische Tabellen* – Kepler,
  first mediavael star table based on measurements of Tycho Brahe **1005 Stars**
* **1690**, *Prodromus Astronomiae* –
  by Johannes Hevelius for his Firmamentum Sobiescanum, **1564 Stars**
* **1725**, *Britannic Catalogue* –
  John Flamsteed for his Atlas Coelestis, Positions of more than **3,000 Stars**
  10“ precision
* **1903**, *Bonner Durchmusterung* –
  by Friedrich Wilhelm Argelander et al., ~ **360,000 Stars**
  (tables of apparent Magnitudines and Positions)

Astronomical Surveys {data sizes}

Year	Survey	Data sizes	Content
1994	Digitzed Sky Survey	~73 Gigabyte	Digitized Photoplates
2001	Catalog of DSS	~16 Gigabyte	89 Mio. Objekte
1997-2001	2 Micron All Sky Survey(2MASS)	~200 Gigabyte	300 Mio. point sources and 1 Mio. extended sources
2000-2006	Sloan Digital Sky Survey	~10 Terabyte	100 Mio. Objects + 1 Mio. Spectra
Start: 2025	LSST (Vera Rubin Observatory)	20+ Terabyte / Night	Images of southern sky w. 3200-megapixel CCD array

Astrophysical Databases connected to the IVOA registry





In total, currently are
27935 services* for astrophysical data registered at the VO registry of databases.

* Table Access Protocol

Data management – Virtual Observatory (2001 -)

Multi-Wavelength Astronomy

- Combine observations from the whole range of the EM spectrum and gravitational wave

International Virtual Observatory Alliance (IVOA):

- **Standards** for
  - Publication of data collections
    - calibrations and units
    - Metadata for machine readable descriptors
- **Protocols**
  - Using HTTP – REST API
  - Table Access Protocol (TAP)
  - Using SQL for selection of data (ADQL => custom dialect)
- Implementation of server and client applications

- Implementation of Registry for data collections
  (based on OAI-PMH Protocol)

IVOA Standards and Protocol specifications (https://www.ivoa.net/documents/index.html)

From inception to now (11/2024)

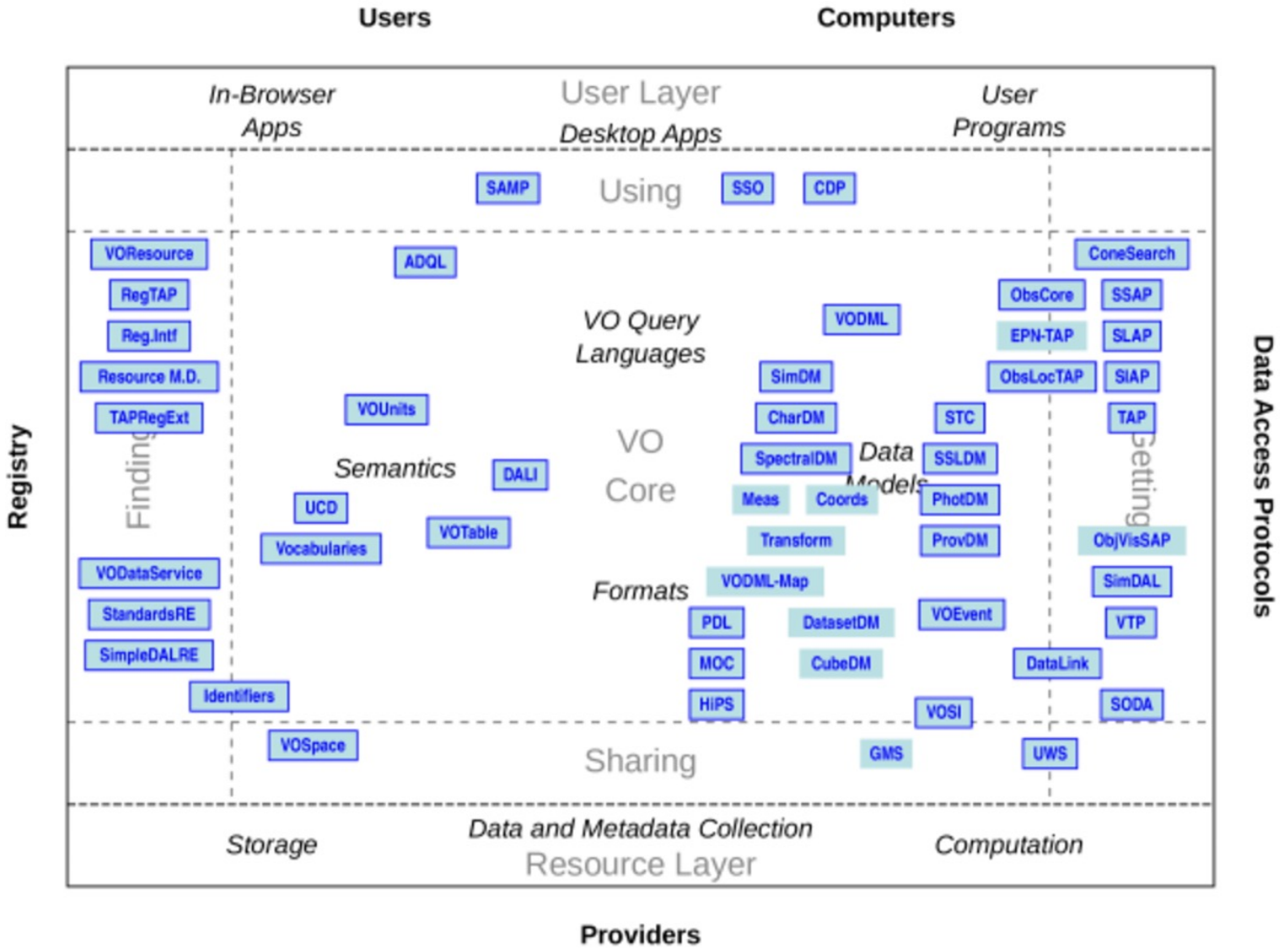
* development through international meetings and collaborations
* solid connections with IAU, the ‘older’ body of international Astronomy collaboration
* working with important international projects

Technical Specifications

Group	Title	Most stable	In progress	Version history
App	SAMP - Simple Application Messaging Protocol	1.3		1.3 1.3 1.3 1.3 1.3 1.2 1.2 1.2 1.11 1.1 1.10 1.00
	VOTable - VOTable Format Definition	1.4	RFC	1.5 1.5 1.5 1.5 1.4 1.4 1.4 1.4 1.4 1.4 1.3 1.3 1.3 1.2 1.2 1.2 1.20 1.20 1.10 1.00
	MOC - HEALPix Multi-Order Coverage Map	2.0		2.0 2.0 2.0 2.0 2.0 2.0 2.0 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0
	HiPS - Hierarchical Progressive Survey	1.0		1.0 1.0 1.0 1.0 1.0 1.0 1.0
DAL	DALI - Data Access Layer Interface	1.1	1.2	1.2 1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	DataLink	1.1		1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	Simple Cone Search	1.03	1.1	1.1 1.03 1.02 1.01 1.00
	SIA - Simple Image Access	2.0		2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 1.0 1.0 1.0 1.0 1.01 1.00
	SLAP - Simple Line Access	1.0	2.0	2.0 2.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	SSA - Simple Spectral Access	1.1		1.1 1.1 1.1 1.1 1.04 1.03 1.02 1.01 1.01 1.01 1.00
	STC-S: Space-Time Coordinate Metadata Linear String Implementation	1.0		1.0
	TAP - Table Access Protocol	1.1		1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.00
	TAPRegExt - A VOResource Schema Extension for Describing TAP Services	1.0		1.1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	ADQL - Astronomical Data Query Language	2.1		2.1 2.1 2.1 2.1 2.1 2.1 2.1 2.00 2.00 2.00 1.01 1.00
	SimDAL - Simulation Data Access Layer	1.0		1.0 1.00 1.00 1.00 1.00 1.00 1.00 1.00
	VOEvent Transport Protocol	2.00		2.00 2.00 2.00 1.00
	SODA - Server-side Operations for Data Access	1.0		1.0 1.00 1.00 1.00 1.00 1.00 1.00 1.00
	Object Visibility Simple Access Protocol		1.0	1.0 0.5 0.4 0.2 0.2
	EPN-TAP: Publishing Solar System Data to the Virtual Observatory	2.0		2.0 2.0 2.0 2.0 2.0 2.0 2.0
	LineTAP: IVOA Relational Model for Spectral Lines	1.0		1.0 1.0

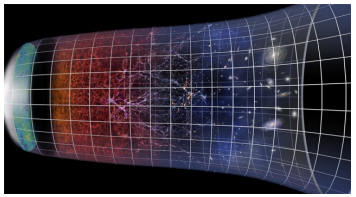
DaM	PHOTDM - Photometry Data Model	1.1		1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	SimDM - Simulation Data Model	1.0		1.0 1.0 1.0 1.0 1.0 1.0
	STC - Space-Time Coordinate Metadata for the Virtual Observatory	1.33		1.33 1.31 1.30 1.21 1.20 1.10 1.00
	Data Model for Astronomical DataSet Characterisation	1.13		1.13 1.12 1.12 1.11 1.10 1.00
	SSLDM - Simple Spectral Lines Data Model	1.0	RFC	2.0 1.0 1.0 1.0 1.0 1.0
	SpectralDM - IVOA Spectral Data Model	1.2		1.2 1.2 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 1.1 1.1 1.1 1.03 1.02 1.01 1.01 1.01 1.00
	ObsCore - Observation Data Model Core Components and its Implementation in the Table Access Protocol	1.1		1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0
	VODML - A Consistent Modeling Language for IVOA Data Models	1.0		1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	DatasetDM - Dataset Metadata Model		1.0	1.0 1.0 1.0 1.0
	CubeDM - N-Dimensional Cube/Image Model		1.0	1.0 1.0
	ProvenanceDM - Provenance Data Model	1.0	1.0	1.0 1.0 1.0 1.0 1.0 1.0 1.0
	Astronomical Coordinates and Coordinate Systems	1.0		1.0 1.0 1.0 1.0 1.0
	WCS Transform Model		1.0	1.0 1.0
	Meas - Astronomical Measurements Model	1.0		1.0 1.0 1.0 1.0
	Observation Locator Table Access Protocol	1.0		1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 0.5 0.4 0.4 0.2 0.2
	MIVOT - Model Instances in VOTable	1.0		1.0 1.0 1.0 1.0
	ObsCoreExtensionForRadioData - IVOA Obscore Extension for Radio data		1.0	1.0 1.0
	ObsCoreTimeExtension - IVOA ObsCore Metadata Extension for Time Properties		1.0	1.0
	CAOM - IVOA Common Archive Observation Model		2.5	2.5
	ProposalDM - A Data model for Observation Proposals		0.6	0.6

	PDL - Parameter Description Language	1.0		1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 0.1
	SSO - Single-Sign-On Profile: Authentication Mechanisms	2.0		2.0 2.0 2.0 2.0 2.0 2.0 2.0 1.01 1.01 1.00 1.00
	VOSpace service specification	2.1		2.1 2.1 2.1 2.1 2.1 2.0 2.0 2.0 2.0 2.0 2.0 2.0 1.15 2.0 1.15 1.15 1.14 1.13 1.12 1.12 1.11 1.10 1.02 1.02 1.01 1.00 1.00
	Credential Delegation Protocol	1.0		1.0 1.0 1.01 1.01 1.00
	UWS - Universal Worker Service	1.1		1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0
	VOSI - IVOA Support Interfaces	1.1		1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0
	GMS - Group Membership Service	1.0		1.0 1.0 1.0 1.0 1.0 1.0 1.0
ReR	IVOA Identifiers	2.0		2.0 2.0 2.0 2.0 1.12 1.11 1.10 1.10 1.10 1.00
	IVOA Registry Interfaces	1.1		1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.00 1.02 1.01 1.00
	RM - Resource Metadata for the Virtual Observatory	1.12		1.12 1.12 1.10 1.10 1.01 1.01 1.00 1.00
	StandardsRegExt: a VOResource Schema Extension for Describing IVOA Standards	1.0	1.1	1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	SimpleDALRegExt - Describing Simple Data Access Services	1.2		1.2 1.2 1.2 1.2 1.2 1.2 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0
	VOResource - an XML Encoding Schema for Resource Metadata	1.1	1.2	1.2 1.2 1.1 1.1 1.1 1.1 1.1 1.03 1.02 1.02 1.01 1.00
	VODataService - A VOResource Schema Extension for Describing Collections and Services	1.2	1.3	1.3 1.2 1.2 1.2 1.1 1.1 1.1 1.1 1.1 1.10
	RegTAP - Registry Relational Schema	1.2		1.2 1.2 1.2 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	DocRegExt - Educational Resources in the VO		1.0	1.0
Semantics	VOUnits - Units in the VO	1.1		1.1 1.1 1.1 1.1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
	UCD - An IVOA standard for Unified Content Descriptors	1.10		1.10 1.10 1.06 1.05 1.03
	UCD1+ Controlled Vocabulary version <= 1.3: recommendation Version >= 1.4: endorsed note	1.5		1.6 1.6 1.5 1.5 1.5 1.5 1.5 1.4 1.4 1.4 1.4 1.3 1.3 1.3 1.3 1.3 1.3 1.23 1.22 1.21 1.20 1.20 1.11 1.11 1.10 1.02 1.00
	Maintenance of the list of UCD words	2.0		2.0 2.0 2.0 1.20 1.20 1.10 1.00
	Vocabularies in the Virtual Observatory	2.1		2.1 2.1 2.1 2.0 2.00 2.00 2.00 2.00 1.19 1.18 1.16 1.15 1.13 1.00
SDP	DocStd - IVOA Document Standards	2.0		2.0 2.0 2.0 2.0 2.0 1.2 1.2 1.2 1.2 1.2 1.1 1.1 1.0 1.0
VOE	VOEvent - Sky Event Reporting Metadata (VOEvent)	2.0	RFC	2.1 2.1 2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0 1.11 1.11 1.10 1.01
	VOEventRegExt - An XML Encoding Schema for Resource Metatdata for Collections of Events		1.0	1.0

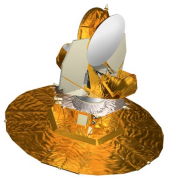


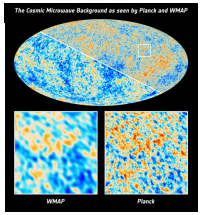
IVOA-Architecture (2023)

Data flows : Cosmological simulations



Initial conditions:
Theory and
Observations (Planck + WMap)





Initial conditions:
(Nbody simulation)

velocity and positions of mass for each particle
N_p ~ o(10^{12} -10^{13})

+ Software

+ Millions of CPU hrs

+ storage space

Raw data:

Snapshots of time steps in simulations

(storing 6d coordinates + mass in binary format)

File based identificators

Result data I:
(w. publications)

Derived:
Mass distribution

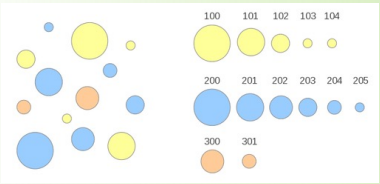
'Halos', filaments etc.

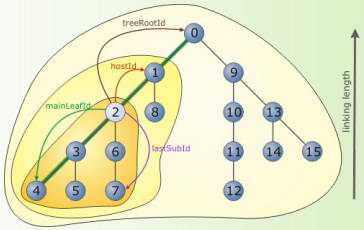
Histories of mass agglomerations

File based identificators

Example: MultiDark Simulations
(https://www.cosmosim.org/cms/data/projects/multidark-bolshoi-project/)

data acquisition | data cleaning & processing | data curation + publication





Data Curation:

* checking consistency of the data

* deciding about the data products to publish

* presenting the data, so scientists not involved in the simulation can use & understand the data sets

Mapping data:

* time steps to redshifts

* history of filaments and halos

* statistical properties

Data Formats:

* files (w. low level read procedures)

* tabluar data as files or in a queryable database

* suitable metadata (community dependant)

* metadata for cross community use

Data Publication:

* assigning units
* adding metadata
*defining datasets
* assigning DOI
* landing pages
* web interface

* REST API
* OAI PMH API
* VO (tap) API

* Website/~`service.

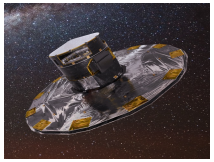
Data Management: Production

Data Management: User Access

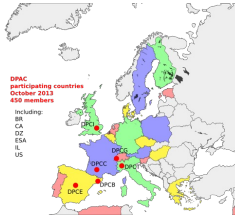
Instrument building | Data taking | Data processing | Data Publication | Data curation | Data exploitation

ESA + Consortium Satellite Construction

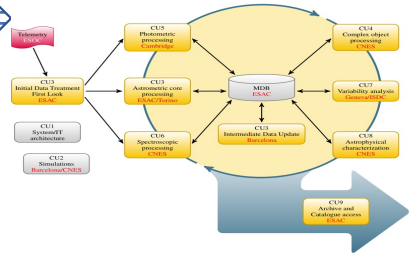
ESA: Satellite Operation



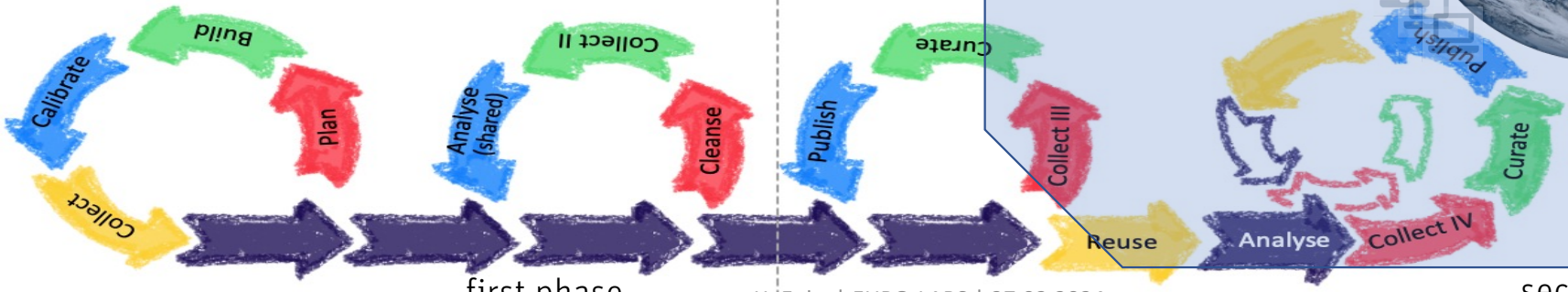
Images: ESA + DPAC



DPAC Consortium



DPAC+ (Partner) DataCenters :

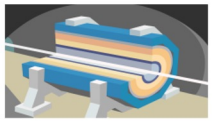


first phase

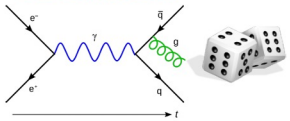
second phase

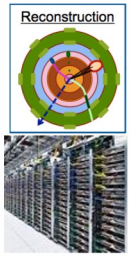
HEP experiment data flow

Real Data

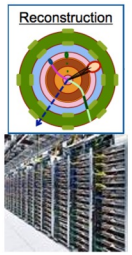


Monte Carlo Simulation
1core min/evt



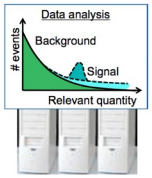


Reconstruction
0.5core min/evt



Reprocessing
0.5core min/evt

Distributed Analysis
A few core sec/evt



Individual Analysis
2-3 PhD brain years

Final Paper
Several brain months

C. Wissing, Desy

Centrally organized

Organized by sub-groups or individually

Data Preprocessing

- Data cleaning
- Data transformation and integration
- Data reduction
- Data normalization
- Data validation
- Data splitting and imputation
- Data sampling

~5000 .root files
max file size ~2Gb

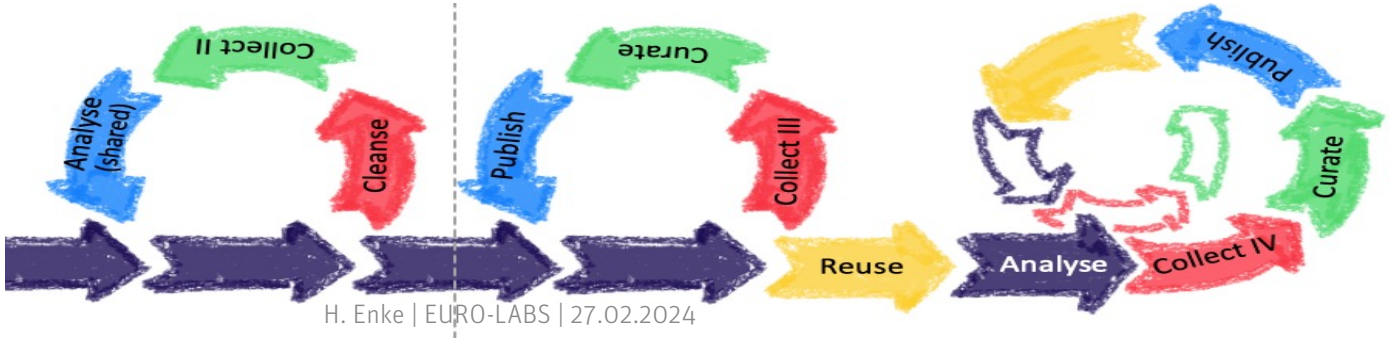
Data Analysis

- Event reconstruction
- Signal-background separation
- Parameter estimation

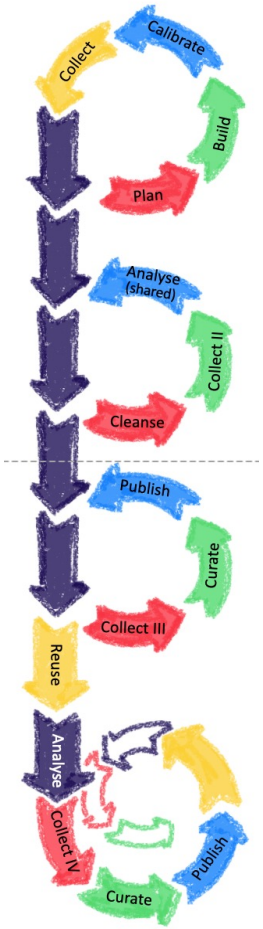
Output ~100
.root files

Data Output

- Root file aggregation
- Creating root file histogram
- Statistical analysis
- Data visualisation



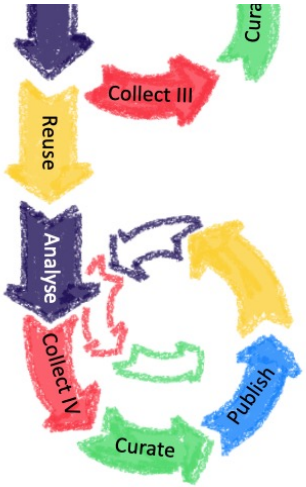
Data life cycles in Physics : not really cycling the same data



- Instrument conception, construction
  - expected observational properties
  - dvelopment of instrumental capabilities
  - construction
- Operations : Data taking
  - Instrument calibration
  - Operation modes
  - Quality monitoring
- Data evalutaion / calibration …
- Data curation
  - Data evalutation,
  - Removal of instrument charcteristics + artifacts
  - Data curation / producing science ready data (NFDI)
- Data exploitation
  - Public (or group based access) data exploitation
  - FAIR data domain. (NFDI)
  - Interdisciplinary exploitation (NFDI)

See also: https://doi.org/10.5281/zenodo.10677953

Infrastructure developments : where to with PUNCH



Current focus of infrastructure suggestions:

- solutions for data analysis processing (ML / FPGA)
- solutions for enabling cloud based analysis processes

First phase RDM

- well developed within in the various builder collaborations
- PI modus not included (mostly)

Second phase (benefitting from first phase)*

- Jupyter Hub
- CoBALD/TARDIS
- Support for Data Caches and time limited storage offers
- REANA (and other cloud-like workflow engines) deployment for integrating the diverse landscapes of many resource providers

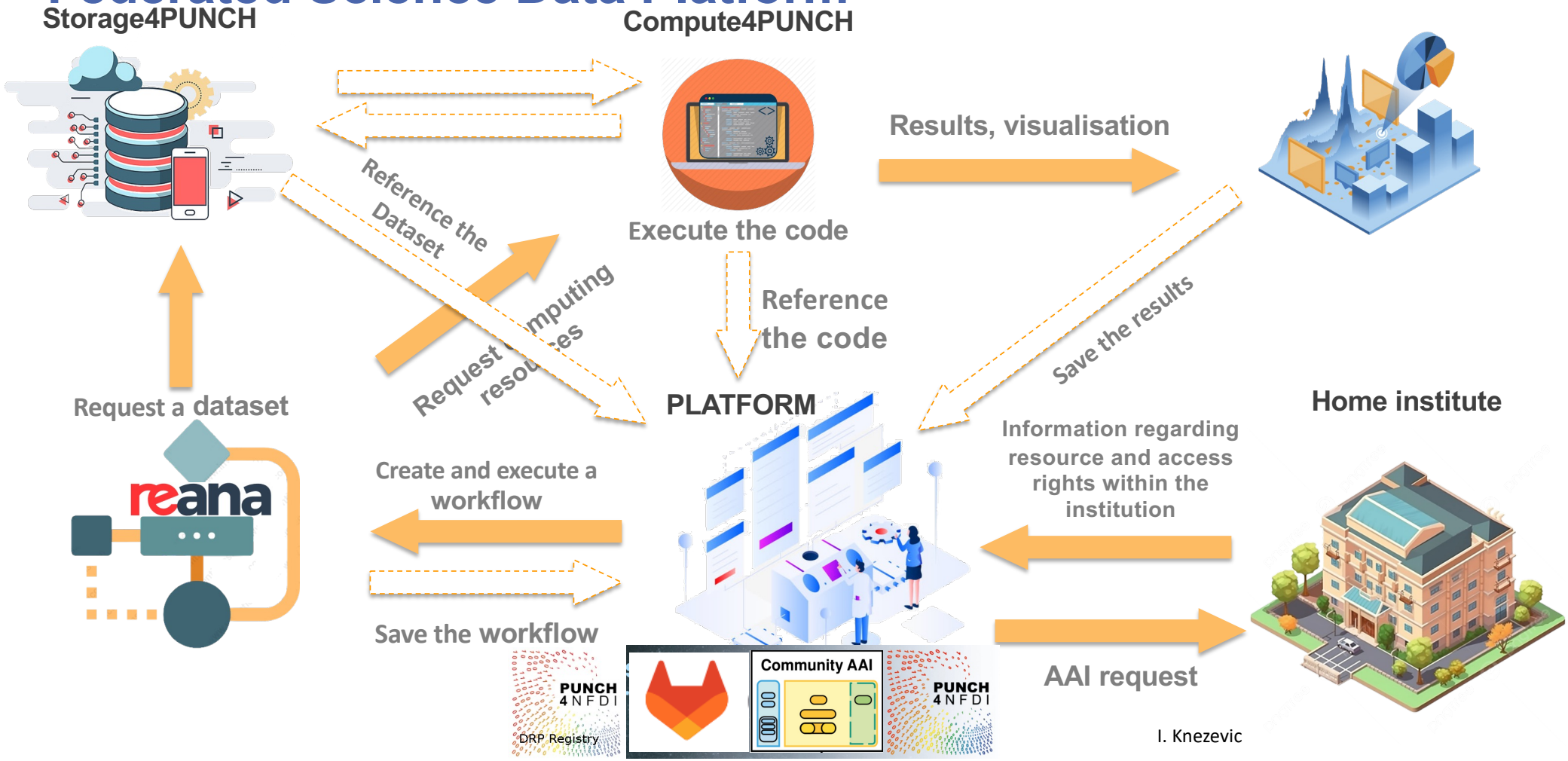
but not well developed:

- processes to curate generated data
- storage for generated data
- support for reproducible data products

'last dirty mile'

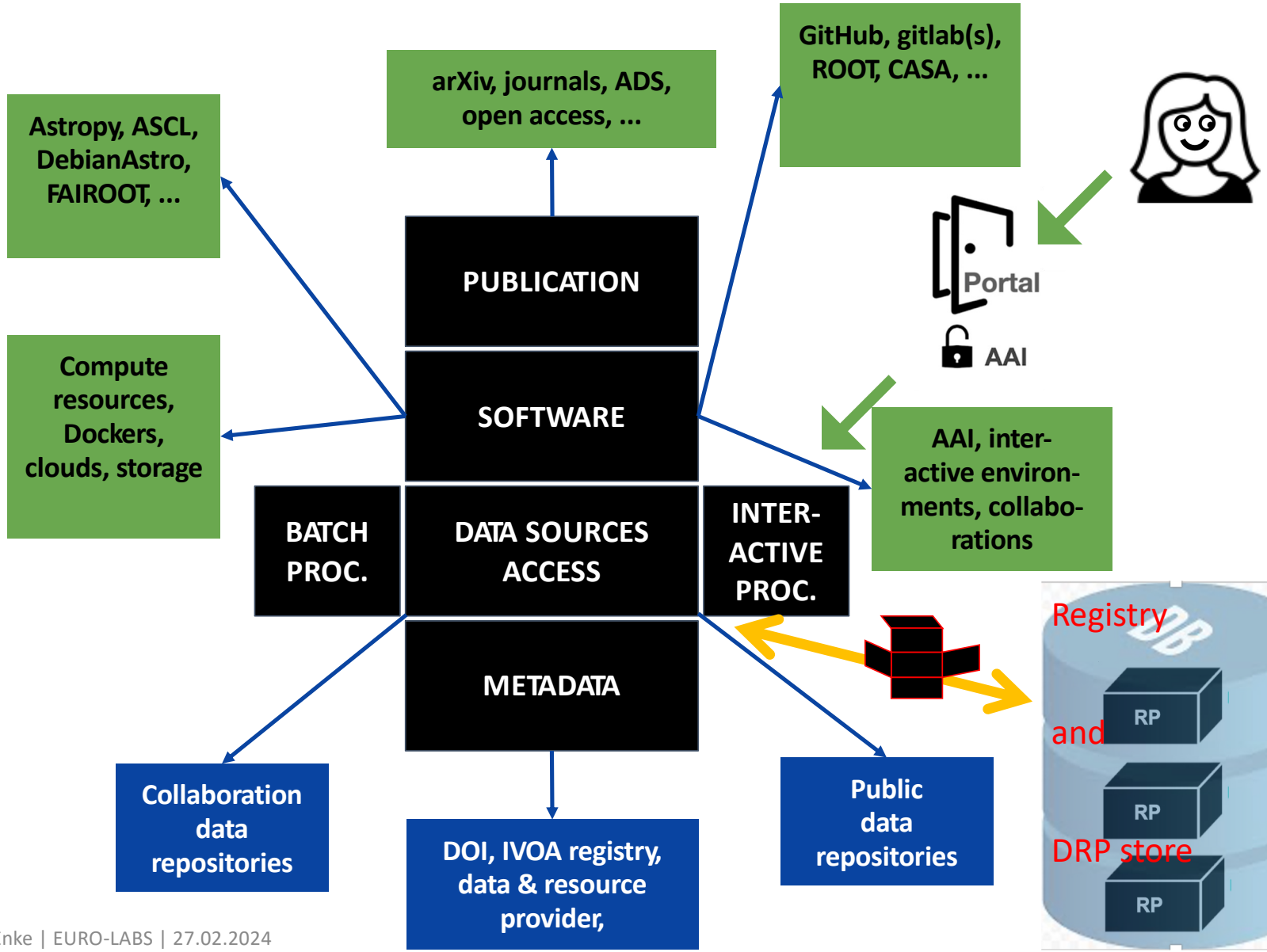
*to name a few developments

Federated Science Data Platform



I. Knezevic

Digital Research Product

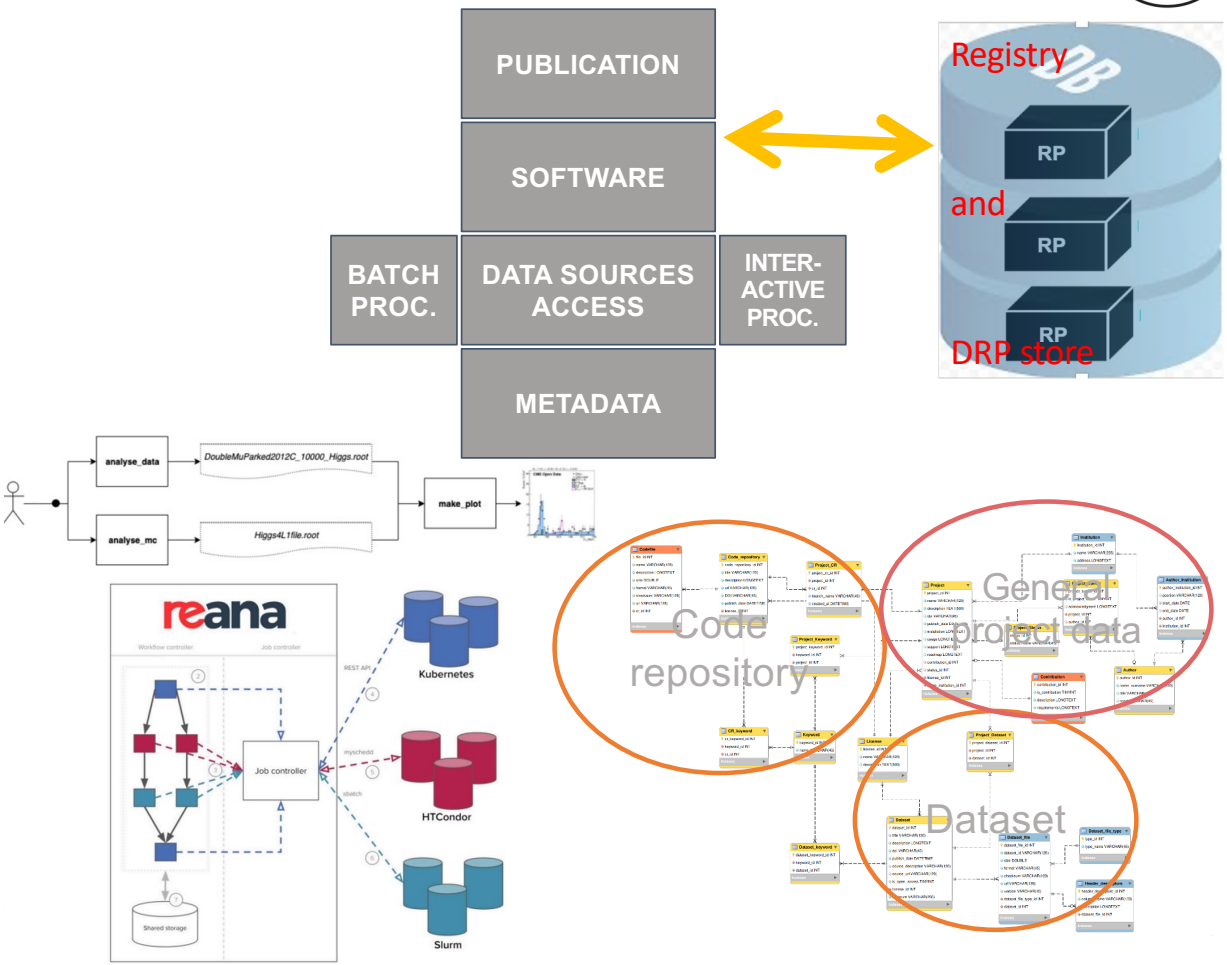


- Improves reproducibility and re-usability
- guided by FAIR
- Access via portal
- Interaction with other RPs
- Interfaces to tools and infrastructures
- Built on available developments of our communities
- Use standards already implemented
- avoid extensive mappings, do the necessary

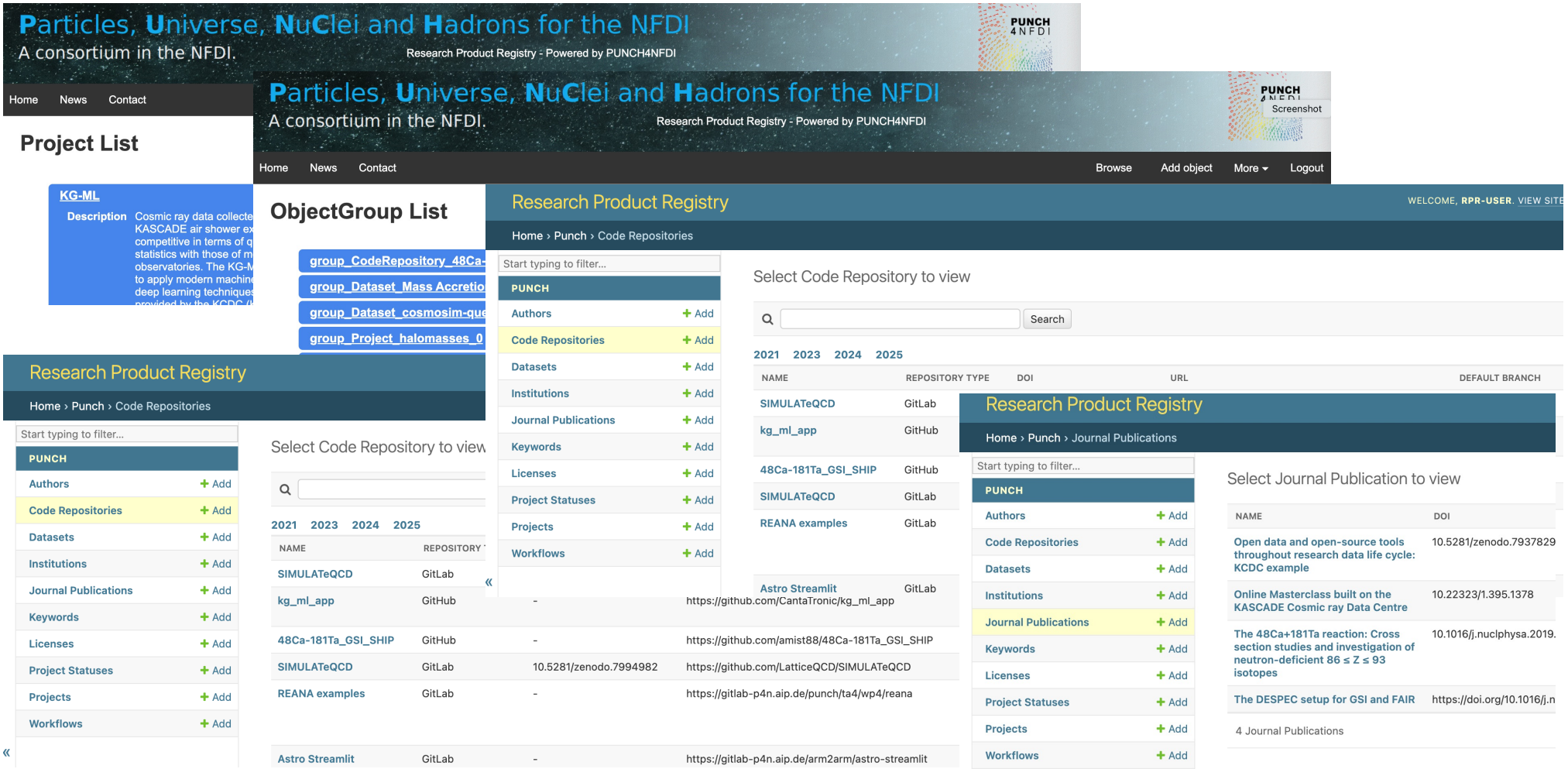
Digital Research Product, Registry, REANA

- DRP : capturing workflow and results
  - Using as much as possible existing metadata, identifiers,
  - working with references to repositories
  - using workflow encapsulation backed by
    - Continous Integration (CI)
    - Gitlab container registry
- REANA:

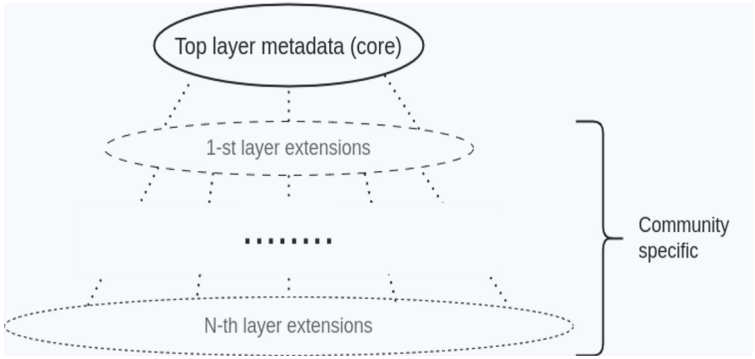
  (Reproducible research data analysis platform)
  - workflow engine
  - connecting multiple storage and computing resources
  - support for Jupyter notebooks
  - multiple workflow languages
- Registry for DRP:
  - based on Django webapp
  - implementing necessary
  - minimal viable product



Registry of Digital Research Products (Pilot)



Findability based on DataCite Kernel (+)



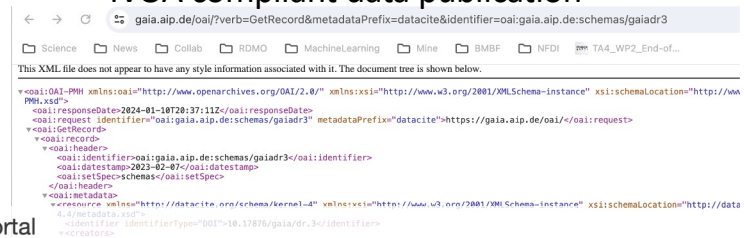
Layered metadata architecture

Metadata (Cross Community)

DataCite Schema (DOI):

- mapping metadata from accessible (public) data collections from HEP, ILDG, RadioAstronomy (LOFAR), Virtual Observatory
- defining reasonable balances between disciplinary metadata management and cross community (= interdisciplinary) schemas and implementations
- published working paper on metadata for real time processing
- webservices for accessing metadata

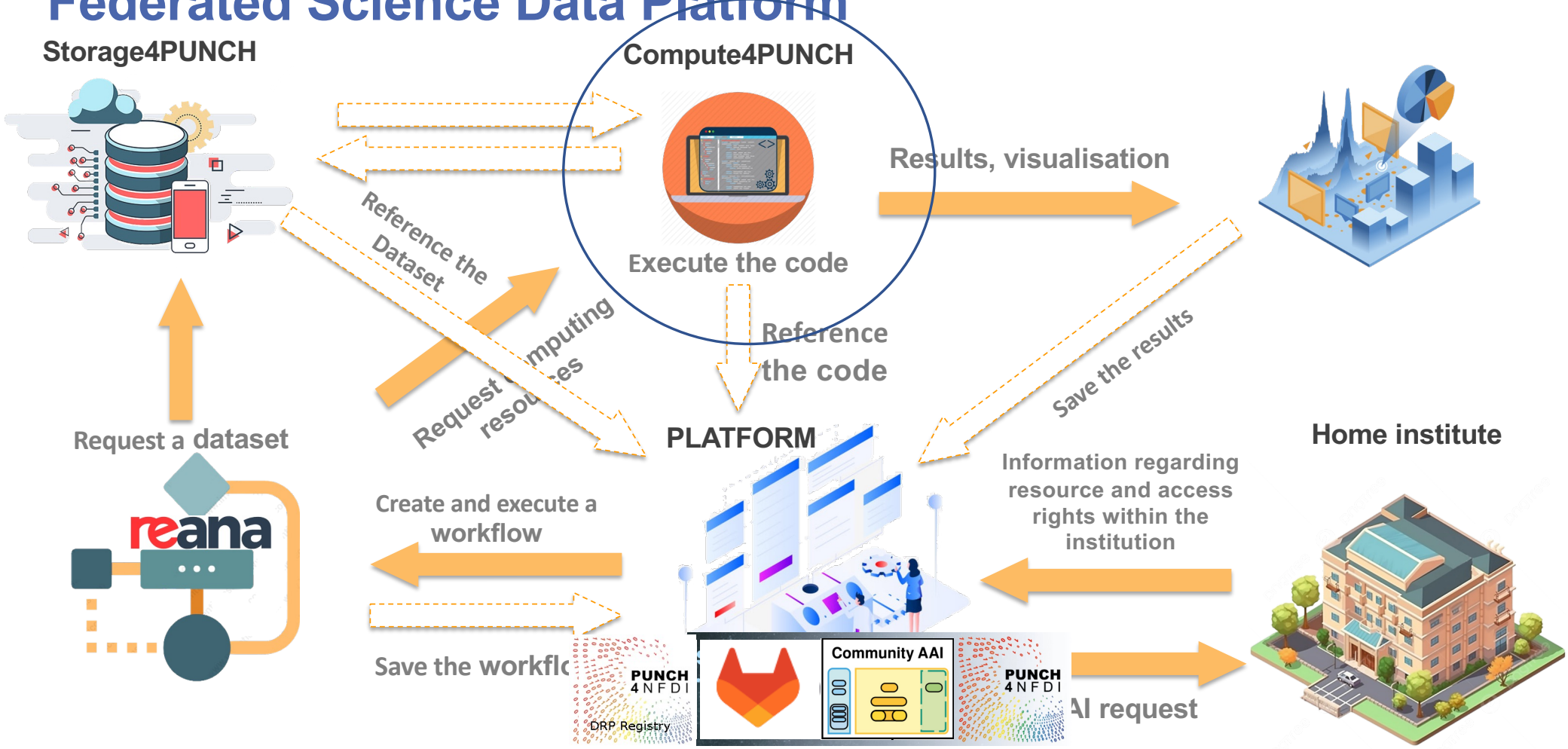
gaia@aip.de,
IVOA compliant data publication



CERN Open Data Portal
Record12341

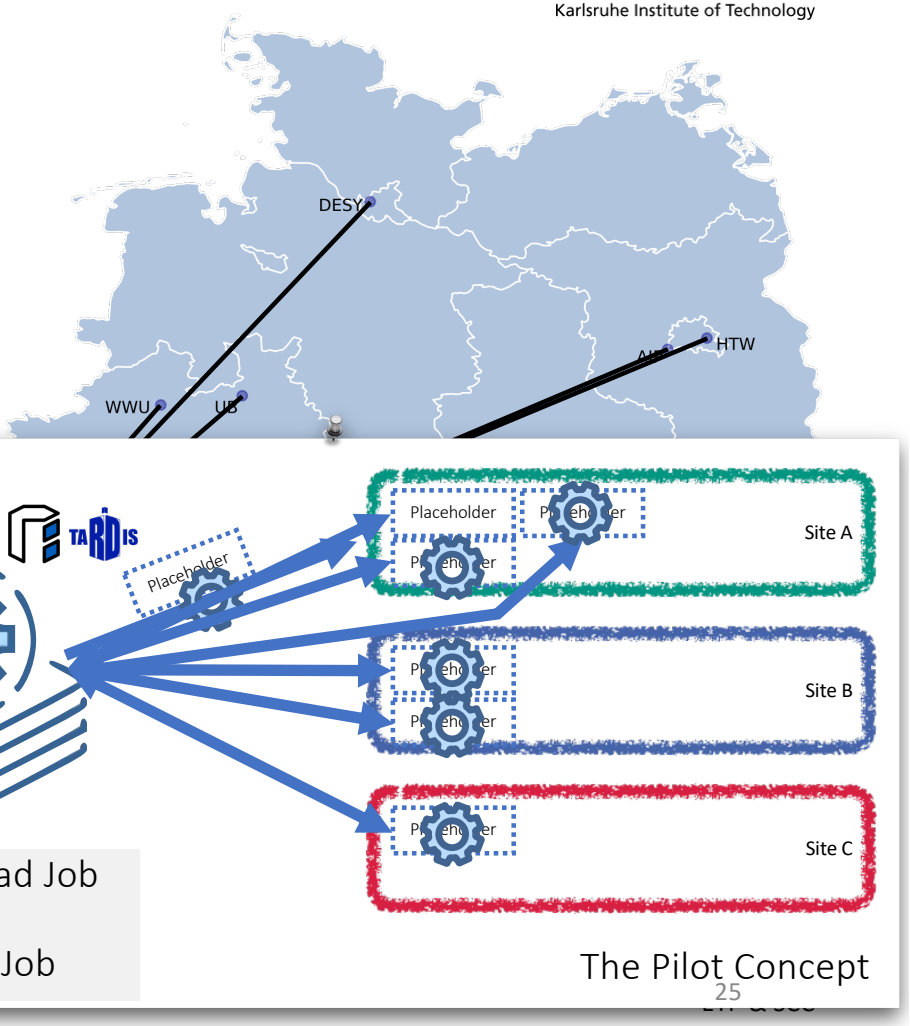
Property	Property specification	Value
Identifier	Doi	10.7483/ OPENDATA.CMS.LVG5.QT81
Creator	creatorName nameType="Personal"	Wunsch, Stefan
	givenName	Stefan
	familyName	Wunsch
	nameIdentifier nameIdentifierScheme="ORCID" schemeURI=	"http:// orcid.org">0000-0002-4485-2972
Title		DoubleMuParked dataset from 2012 in NanoAOD format reduced on muons
Publisher		CERN Open Data Portal
publicationYear		2019
resourceType	resourceTypeGeneral=	"Dataset">Derived<
Subject	subjectScheme=	"experiment">CMS<
Dates	dateType="Created" dateType="Issued"	2012 2019
alternateIdentifier	alternateIdentifierType=	"recid">12341<
relatedIdentifiers	relationType="HasPart" relatedIdentifierType=	„uri_http" >http://opendata.cern.ch/record/ 12341/files/ Run2012BC_DoubleMuParked_M

Federated Science Data Platform



Available Resources of PUNCH4NFDI Institutions

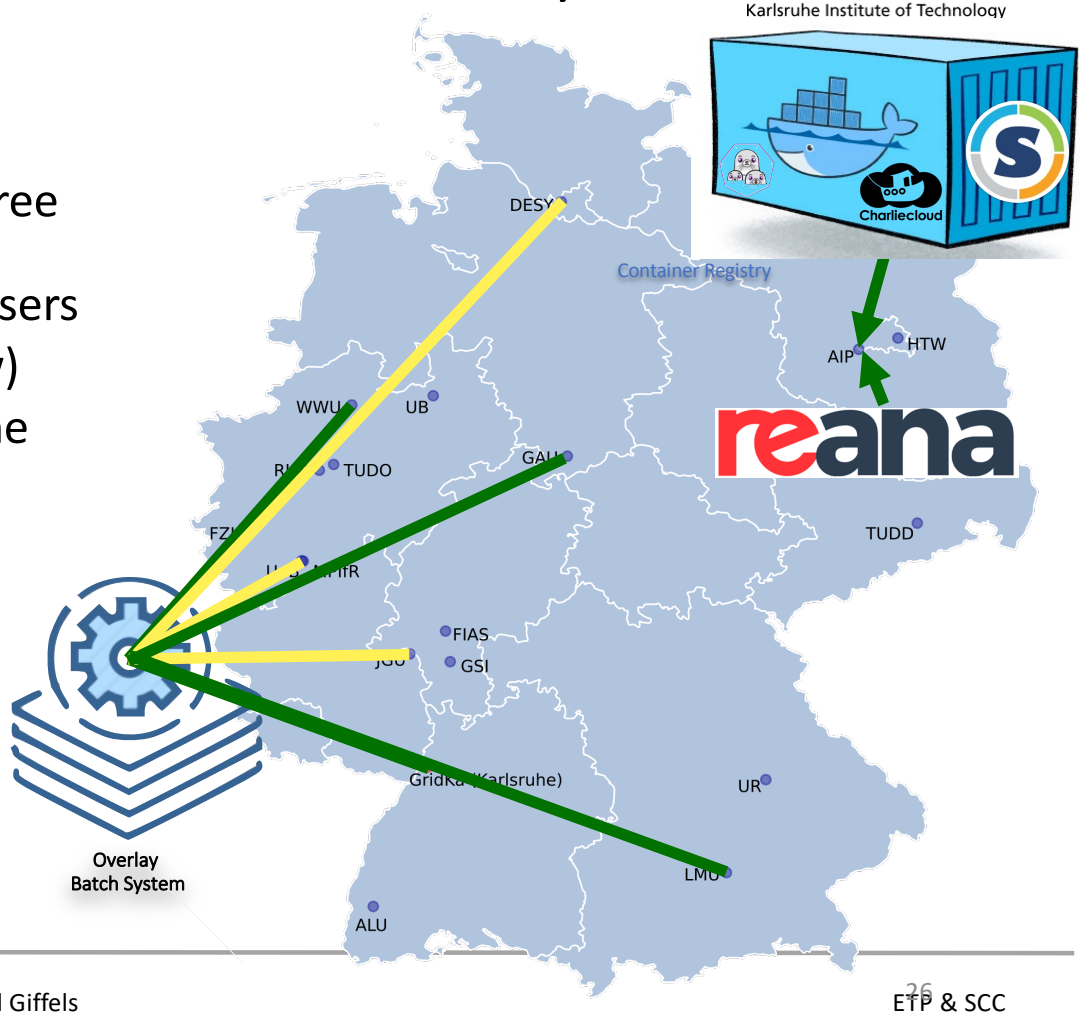
- Substantial amount of HTC, HPC, Cloud compute resources are provided to PUNCH4NFDI
- **Idea:** Establish a federated heterogenous compute infrastructure for PUNCH4NFDI
- Dynamically integrate compute resources into one HTCondor overlay batch system using the COBaLD/TARDIS meta scheduler [1,2]
- Provide single point(s) of entry to users:
  - Traditional login nodes (available)
  - JupyterHubs (in development)
  - REANA (available)
  - Grid Compute Elements (if necessary)
- Provide necessary software environment using container technology + CVMFS [3]



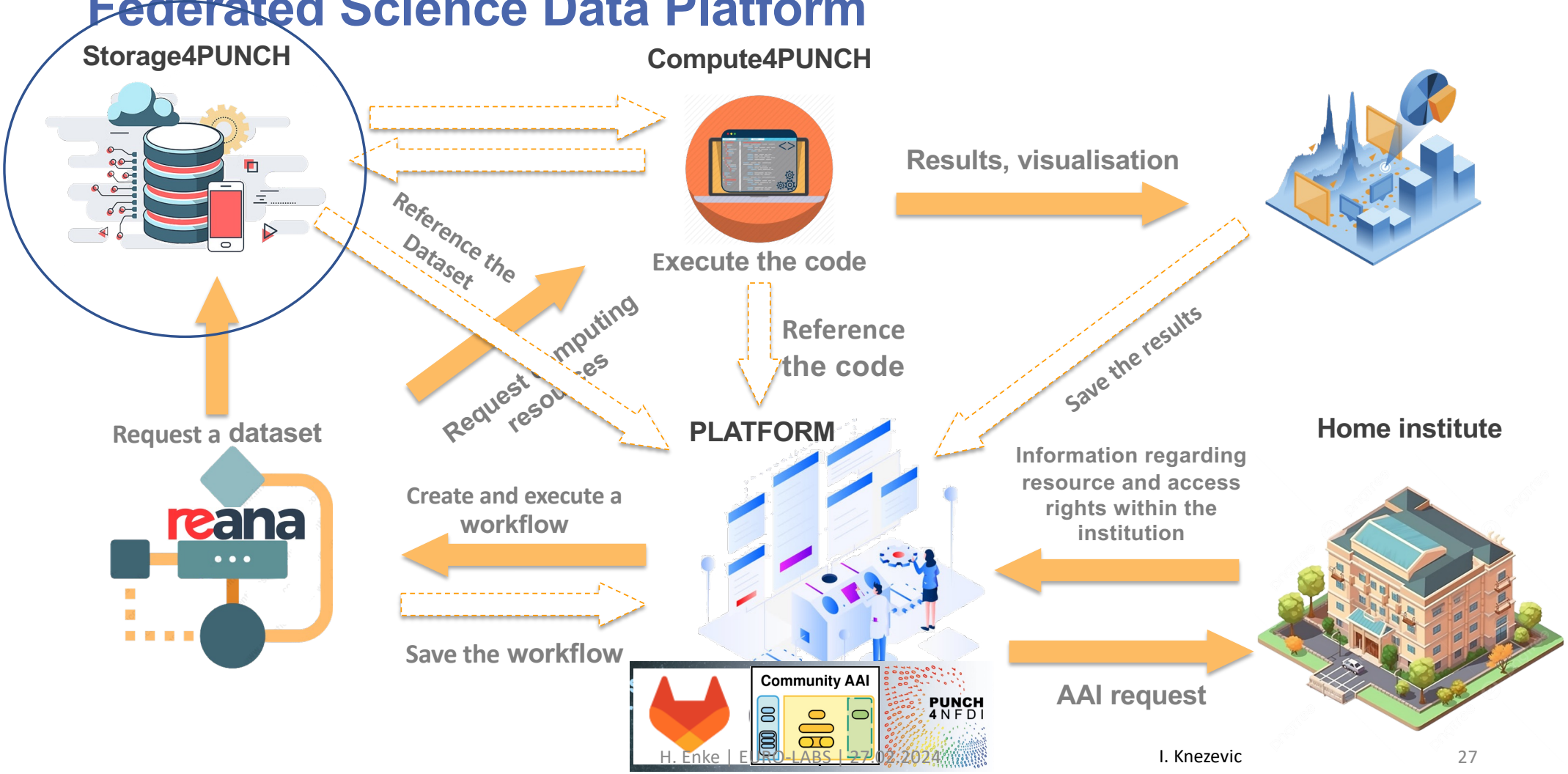
The Compute4PUNCH Infrastructure Today

- Prototype of federated Compute4PUNCH infrastructure is available
- Dynamic integration of four compute sites, three more will follow soon
- AAI based login node available to all PUNCH users
- Container registry available (+ CI/CD workflow)
- Container distributed via CERN Virtual Machine File System (CVMFS) for scaling
- REANA instance available

c4p-login.gridka.de

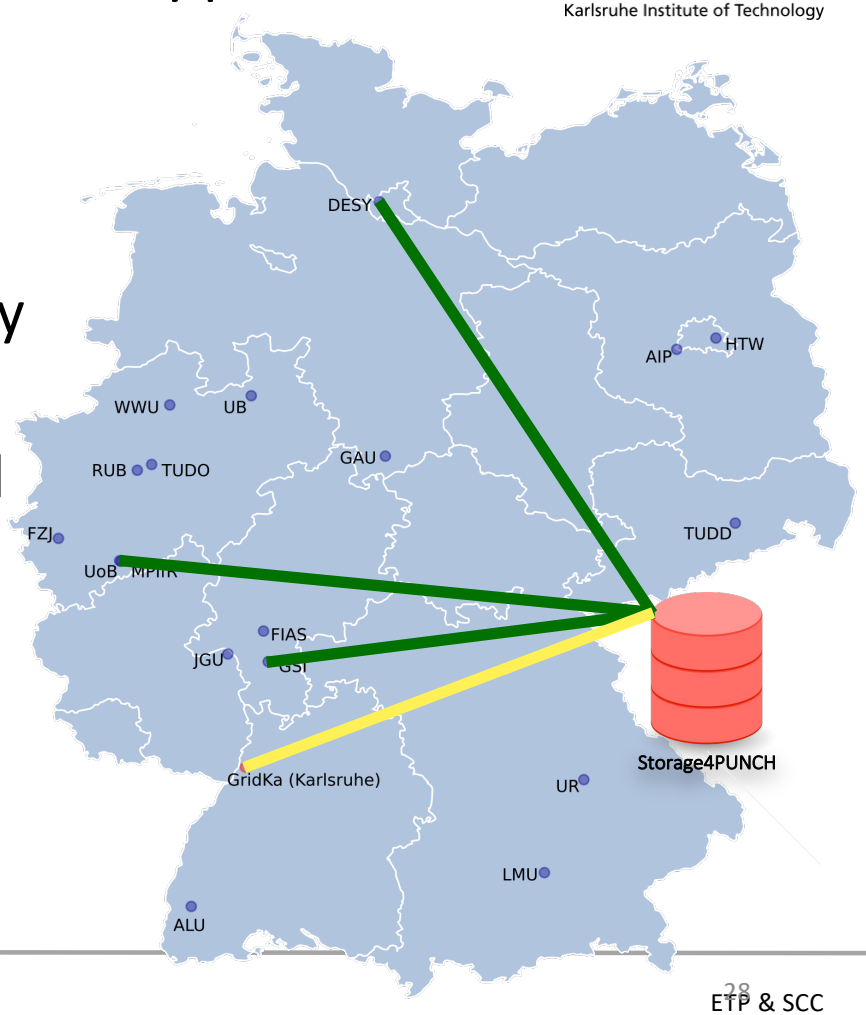


Federated Science Data Platform



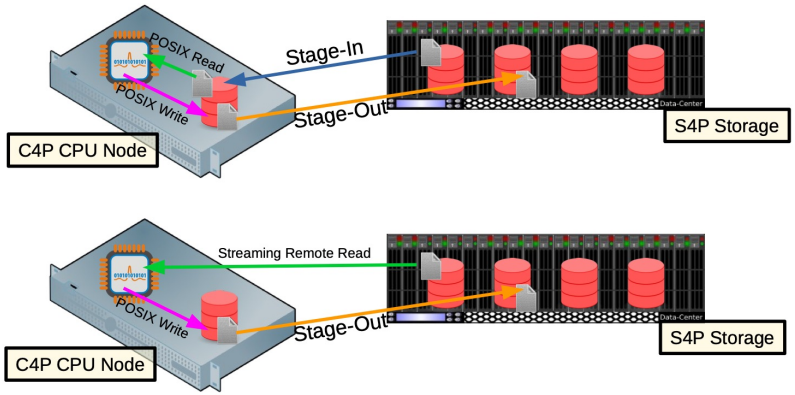
Storage4PUNCH - Distributed Prototype

- Based upon different technologies
  - dCache (Test Endpoint at DESY)
  - XRootD (Test Endpoints Bonn & GSI)
- Token based access using PUNCH AAI (Unity IdM [4])
- Using WebDav/XRootD as transfer protocol

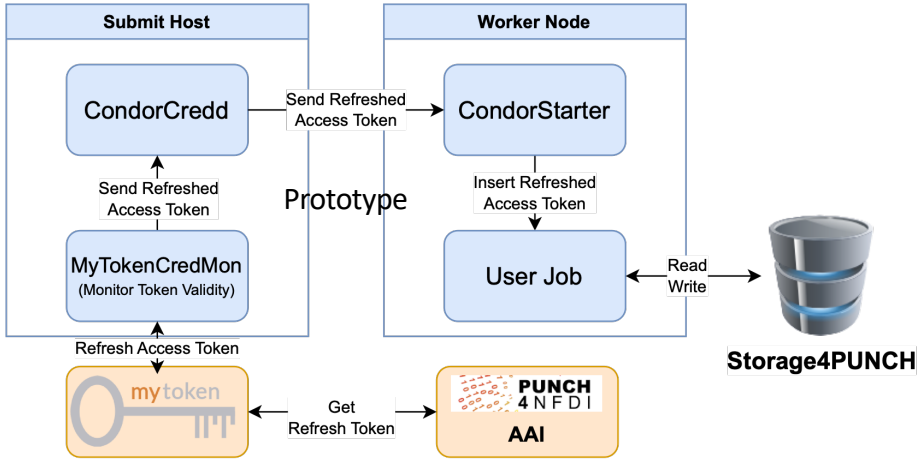


Integration of Compute4PUNCH & Storage4PUNCH

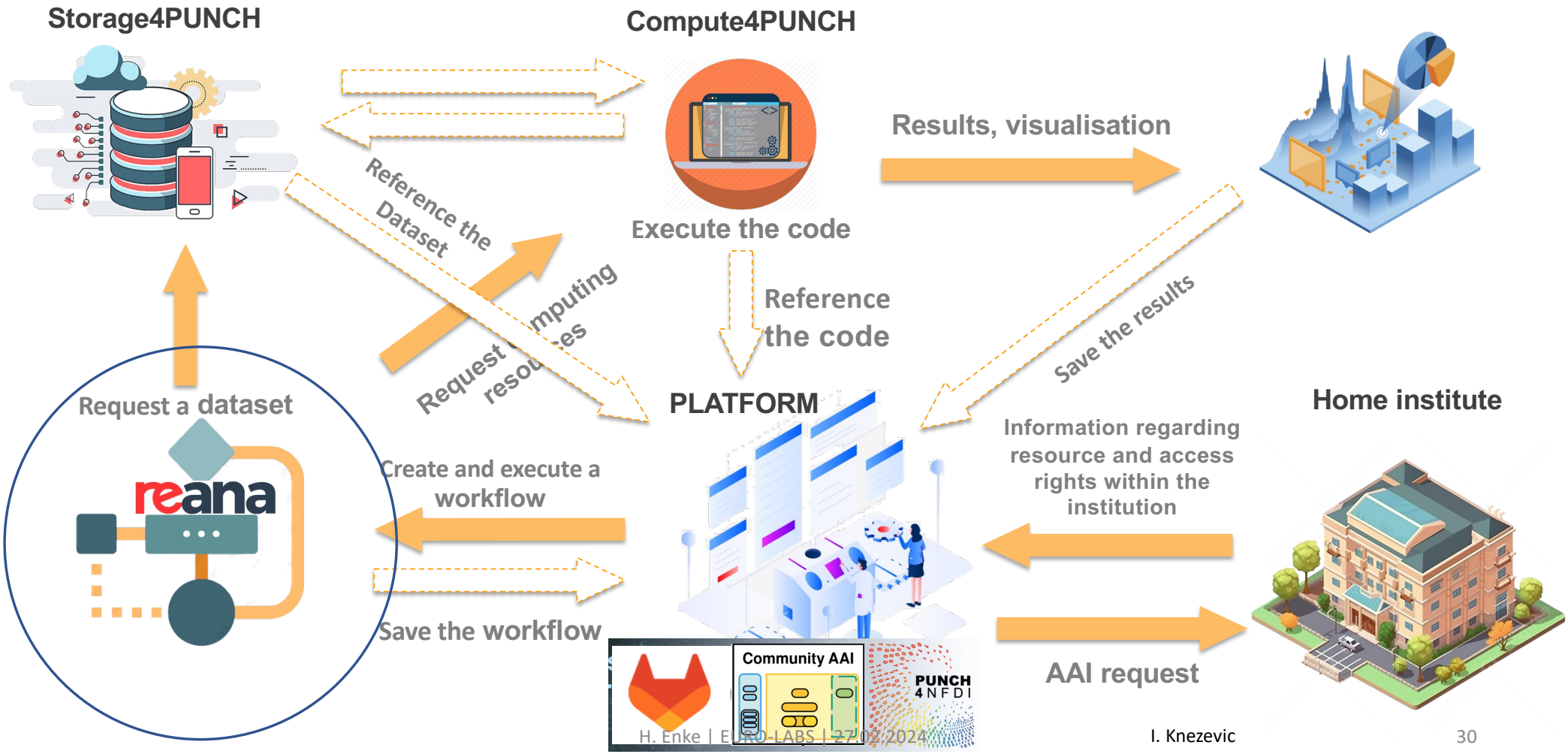
- Storage4PUNCH is not POSIX accessible
  - Files need to be staged to local POSIX compliant storage (usually inefficient)
  - Application needs to support streaming (preferred method, not always supported)



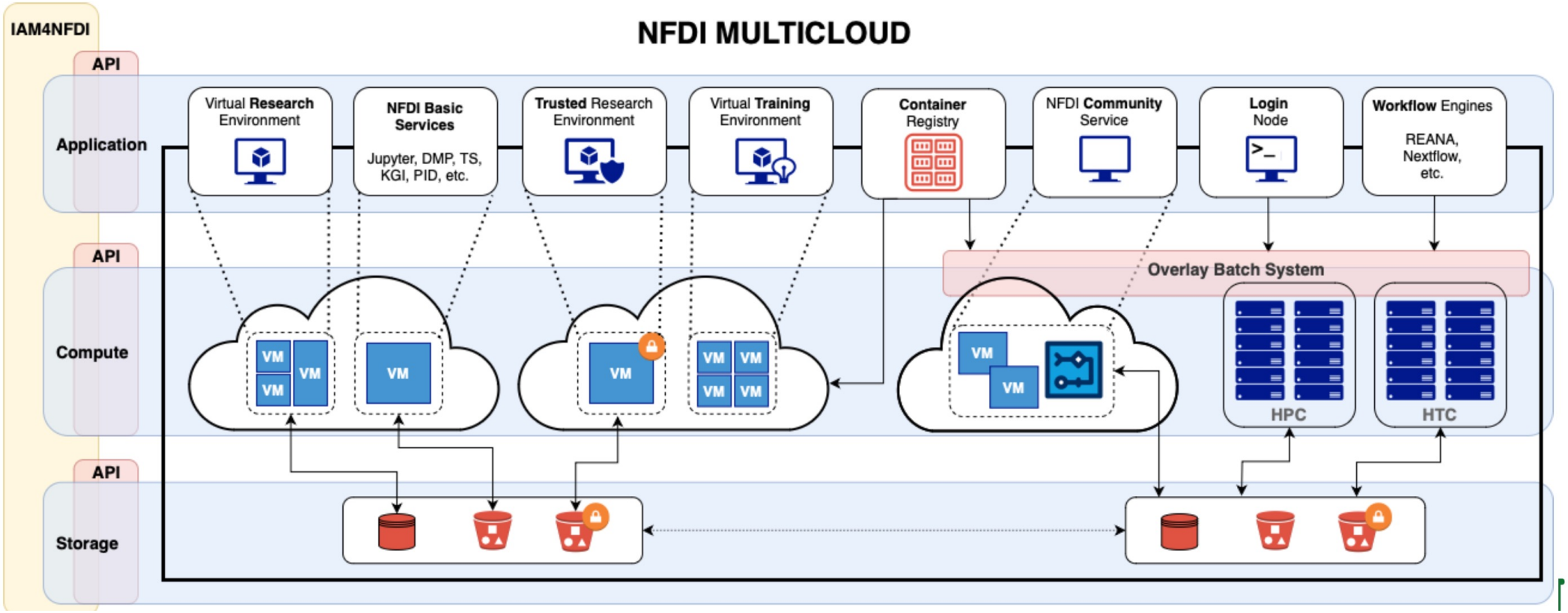
- Access token has a limited lifetime, usually shorter than the job runtime
  - Add refresh token to MyToken service
  - Use HTCondor CredMon to create, monitor and refresh access token of the user
  - Use HTCondor Credd to synchronize access token to user jobs on worker nodes



Federated Science Data Platform



Diverse and distributed infrastructure



NFDI MultiCloud WG, Oct. 2024