

Pioneering Digital Research Landscapes: Innovations at HZDR

Towards Open Digital Research Ecosystems – Interconnecting Infrastructures, Open Science Forum, February 14, 2024

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Our Research Facility and our Large Scale Research Infrastructures

The Helmholtz-Zentrum Dresden - Rossendorf

- Employees approx. 1,470. Thereof 670 scientists



Research Fields

- Energy, Health and Matter

ELBE – Center for High-Power Radiation Sources

- Electron accelerator, free-electron lasers & THz source.
- Positrons, protons, neutrons as well as X-ray and gamma radiation

Dresden High Magnetic Field Laboratory (HLD)

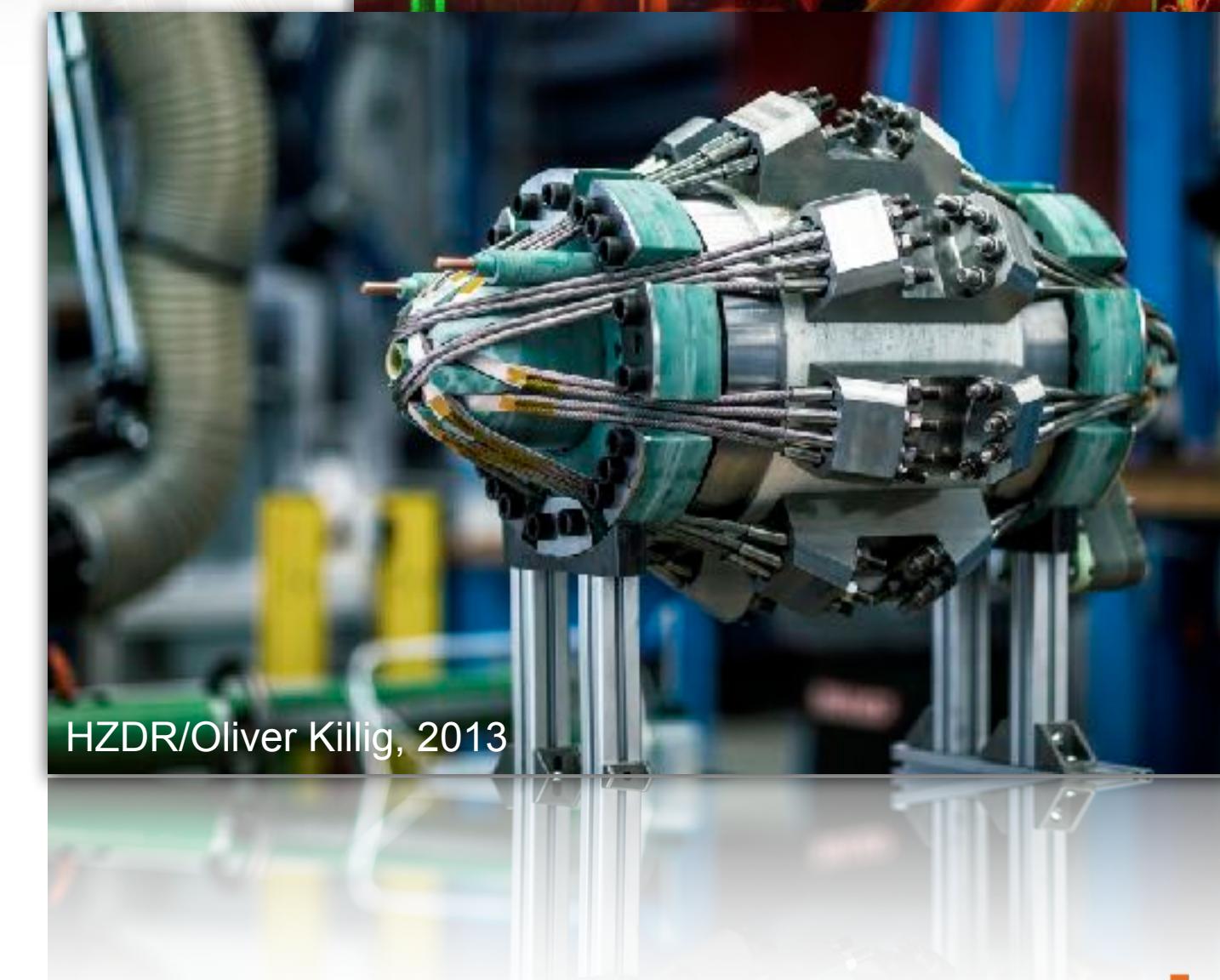
- Europe's highest pulsed magnetic fields

Ion Beam Center (IBC)

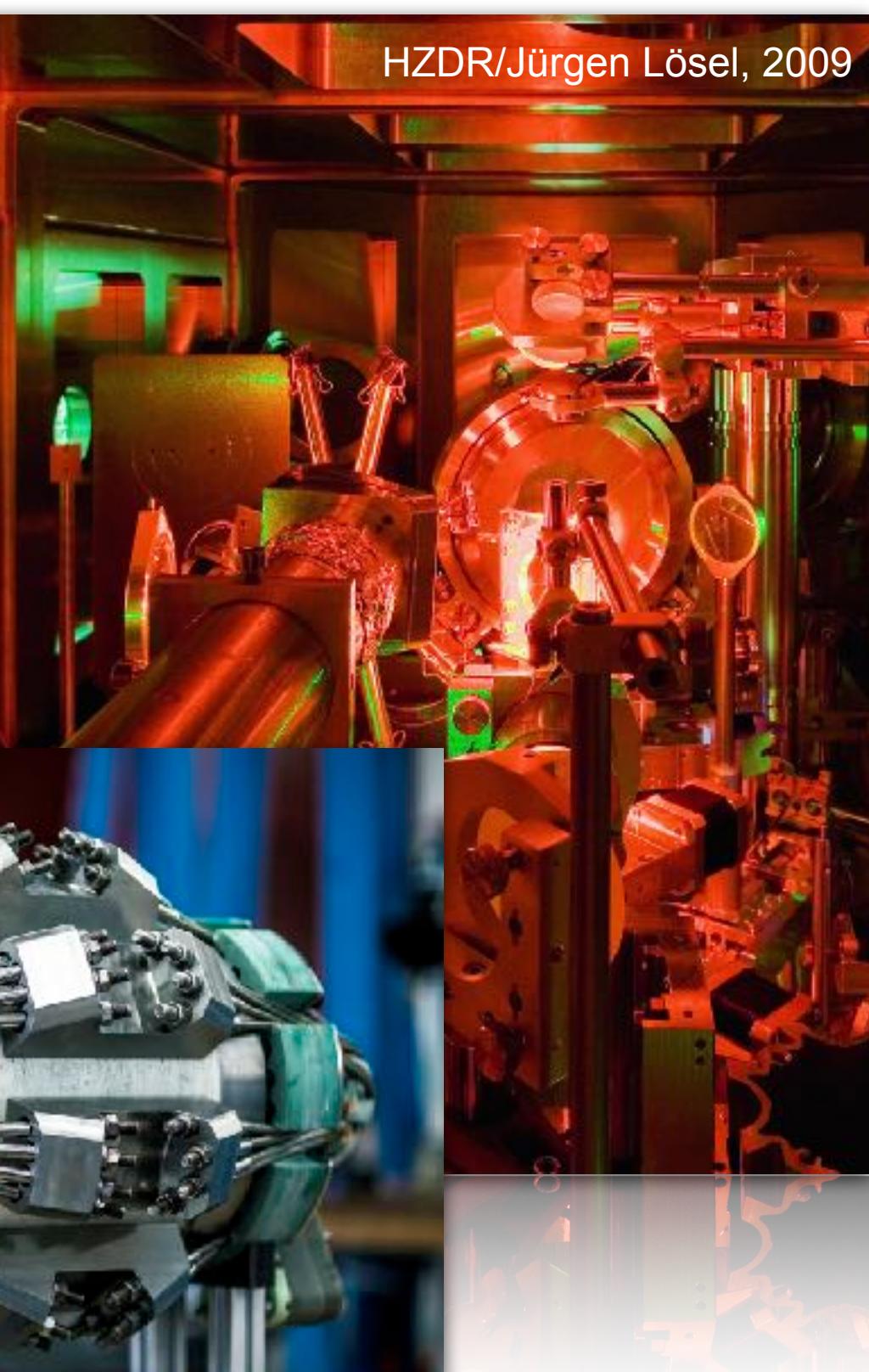
- Nanoscale surface analysis and modification



HZDR/André Wirsing, 2017



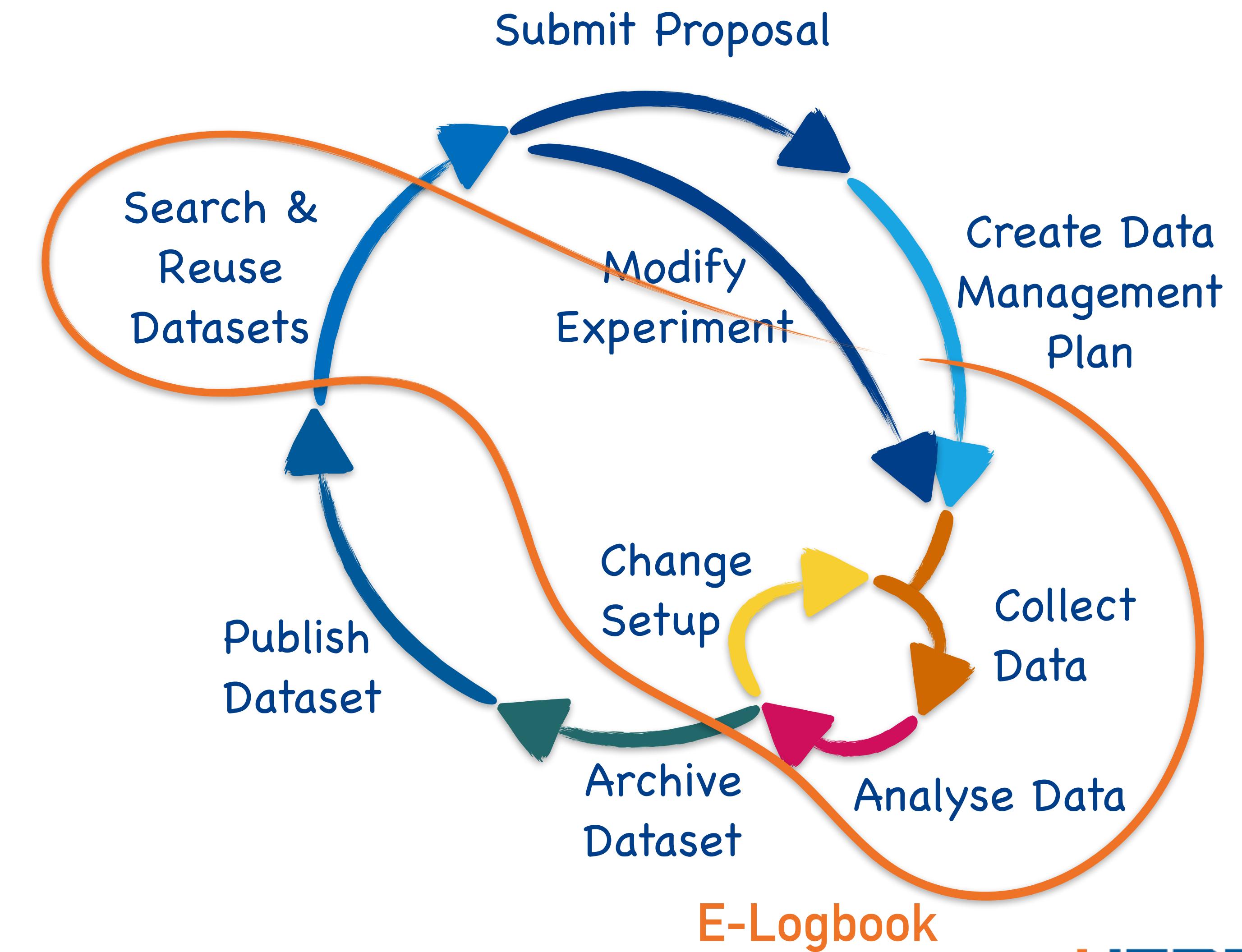
HZDR/Oliver Killig, 2013



HZDR/Jürgen Lösel, 2009

Our Challenge: An End-to-End Digital Data Lifecycle

- We support many steps of our different research experiment (matter, energy and health) with a wide range of tools:
 - Electronic lab notebook (**E-Logbook**),
 - Interactive analysis,
 - **FAIR Publication** of datasets,
 - Scientific **workflow** management,
 - **Handle** (PID) generation and management.
- A uniform and smooth access to and **between** all services and systems in our ecosystem is necessary.
- The documentation of all these linked resources is essential to create a **comprehensible** and **FAIR** data lifecycle.

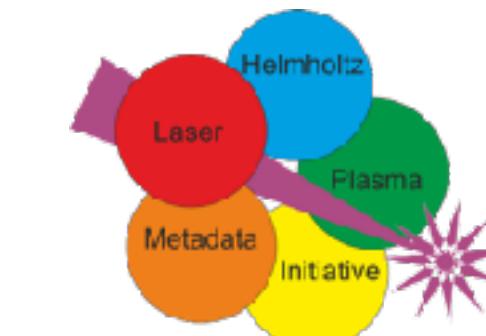


The Foundation for our Digital Data Lifecycle: HZDR Data Policy

- The HZDR has a data policy since **May 2018**
- Reasons for the development:
 - Legal framework for data management and publication,
 - Establishment and legitimisation of coordinated research data management at HZDR,
- Foundation for the development of tools and services to support our scientists:



HELIPORT HELmholtz Scientific Project W ORkflow PlAtform



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<https://os.helmholtz.de/open-research-data/forschungsdaten-policies/>

HZDR Data Policy
HZDR-Regulation No. B 220
Date: 01.05.18
Rev.: 0
Page: 1 of 9

DOI 10.14278/rodare.2269

Terms and Conditions for the Storage, Access and Curation of Research Data

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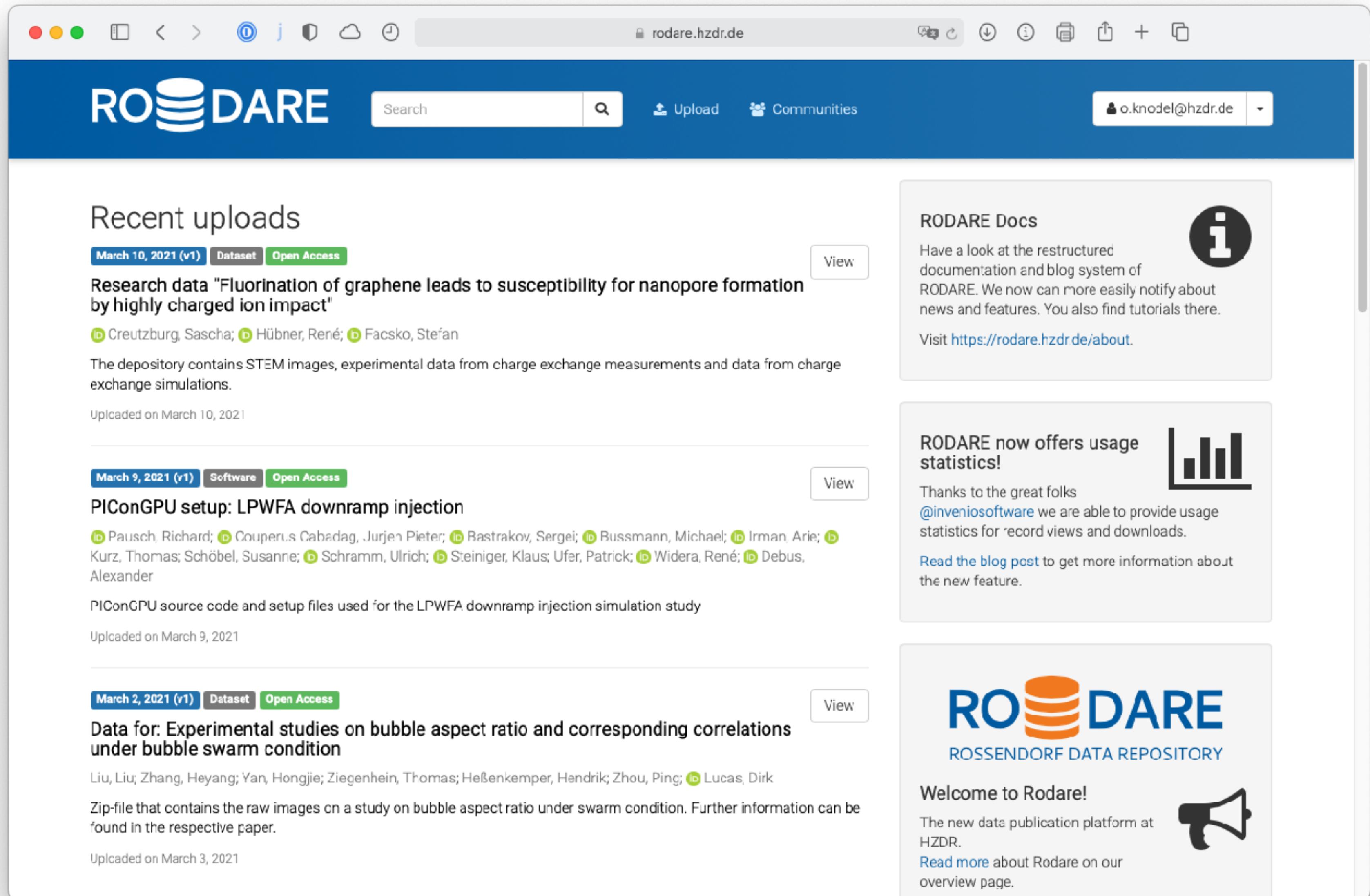
List of Revisions

Page	Rev.-No	Date	Reason for revision
1-9	0	01.05.2018	New Regulation

List of Abbreviations

CC BY	Creative Commons Attribution License
CC0	Creative Commons Universal License
DMP	Data Management Plan
DOI	Digital Object Identifier
FAIR data	Data that is findable, accessible, interoperable and reusable
HZDR	Helmholtz-Zentrum Dresden - Rossendorf e. V.
PI	Principal Investigator
RODARE	Rossendorf research Data Repository

Starting Point in 2018: Data Publication Platform RODARE rodare.hzdr.de



The screenshot shows the Rodare website interface. At the top, there's a navigation bar with icons for back, forward, search, upload, and communities. The main header features the Rodare logo and a user account dropdown. Below the header, a "Recent uploads" section displays three datasets:

- March 10, 2021 (v1) Dataset Open Access**
Research data "Fluorination of graphene leads to susceptibility for nanopore formation by highly charged ion impact"
View
by Creutzburg, Sascha; Hübner, René; Facsko, Stefan
The depository contains STEM images, experimental data from charge exchange measurements and data from charge exchange simulations.
Uploaded on March 10, 2021
- March 9, 2021 (v1) Software Open Access**
PIConGPU setup: LPWFA downramp injection
View
by Pausch, Richard; Couperus Cabadag, Jurjen Pieter; Bastrakov, Sergei; Bussmann, Michael; Irman, Arie; Kurz, Thomas; Schöbel, Susanne; Schramm, Ulrich; Steiniger, Klaus; Ufer, Patrick; Widera, René; Debus, Alexander
PIConGPU source code and setup files used for the LPWFA downramp injection simulation study
Uploaded on March 9, 2021
- March 2, 2021 (v1) Dataset Open Access**
Data for: Experimental studies on bubble aspect ratio and corresponding correlations under bubble swarm condition
View
by Liu, Liu; Zhang, Heyang; Yan, Hongjie; Ziegenhein, Thomas; Heßenkemper, Hendrik; Zhou, Ping; Lucas, Dirk
Zip-file that contains the raw images on a study on bubble aspect ratio under swarm condition. Further information can be found in the respective paper.
Uploaded on March 3, 2021

On the right side of the page, there are three informational boxes:

- RODARE Docs** 
Have a look at the restructured documentation and blog system of RODARE. We now can more easily notify about news and features. You also find tutorials there.
Visit <https://rodare.hzdr.de/about>.
- RODARE now offers usage statistics!** 
Thanks to the great folks @inveniosoftware we are able to provide usage statistics for record views and downloads.
Read the [blog post](#) to get more information about the new feature.
- RODARE** 
ROSSENDORF DATA REPOSITORY
Welcome to Rodare! 
The new data publication platform at HZDR.
Read more about Rodare on our overview page.

Powered by:



Registered in:

re3data.org
REGISTRY OF RESEARCH DATA REPOSITORIES



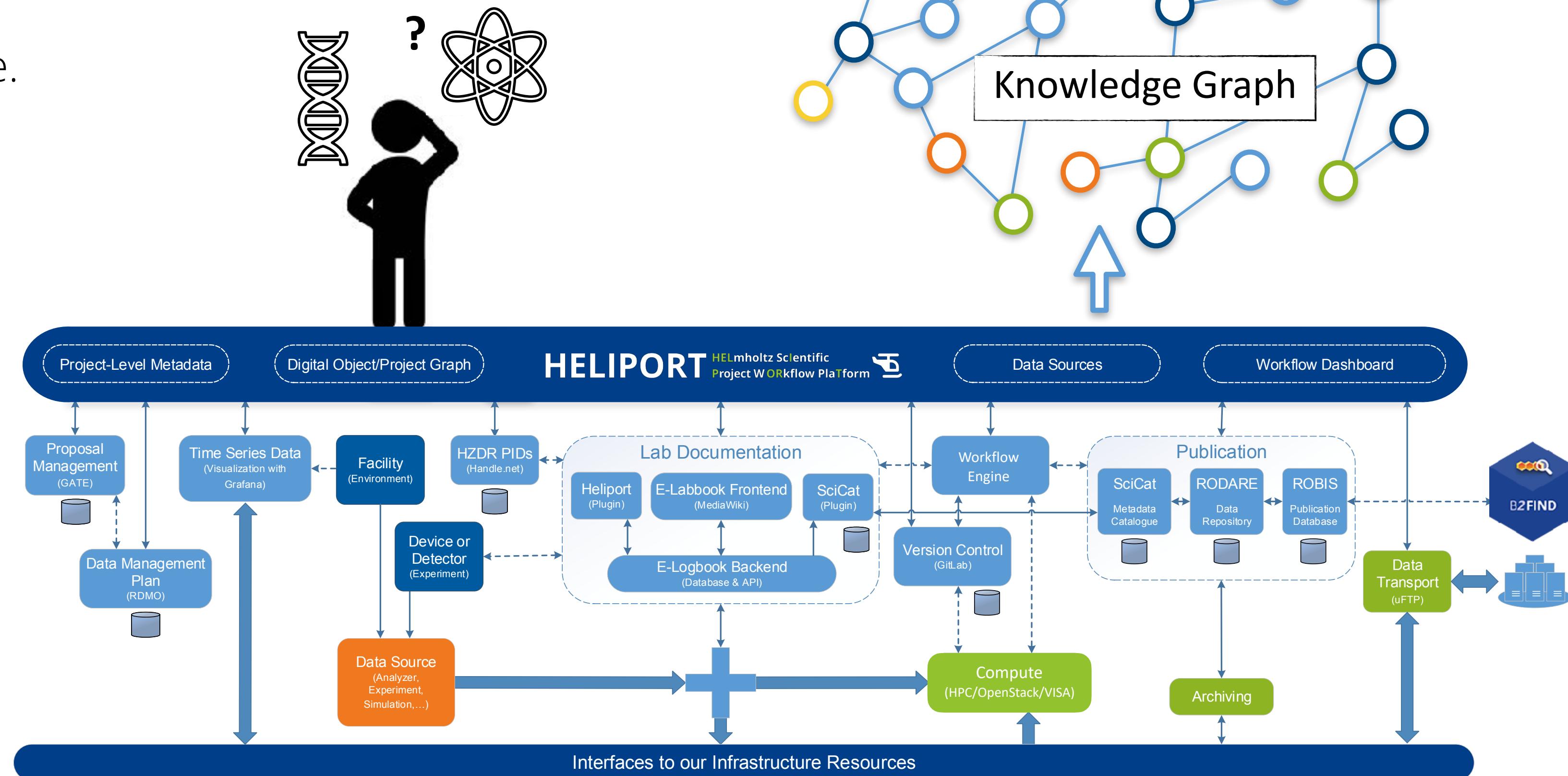
<http://doi.org/10.17616/R3BR40>

Findable with:



Our Observations Over the Following Years...

- We need to support the entire experiment with reliable **interconnected tools** to enable comprehensible and FAIR science.
- The resulting IT infrastructures are complex.
- Documentation is necessary, but typically time is missing.
- Scientists often don't know which services are available at facilities and how to use them.
- An overarching system **guiding our scientists** (and visitors) through the lifecycle of their research project is essential.





The HELIPORT project aims at developing a platform which accommodates the **complete life cycle** of a scientific project and links all corresponding programs, systems and workflows to create a more **FAIR** and comprehensible project description.

Project Members:



Funded by:



Phase-resolved Higgs response in superconducting cuprates

Tags Project Timeline Object Graph Project

Systems Resources Automation Results

- Version Control
- Data Source
- UNICORE Jobs
- Archive

- Data Management Plan
- SSH Files/Directories
- UNICORE Storages
- Publication

- Documentation
- + Digital Objects
- + Data Source
- + UNICORE Jobs
- + Archive

To Do: Metadata crosswalk to schema.org ResearchProject

```
{
  "namespaces": {
    "datacite": "http://purl.org/spar/datacite/",
    "rdfs": "http://www.w3.org/2000/01/rdf-schema#",
    "heliport": "https://heliport/schema/",
    "time": "http://www.w3.org/2006/time#",
    "dc": "http://purl.org/dc/terms/"
  },
  "heliport:project_id": 28,
  "datacite:hasIdentifier": "HZDR.FWCC.2021.84769",
  "heliport:uuid": "09779261-200c-48c4-be9c-1298369d6a1c",
  "datacite:handle": "https://hdl.handle.net/None",
  "heliport:project_name": "PaN Research Project",
  "time:hasBeginning": "2021-04-01 09:14:34.295524+00:00",
  "datacite:hasDescription": "",
  "heliport:group": "FWCC",
  "heliport:owner": {
    "datacite:hasIdentifier": "132739",
    "datacite:orcid": null,
    "rdfs:label": "Knodel, Dr. Oliver (FWCC) – 132739"
  },
  "heliport:has_VersionControl": [
    {
      "heliport:version_control_id": 15,
      "dataciteuri": "https://datacite.org/works/10.5281/zenodo.5300000",
      "rdfs:label": "DataCite XML"
    }
  ],
  "heliport:has_DataSource": [
    {
      "heliport:data_source_id": 11,
      "dataciteuri": "http://ddd.hzdr.de/zenodo/5300000",
      "heliport:use_computer": null,
      "rdfs:label": "ddd",
      "datacite:hasDescription": ""
    }
  ]
}
```

Requirements and Expectations

- HELIPORT was intended to provide only the **proposal's metadata**, from internal and external scientists, to allow the assignment of resources.
- Over time, we realised that HELIPORT can also answer our scientists' most important questions, such as:

How can we **automate recurring processes** and keep track of status and data products?

How can we bring **new team members** or **visiting/external scientists** into our project lifecycle and all associated tools?

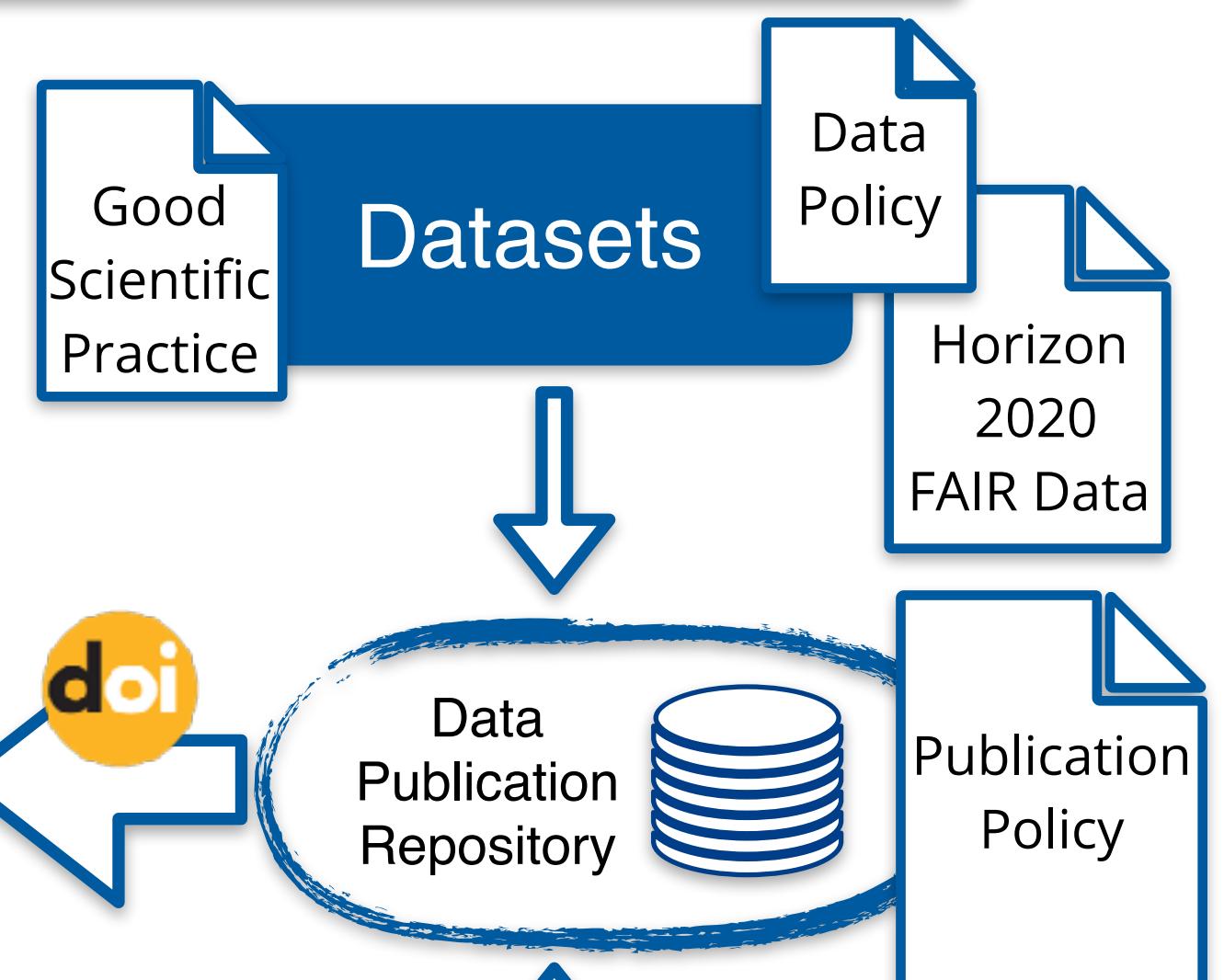


Which datasets or software can be **published** (and how)?

Where are data, software and how can I gain **access** to both of them?

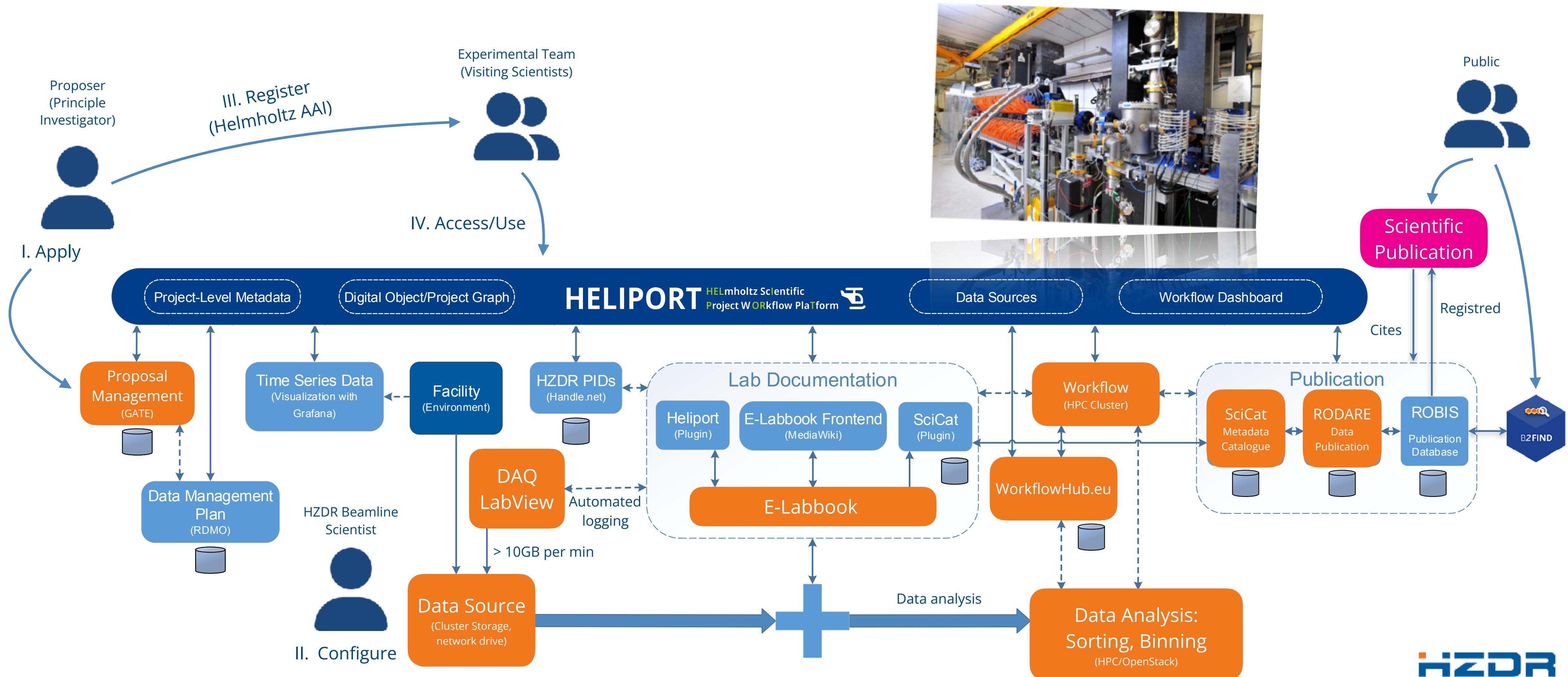
And how we can support them?!

What are the necessary steps towards a full comprehensible and FAIR research experiment ensuring data provenance?



Example: HELIPORT Supported Experiment at The TELBE Beamline

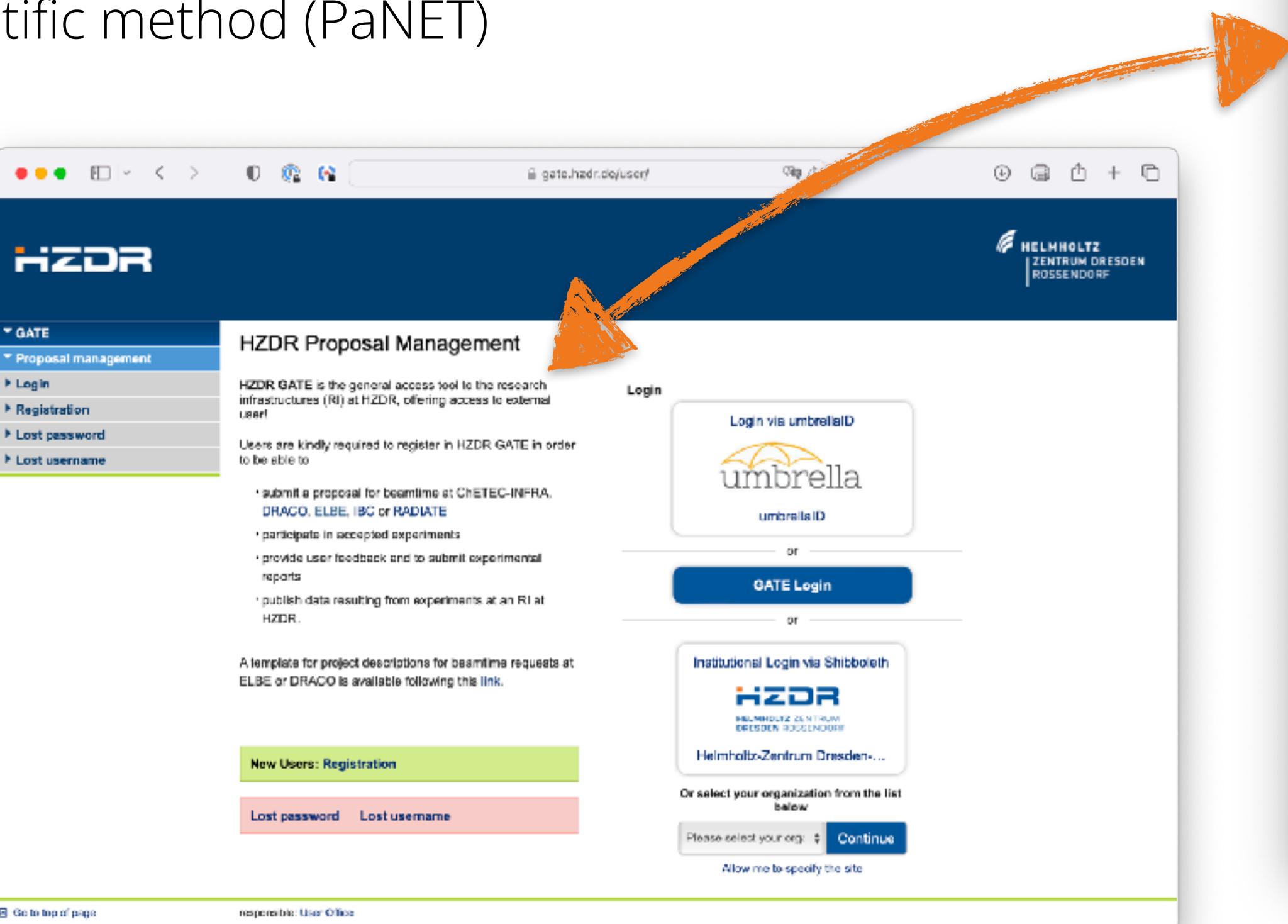
- HELIPORT provides access to our services and guides **external/visiting scientists** through the entire experiment.
- This requires the experiment to be mapped to systems in the HZDR infrastructure.



I. Proposal Submission

Automated transfer of project metadata from the proposal system (GATE) into HELIPORT:

- Title, Authors, Description,
- Beamtime schedule,
- Large-scale facility used,
- Scientific method (PaNET)



The screenshot shows the HELIPORT project properties page for a project titled 'Phase-resolved Higgs response in superconducting cuprates'. The page includes sections for 'Project Properties' (with fields like HZDR-ID, Digital Object ID, uuid, Landing Page, Created, Department, and Title), 'Tags' (with 'TELBE' selected), and 'Members and Contributors' (listing Gruber, Deinert, Knodel, Lokamani, and Mueller with their respective ORCID IDs and roles: Owner, Member, Member, Member, Member). An orange arrow points from the left side of this screen towards the HZDR GATE interface.

II. Project List and Dashboard

- Typically, a beam line scientist is the owner of a HELIPORT project and the proposer has the role of the manager and can add additional project members.
- Tags and sub-projects including inheritance are possible in the project list.

The image displays two side-by-side screenshots of the HELIPORT web application interface.

Left Screenshot (Project List):

- Header:** HELIPORT
- Search:** Search bar with a magnifying glass icon.
- Navigation:** About, Docs, knodel39
- Section:** Project List
- Table:** A list of projects with columns: Project Name, Last Modified, and Owner.
- Projects:**
 - Semantic x-Lab (Last Modified: Jul 11, 2023, Owner: Voigt, Martin (FWCC-D) - 141575)
 - gELBE Projects (Last Modified: Apr 24, 2023, Owner: Mueller, Dr. Stefan (FWCC) - 7394)
 - gELBE beamtime 21102205-ST (Last Modified: Sep 11, 2023, Owner: Mueller, Dr. Stefan (FWCC) - 7394)
 - gELBE beamtime 21202619-ST (Last Modified: Sep 11, 2023, Owner: Mueller, Dr. Stefan (FWCC) - 7394)
 - Example parent project (Last Modified: Apr 24, 2023, Owner: Voigt, Martin (FWCC-D) - 141575)
 - ML Ops Project (Last Modified: Jun 06, 2023, Owner: Knodel, Dr. Oliver (FWCC) - 132739)
 - SOTA on Uncertainties (Last Modified: May 23, 2023, Owner: Pape, David (FWCC) - 139658)
 - Phase-resolved Higgs response in superconducting cuprates (Last Modified: May 23, 2023, Owner: Gruber, Thomas (FWCC-D) - 141575)
 - Digital Twin Showcase (Last Modified: Jun 07, 2023, Owner: Voigt, Martin (FWCC-D) - 141575)
 - Beamtime Dashboard Test (Last Modified: May 31, 2022, Owner: Voigt, Martin (FWCC-D) - 141575)
 - Rodare Data Publication Project (Last Modified: Aug 09, 2022, Owner: Knodel, Dr. Oliver (FWCC) - 132739)
- Buttons:** Create Project, Page navigation (1, 2, 3, 4, 5).
- Footer:** Powered by HZDR, FZJ, HU & HMC, Member of Helmholtz, Imprint, Privacy Policy, Terms of Use.

Right Screenshot (Project Dashboard):

- Header:** HELIPORT
- Search:** Search bar with a magnifying glass icon.
- Navigation:** About, Docs, knodel39
- Title:** Phase-resolved Higgs response in superconducting cuprates
- Section:** Project Timeline, Object Graph, Project
- Diagram:** A central graph illustrating the project's structure and workflow across four main categories: Systems, Resources, Automation, and Results.
- Systems:** Version Control, Data Management Plan, Documentation, Digital Objects.
- Resources:** Data Source, SSH Files/Directories, UNICORE Storages.
- Automation:** UNICORE Jobs.
- Results:** Archive, Publication.
- Interactions:** Arrows show relationships between components, such as Version Control feeding into Data Source, and UNICORE Jobs leading to Archive.
- Footer:** Powered by HZDR, FZJ, HU & HMC, Member of Helmholtz, Imprint, Privacy Policy, Terms of Use.

III. Resources: Documentation and Repositories

The documentation section is typically used to refer to all internal and external systems or services used:

- E-Labbook (Mediawiki),
- GitLab, Github, Workflowhub, ...

HELIPORT Documentation

ID	Description	System	Actions
67	Project documentation in Mediawiki	MediaWiki	<button>Open</button> <button>Edit</button> <button>Remove</button>

Add a Documentation

SEEK ID: https://workflowhub.eu/workflows/473?version=1

Version History

Version 1 (earliest) Created 17th May 2023 at 13:08 by Thomas Gruber
Initial commit

FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar 01

Main page ELN (public) How To Recent changes Random page Help about Mediawiki FWCC group FWCC FWCA FWCB FWCC FWCI FWCS Tools What links here Related changes Upload file Special pages Printable version Permanent link Page information Browse properties Create this page Page values

Data File: File:FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar 01_loops.dat

Workflowhub URL: https://workflowhub.eu/workflows/473/re.create?version=1

Workflowhub Version: 1

Repetition Rate: 50000 Hz

time on single step measurement: 1

FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar 01

Log Name: 22_DAQ_CdAs_120degs_WP_45degs_SHG_V_polar

Start Date: 2022/03/13 00:00:00

Belongs to Measurement: Measurement Day March 13 2022

Day Name: Day March 13 2022

BDA Power: mW

Frequency: THz

Polarizer: V

Angle: 45

Filter Used: No

AI2 Three: No

Pyro Channel No: 1

Stage1 Start Pos: mm

Stage1 Stop Pos: mm

Path binned: /bigdata/Sorted_data/2022/2022-03-March_datalog/2022-03-13/mm

Selcat Export No: 1

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MediaWiki

WorkflowHub

Sorting and registration of Terahertz ELBE raw data Version 1

Overview Files Related Items

Creators and Submitter

Creators Not specified

Submitter Thomas Gruber

License Creative Commons Attribution 4.0

Activity Views: 139
Created: 17th May 2023 at 13:08
Last updated: 17th May 2023 at 13:12

Tags

This item has not yet been

SEEK ID: https://workflowhub.eu/workflows/473?version=1

Version History

Version 1 (earliest) Created 17th May 2023 at 13:08 by Thomas Gruber
Initial commit

Version Control

ID	Name	Actions
7	Terabe sorting script	<button>View</button> <button>Open</button> <button>Edit</button> <button>Remove</button>

Add a Source Code Repository

HZDR GitLab Other New

Select where you want to create your new repository

HZDR GitLab repository GitHub repository

Powered by HZDR, FZJ, HU & HZMC

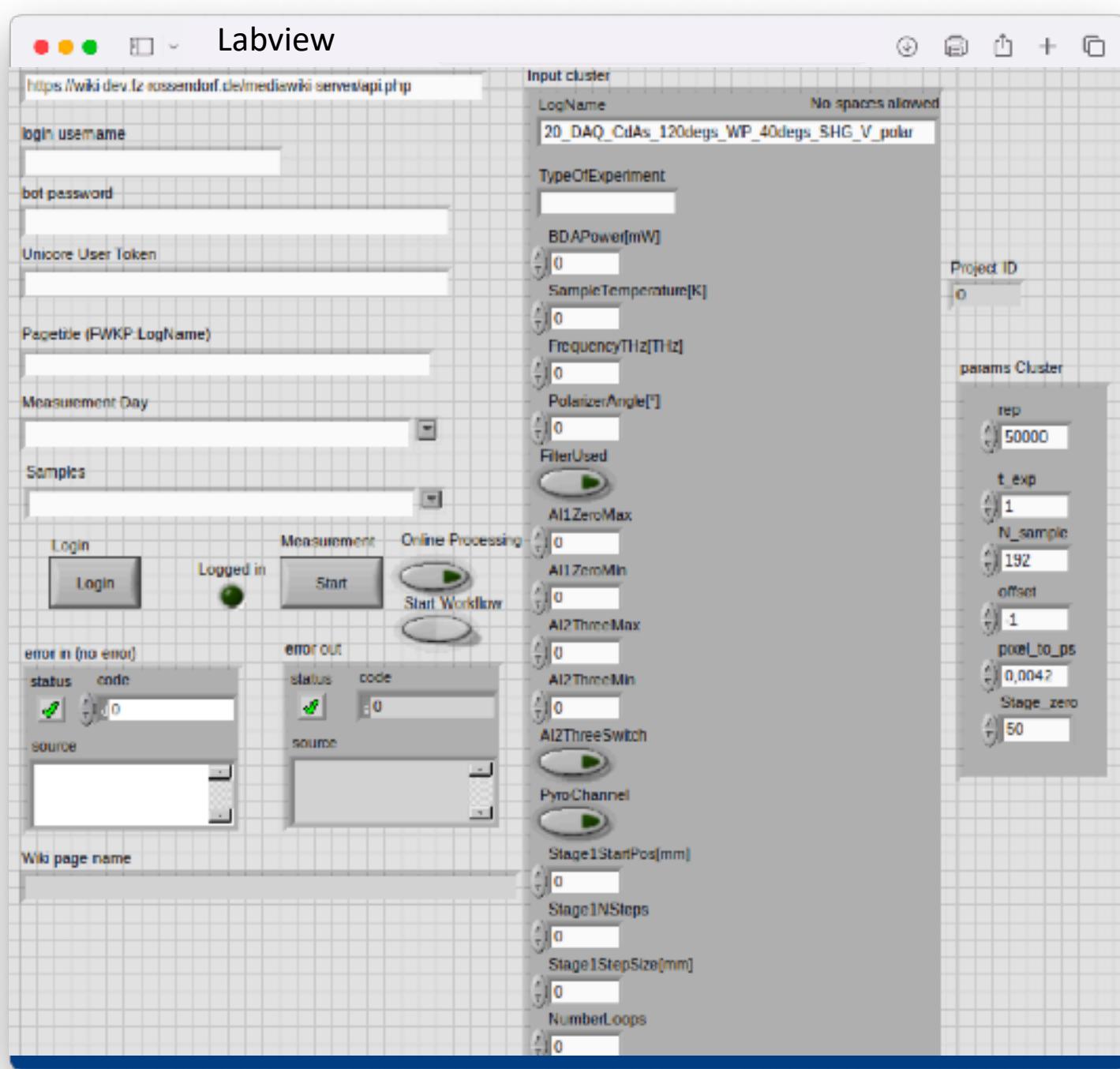
Member of Helmholtz

Imprint Privacy Policy Terms of Use

HZDR

IV. Detector Control and Workflows

- The **HELIPORT REST-API** enables the transfer of metadata between HELIPORT and external systems (e.g. detector control in LabView).
- The integrated job/workflow submission system collects metadata with **provenance information** provided by HELIPORT.
- Workflows (on our HPC cluster) can be accessed by any project member using the HELIPORT web frontend.



The screenshot shows the HELIPORT web interface. At the top, it displays the URL "https://vlsdms.fz-rossendorf.de/unicore/notify". The main content area is titled "Interaction between HELIPORT and UNICORE". It shows a section for "Project Jobs:" with a list item: "HELIPORT Test Job (27ed033...) @ HEMERA" with a green checkmark and a trash icon. Below this, it says "Submitted June 10, 2023, 4:20 p.m.". At the bottom, there are footer links: "Powered by HZDR, FZJ, HIJ & <HMC>", "Member of Helmholtz", and "Imprint Privacy Policy Terms of Use".

The screenshot shows the HELIPORT log output in a browser window. The log starts with "Sat Jun 10 16:20:01 CEST 2023: Created with ID 27ed0332-842e-4a07-bba8-85e8cf94dc9d" and continues with various log entries including security tokens, client details, and command execution. It ends with "TSI_EXECUTESCRIPT" and a series of commands like "#TSI_DISCARD_OUTPUT true", "#TSI_SCRIPT", "#TSI_UMASK 77", and "umask 77". The log concludes with notifications about the job's status and completion.

V. Data Sources

- Folders and files in our internal filesystems can be registered in HELIPORT as **data source**.
- Each **project member** has access to the files and folders using HELIPORT.
- The provenance of the data sets generated from an experiment is entirely comprehensible.

The screenshots illustrate the HELIPORT interface for managing data sources. The top screenshot shows the 'Add a Data Source' page with a protocol selection dropdown menu open, listing options such as https, http, ftp, ftps, file, ssh, and other. The bottom screenshot shows a list of data sources under the 'Beamtime_DSPEC_data' project, including various folders and files with their respective publish status, sizes, and timestamps.

Protocol Selection:

- ✓ Choose a Protocol
- https
- http
- ftp
- ftps
- file
- ssh
- other

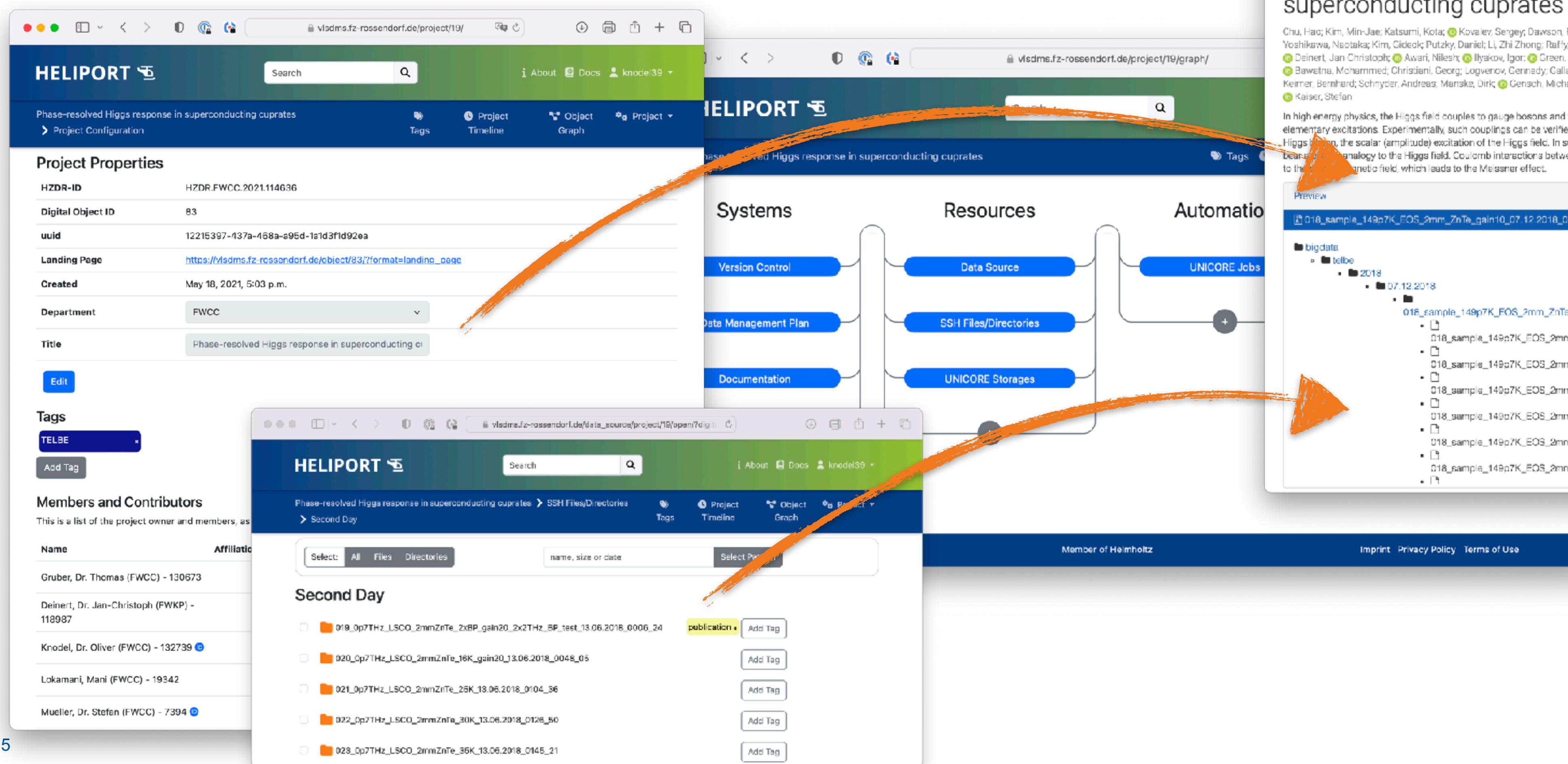
Data Sources List:

Name	Action	Size	Last Published
15092021	Publish Zipped		Sept. 21, 2021, 2:18 p.m.
16092021	Add Tag		Sept. 21, 2021, 3:05 p.m.
20092021	Add Tag		Sept. 21, 2021, 2:16 p.m.
ELBE TI Current-data-2021-09-17 16_52_59.xlsx	Publish	53 Kib	Sept. 21, 2021, 2:16 p.m.
ELBE_2021-09-15.png	Publish	121 Kib	Sept. 21, 2021, 2:16 p.m.
ELBE_2021-09-16.png	Publish	112 Kib	Sept. 21, 2021, 2:16 p.m.

VI. Integration in an Overall Data Publication Workflow

Automated data publication with:

- Metadata from Proposal System,
- Files and folders registered and selected in HELIPORT.



RODARE

December 16, 2021

Phase-resolved Higgs response in superconducting cuprates

Chu, Hao; Kim, Min-Jae; Katsumi, Kolar; Kovalev, Sergey; Dawson, Robert David; Schwarz, Lukas; Yoshikawa, Nectala; Kim, Cideck; Putzky, Daniel; Li, Zhi Zhong; Raffy, Hélène; Germanakos, Serafim; Deinert, Jan Christoph; Awari, Niles; Ilyakov, Igor; Green, Bertram Würdich; Chen, Min; Bawelina, Mohammed; Christiani, Georg; Logvenov, Gennady; Gallais, Yann; Boris, Alexander V.; Keimer, Bernhard; Schryer, Andreas; Manske, Dirk; Gensch, Michael; Wang, Zhe; Shimano, Ryosuke; Kaiser, Stefan

In high energy physics, the Higgs field couples to gauge bosons and fermions and gives mass to their elementary excitations. Experimentally, such couplings can be verified from the decay product of the Higgs boson, the scalar (amplitude) excitation of the Higgs field. In superconductors, Cooper pairs bear a similar analogy to the Higgs field. Coulomb interactions between the Cooper pairs give mass to the magnetic field, which leads to the Meissner effect.

Preview

018_sample_149a7K_EOS_2mm_ZnTe_gain10_07_12_2018_0527_47.zip

bigdata

telbe

2018

07.12.2018

018_sample_149a7K_EOS_2mm_ZnTe_gain10_07_12_2018_0527_47

018_sample_149a7K_EOS_2mm_ZnTe_gain10_A10_Experiment

38.4 MB

Versions

Version 2 Dec 16, 2021

10.14278/rodare.1289

See more details

VII. Search & Reuse: Metadata Catalogue SciCat

- With our data publication repository RODARE we provide a platform for publishing datasets.
- In RODARE, bibliographic metadata is based on **DataCite**.
- For additional **scientific metadata** we use SciCat and reference the specific datasets in RODARE or HELIPORT.



A screenshot of the SciCat search interface. The top navigation bar shows 'Datasets /'. Below it is a search bar with 'Text Search' and filters for 'My Data', 'All Public Data', 'All', 'Archivable', 'Retrievable', 'Work In Progress', 'System Error', and 'User Error'. A sidebar on the left contains filters for 'Location', 'Group', 'Type', 'Keywords', and 'Start Date – End Date', with a '+ Add Condition' button. The main area displays a table of three datasets:

Name	Run No.	Source Folder	Size	Start Time	Type
upload/nfs	0 B	2022-07-05 Tue 11:28		derived
Second dataset/nfs	0 B	2022-07-05 Tue 10:29		derived
Dataset/nfs	0 B	2022-07-05 Tue 10:15		derived

A screenshot of the SciCat dataset details page for 'Raw Dataset Example 300'. The page is divided into several sections:

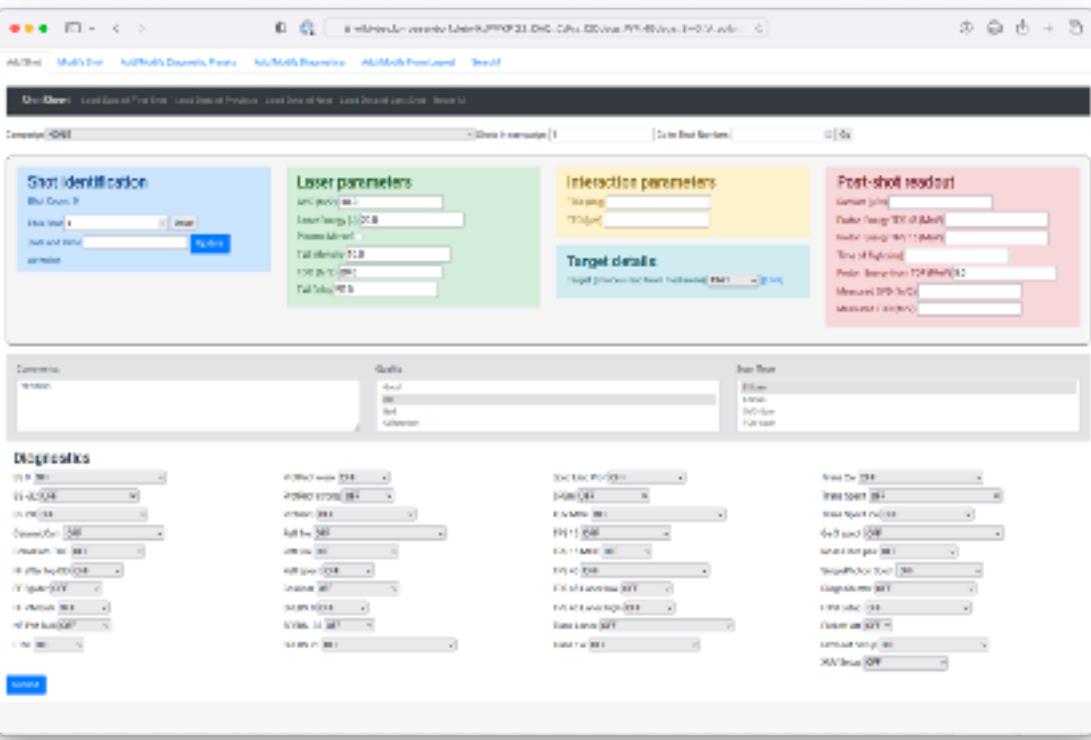
- General Information:** Name: Raw Dataset Example 300, Description: This input file was created to study a aluminum oxide film on rough aluminum surface with high spatial resolution. Load the dataset folder with nxs files to do analysis., PID: HZDR/73da2dfa-176f-4c5c-853a-b2ffbfca4e3d7, Type: raw, Creation Time: 2022-07-15 17:47:47, Keywords: Rough surface, aluminum oxide film, Smile simulation.
- Creator Information:** Owner: hzdr_ingestor, Principal Investigator: hzdr@scicat.hzdr.de, Orcid: orcid.org/0000-0000-9261-7643, Contact Email: hzdr@scicat.hzdr.de, Owner Group: hzdr_ingestor, Access Groups: hzdr_ingestor.
- File Information:** Source Folder: /bigdata/hpseim/scratch/lisa/Houghness, Size: 5 KB, Data Format: py.
- Deleted Documents:** Creates location: HZDR/Smile, Techniques: Simulation via Smile.
- Scientific Metadata:** A table with columns 'Search' and 'Value' containing various parameters like 'DigParticleBinningNc', 'DigProbNo', 'E_to_e0', 'Et_max', 'Et_max_D', 'GVD', 'LSI', 'J', 'L', 'N_steps', 'T00', 'Tsim', and 'Tsim_G'.

On the right side of the page, there is a small thumbnail image of a grayscale 2D plot showing a textured surface profile.

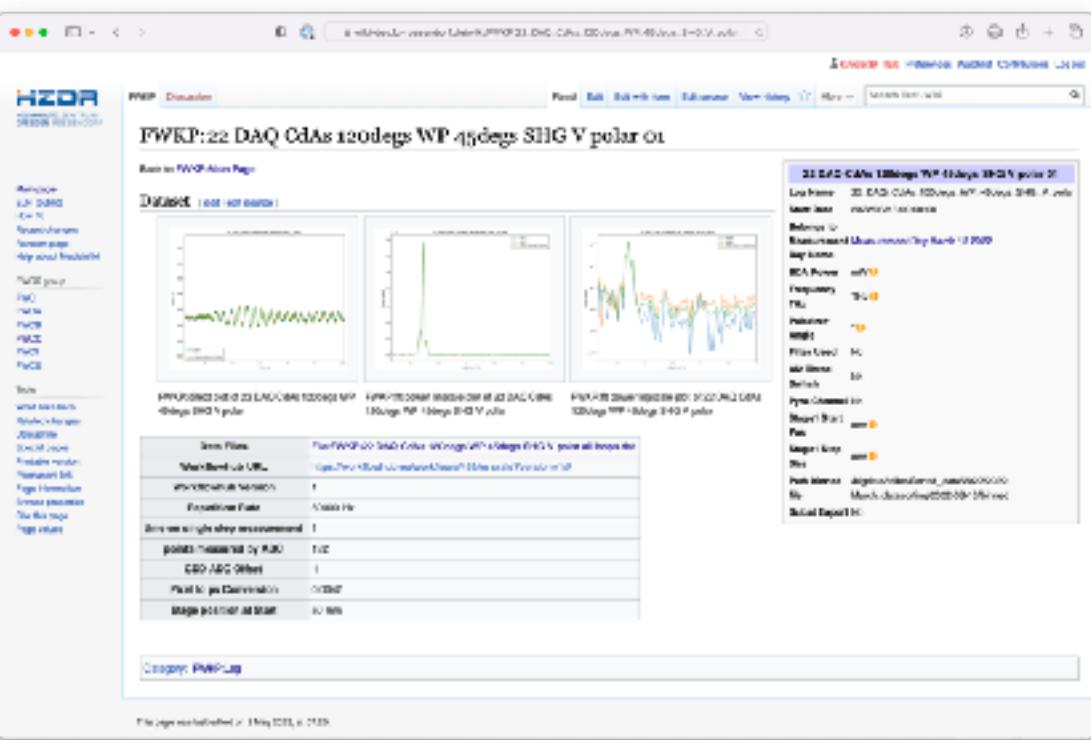
Metadata Catalogue SciCat and Data Repository RODARE (Draft)

Curated Metadata Source

ExperimentLogging app (ExL)



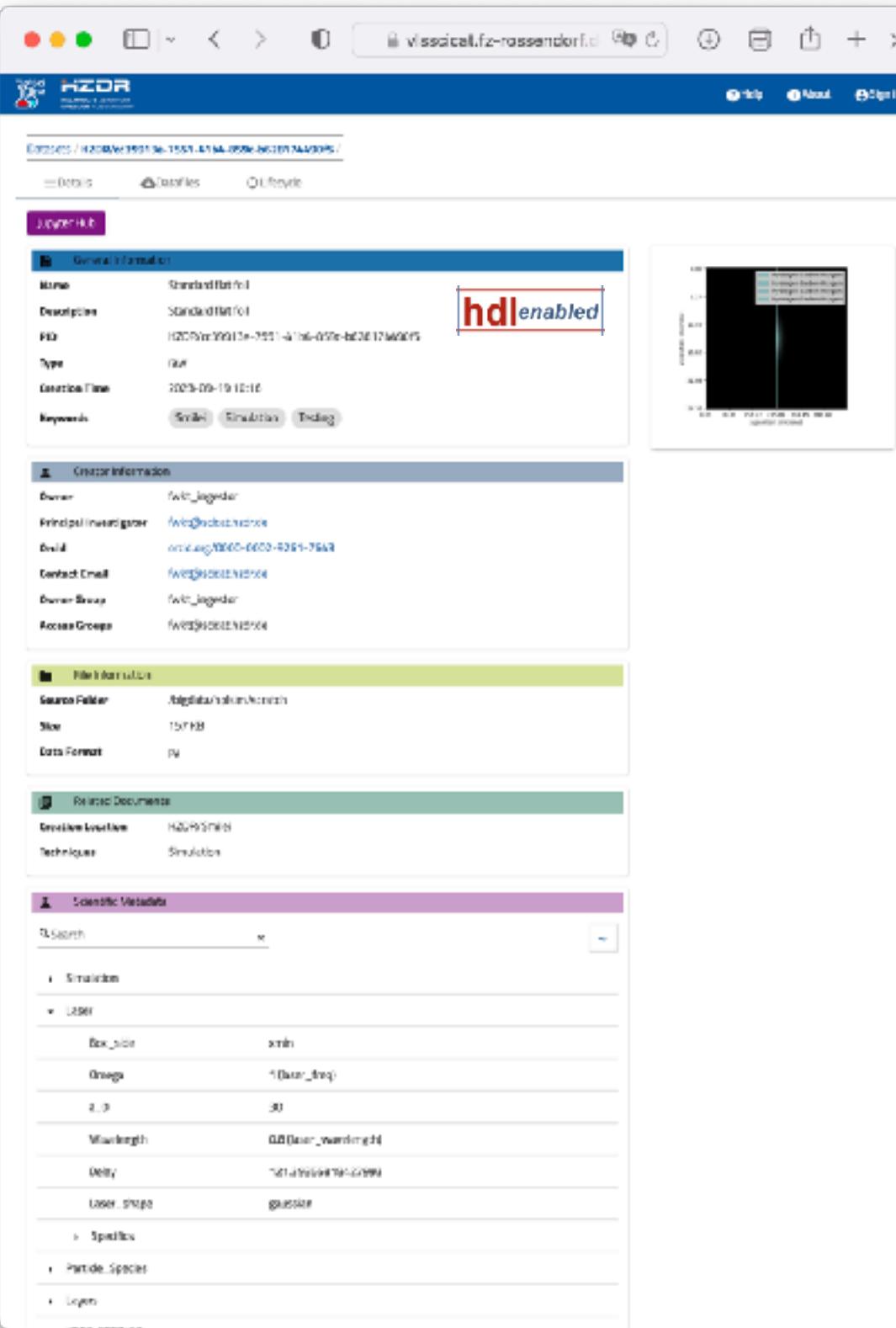
E-Logbook



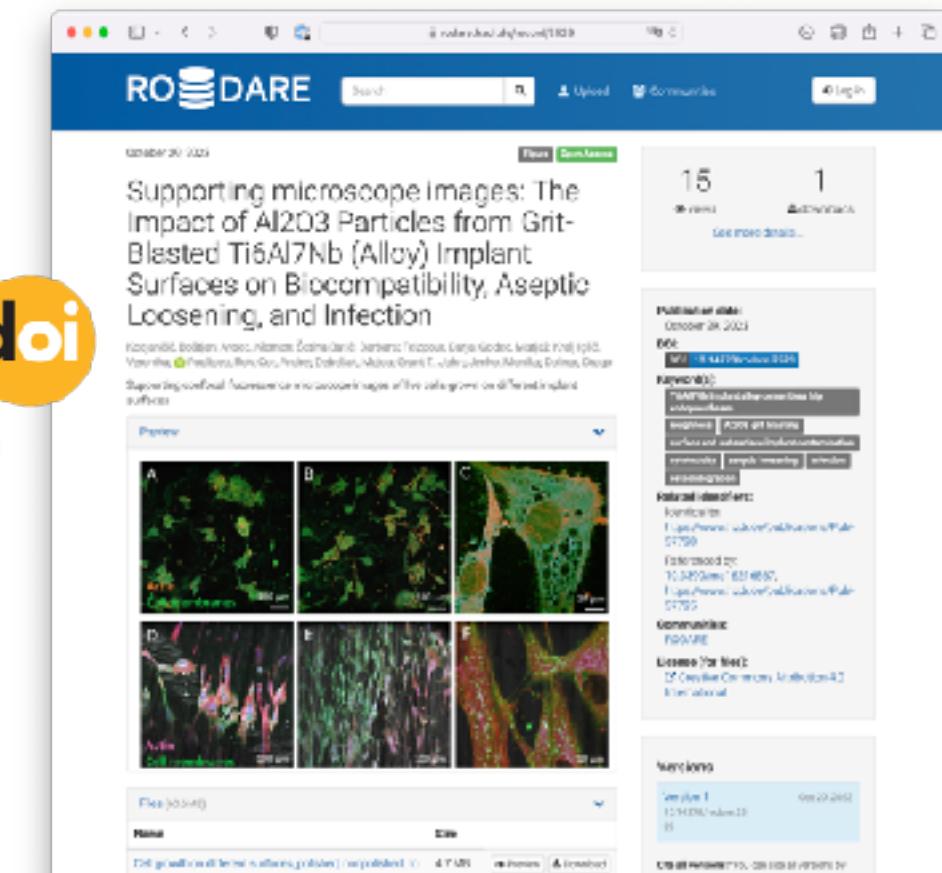
Direct API Call

Public Metadata Catalogue

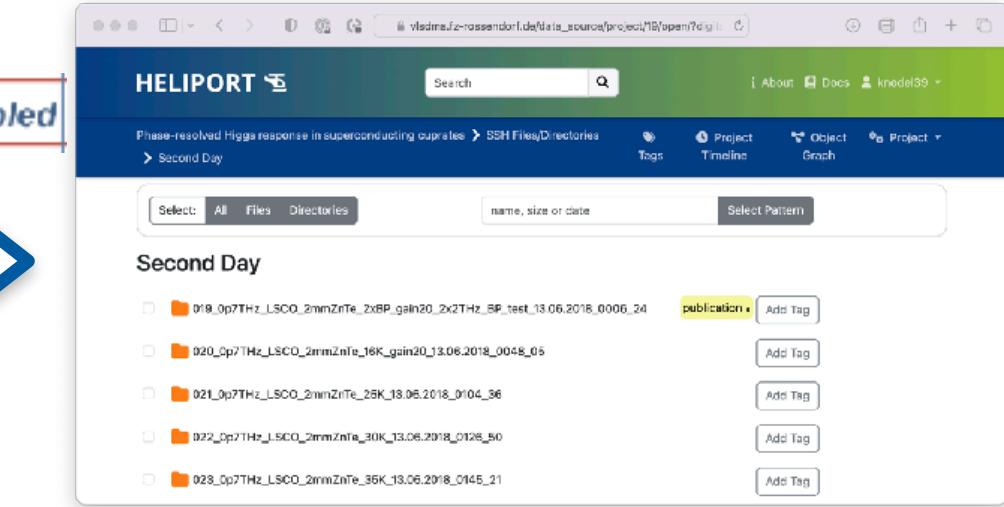
SciCat



RODARE

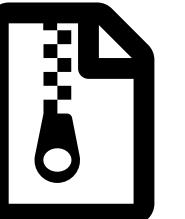


HELIPORT

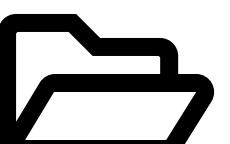


Data Access

Dataset



Filesystem



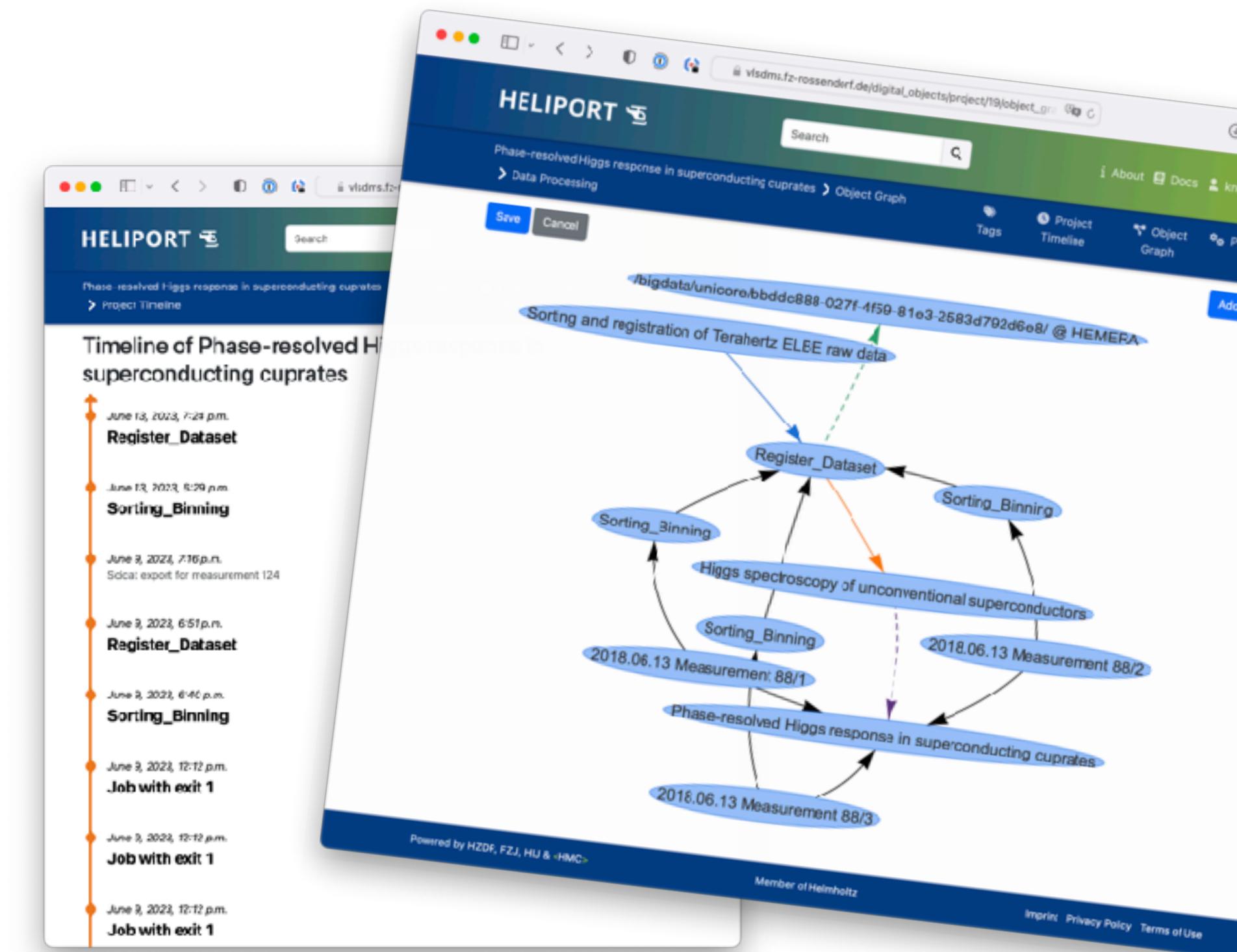
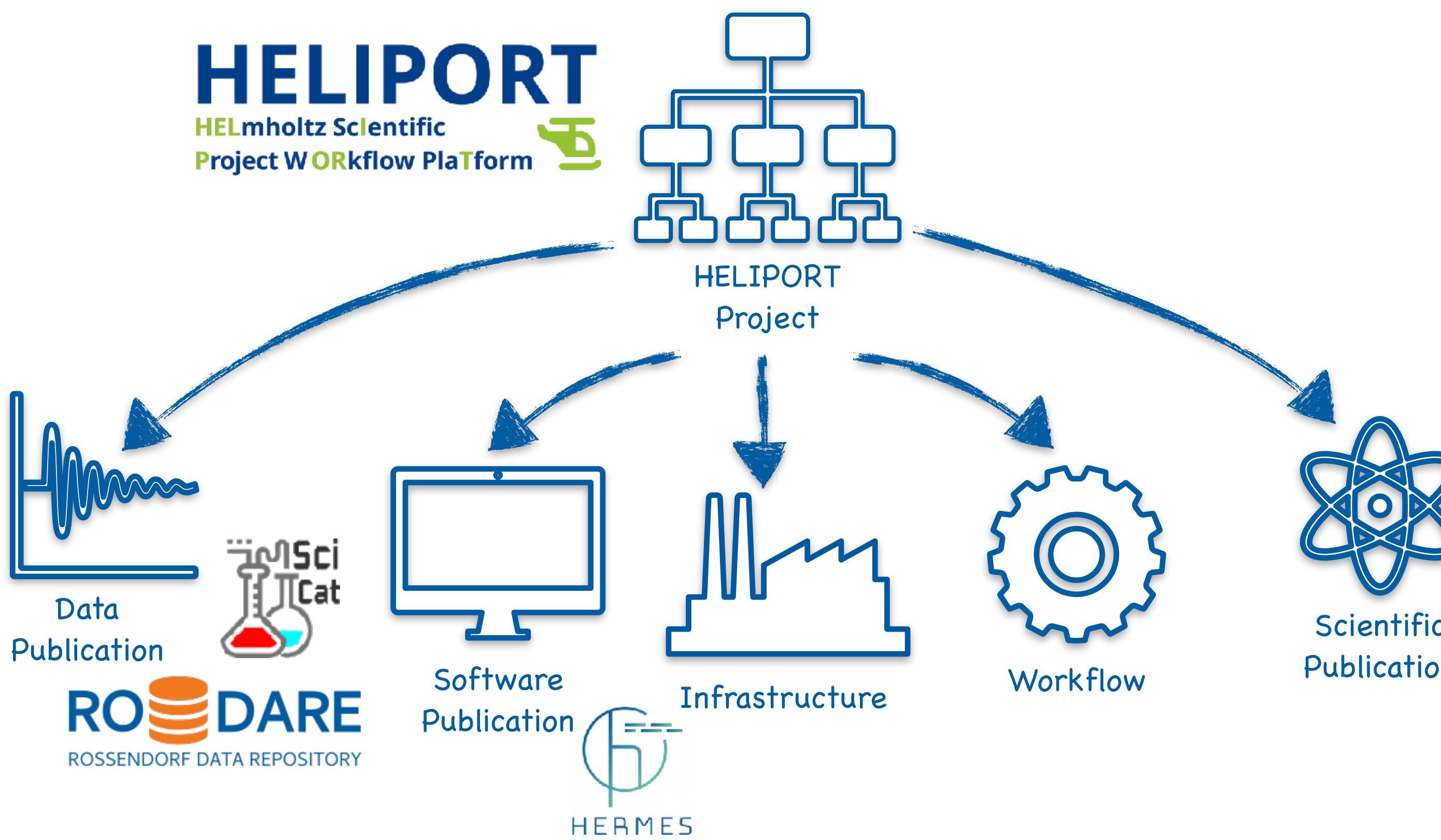
Tape Archive



Metadata from Experiment/Simulation

Conclusions

- Close and automated interaction of services and systems in our digital research landscape is essential to provide **FAIR** and **comprehensible** research projects.
- HELIPORT describes and **collects metadata** from services and systems involved in experiments.
- APIs and workflows are used to transfer metadata between our services and systems.



Resources

Website: heliport.hzdr.de



The guidance system HELIPORT aims to make the entire life cycle of a project at the HZDR findable, accessible, interoperable and reusable according to the FAIR principles, mentioned below. In particular, our data management solution deals with the areas from the generation of the data to the publication of primary research data, the workflows carried out and the actual research results. For this purpose, a concept was developed which shows the various essential components and their connections. Descriptions of the individual components can be found in our HZDR Data Management Strategy.

Intuitive and structured user interface

listProjects

Showing the most general HELIPORT project properties. Request more detailed information by appending `?id` to the url. Go to a specific project by appending its `?id` to the url. For more information on how to authenticate look in HELIPORT (user settings).

QUERY PARAMETERS

- `limit`: Integer. Number of results to return per page.
- `offset`: Integer. The initial index from which to return the results.
- `search`: String. A search term.
- `group`: String. group
- `cverz`: String. owner

Documentation Powered by Redoc

API Doc: heliport.hzdr.de/redoc/

Repository: codebase.helmholtz.cloud/heliport

HELIPORT Project ID: 1287

1,941 Commits | 5 Branches | 2 Tags | 3.4 GiB Project Storage

version 0.6.0 pipeline passed coverage 61.00% lifecycle experimental python ^3.8 code style black license GPL-3.0-or-later DOI [10.1145/3456287.3465477](https://doi.org/10.1145/3456287.3465477)

Bump django from 4.2.4 to 4.2.5 by HIFIS Bot authored 40 minutes ago

master / heliport / + History Find file Edit Clone

README GNU GPLv3 CHANGELOG CI/CD configuration Add Kubernetes cluster Add Wiki

Configure Integrations

Name	Last commit	Last update
.gitlab	Enable pydocstyle checks	1 month ago
.vscode	Fix djlint and prettier formatting and lint...	5 months ago
.yarn/releases	Frontend Package Management and Lint...	8 months ago
LICENSES	Resolve "Separate SVCs of workflow vis...	5 months ago
config	Resolve "Remove unused Flower stuff"	9 months ago
docs	Enable pydocstyle checks	1 month ago
heliport	Enable flake8-return- checks	3 days ago
heliport_config	Ruff: Enable E501 (lines too long)	1 month ago

Privacy | Imprint | Support | Status | Documentation | Changelog
<https://doi.org/10.1145/3456287.3465477>

1 INTRODUCTION

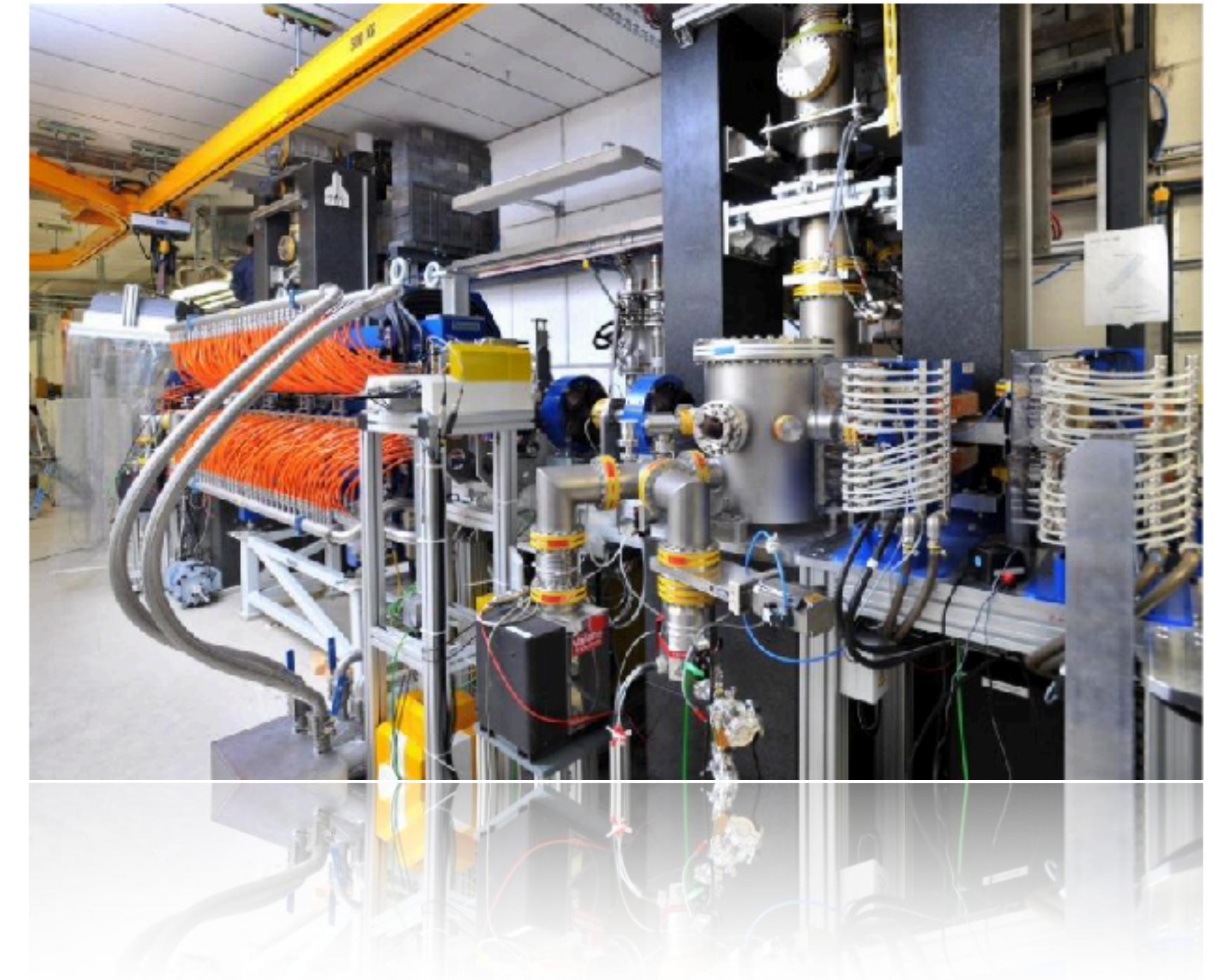
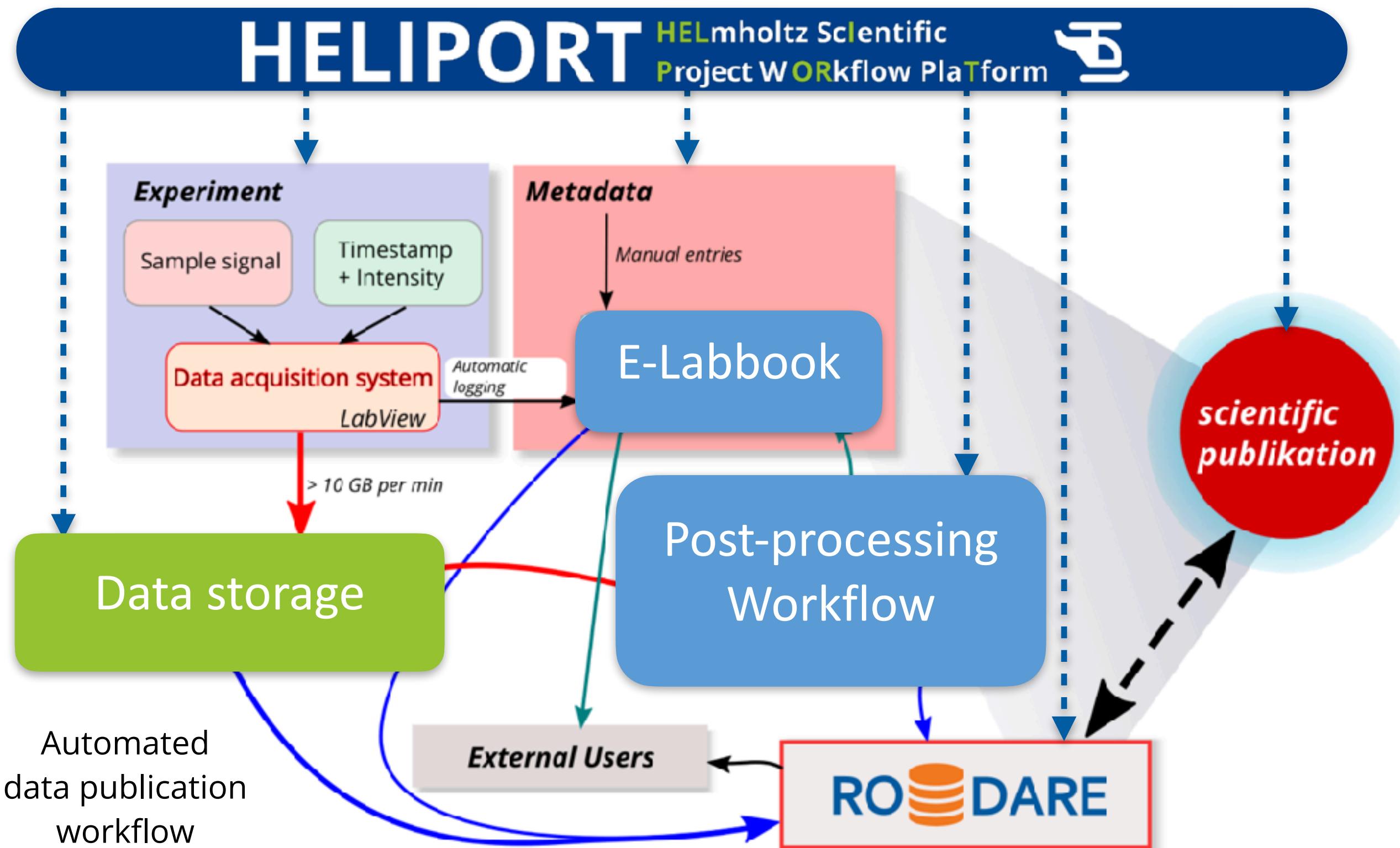
An essential objective of modern cutting-edge research should be to enable accessibility of the acquired research data and its re-usability across different research fields and their respective communities. The current generation of scientists is therefore faced with the challenging task of transferring experimental investigations into a data oriented research flow with strong focus on documenting every step closely following the FAIR [41] principles. The FAIR principles are well-established as standards in the field of research data management. The three pillars F (Findable), A (Accessible) and

Appendix



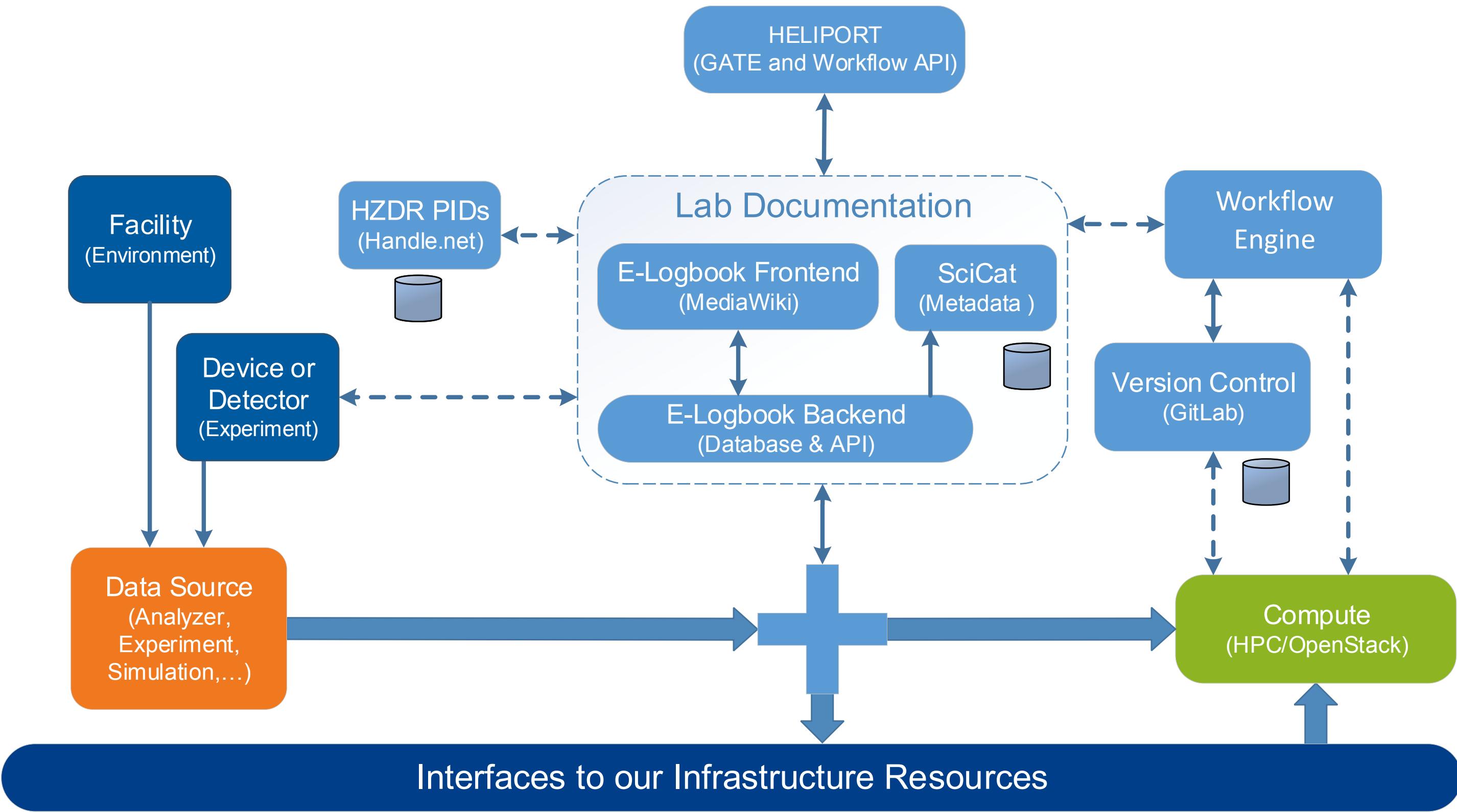
Example: Data Management View of the TELBE Experiment

- Terahertz facility at the ELBE center for High-Power Radiation Sources.
- In the future HELIPORT guides (external) scientists through the complete experiment.
- Submission of data analysis Jobs from LabView to UNICORE with visualisation in HELIPORT.



Documentation Ecosystem at HZDR

- Our **Electronic Lab Documentation** is a central database gathering information from various systems:
 - Proposal management (GATE),
 - Environmental data,
 - Devices (e.g. Labview),
 - Workflows,
 - (Meta)data databases.
- Different frontends are available:
 - SciCat (metadata only),
 - MediaWiki (structured user-definable views).
- The system is build on-top:



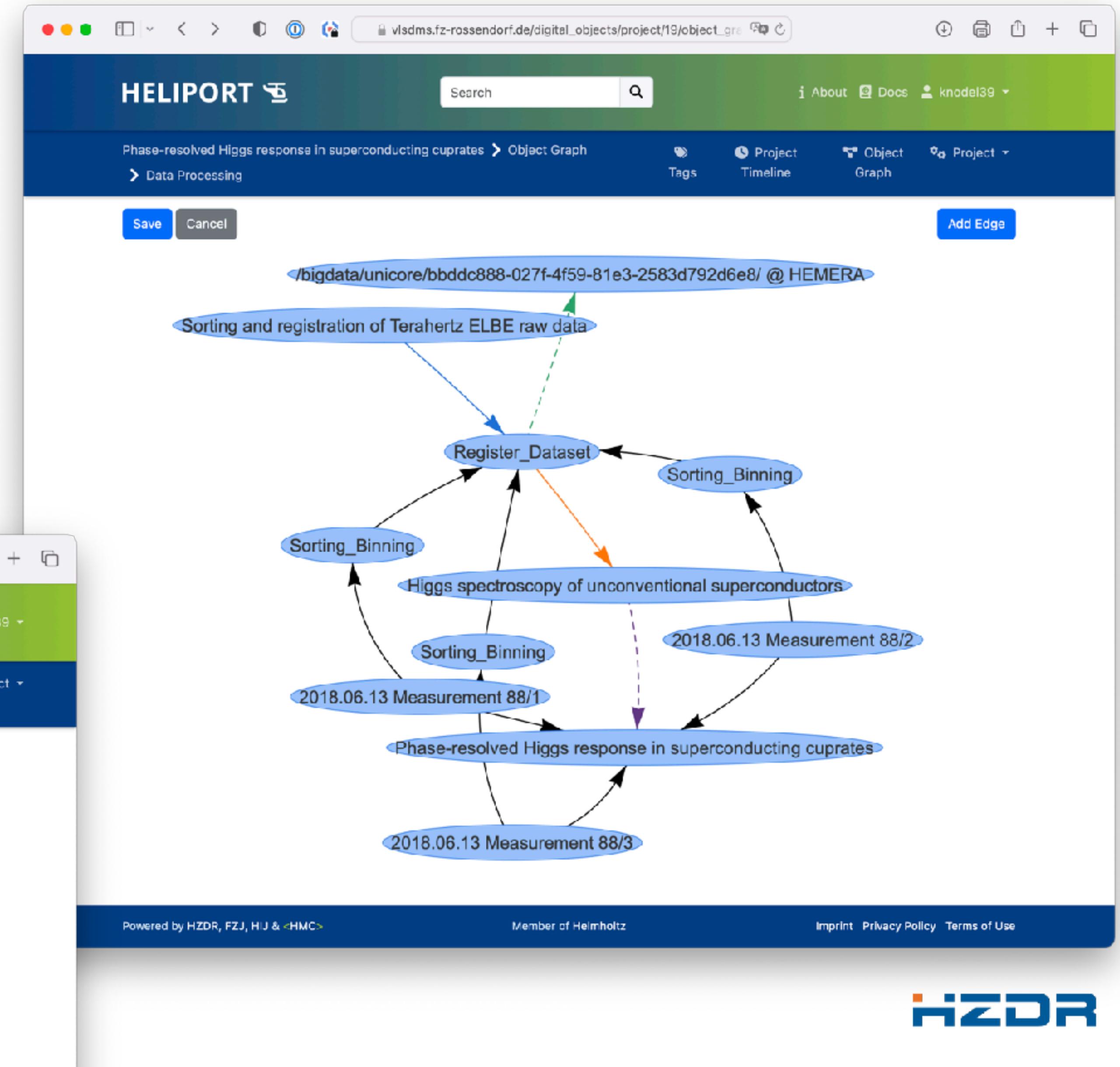
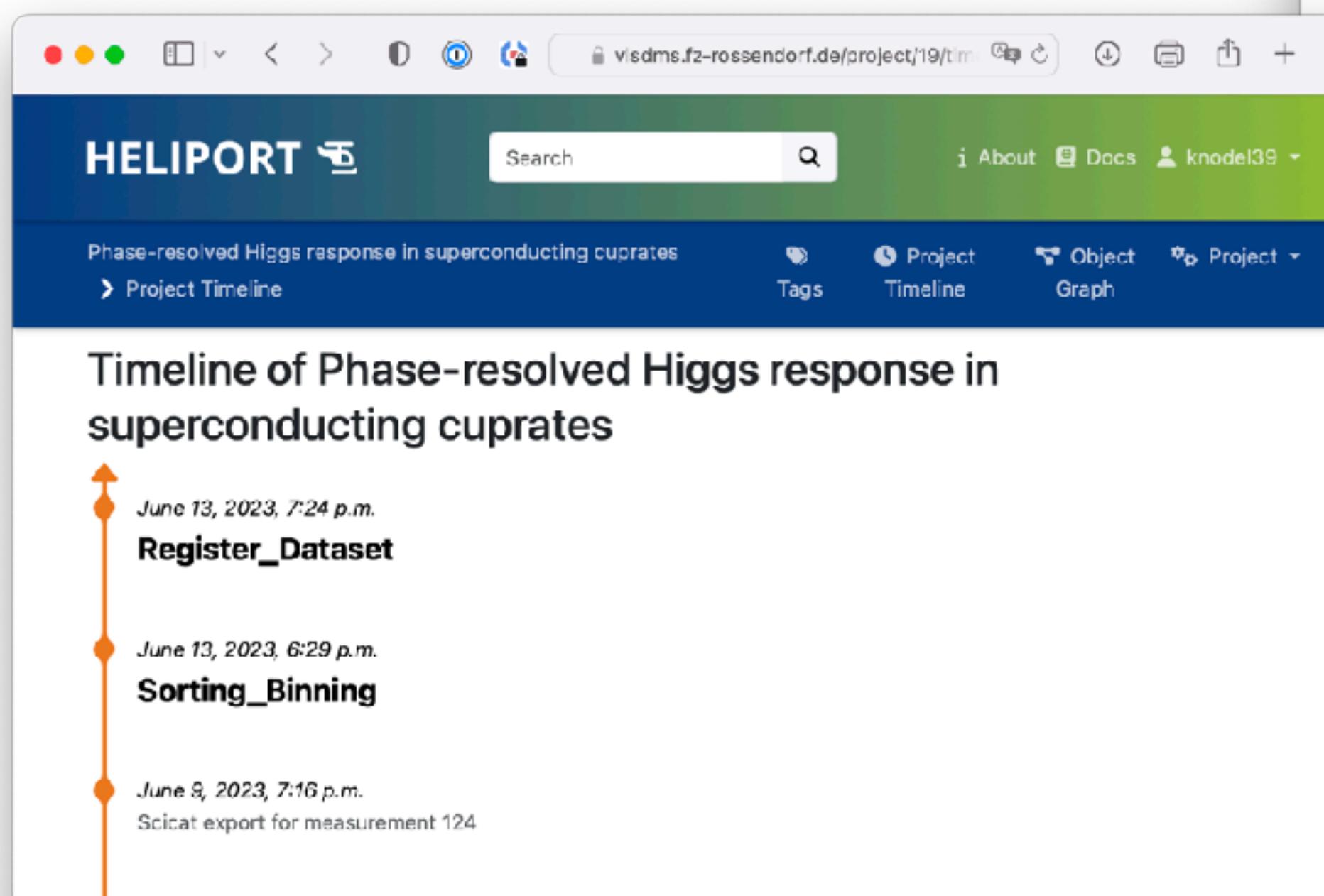
Semantic
MediaWiki



Cognitive Process Designer

Relations Between Digital Objects and

- Relations between digital objects are visualized to provide a top-level view on the project with dependencies.
- The relationships between simulation (surrogate model) and experiment can also be demonstrated.
- The versioning of an experiment is an essential extension, and first approaches via a timeline are being evaluated.



Workflow Architecture (in development)

- HELIPORT offers an infrastructure which permits the integration of various workflow languages and access modes to HPC infrastructures.
- The infrastructure keeps track of and collects the metadata and enables access to all resources involved.
- Next steps:
 - Python library sending workflow information directly to HELIPORT,
 - Provision of provenance information from Jupyter notebooks,
 - Use case: **PIConGPU**

