

Overarching Data Management Ecosystem HELIPORT

From Small Experiments to Large-Scale Research Facilities

1st Workshop on Open Science at GSI/FAIR, 19. October 2023

Oliver Knodel, Thomas Gruber, Martin Voigt, Jeffrey [Kelling](#), Mani Lokamani, Stefan E. Müller, David Pape and Guido Juckeland // contact: o.knodel@hzdr.de



Our Research Facility and our Large Scale Research Infrastructures

The Helmholtz-Zentrum Dresden - Rossendorf

— Employees approx. 1,470. Thereof 670 scientists.

— **HELMHOLTZ**

RESEARCH FOR GRAND CHALLENGES

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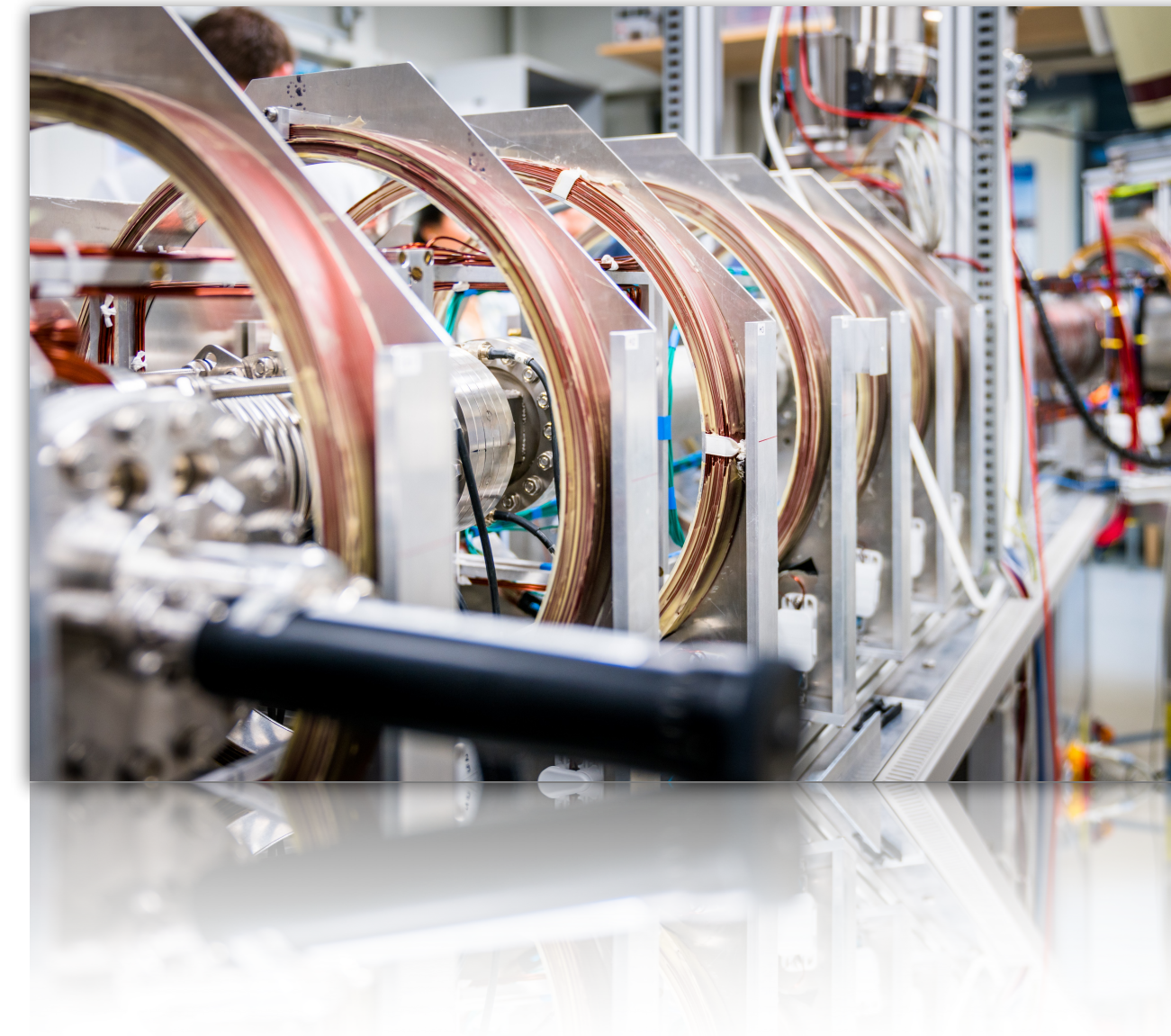
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— Energy, Health and Matter.



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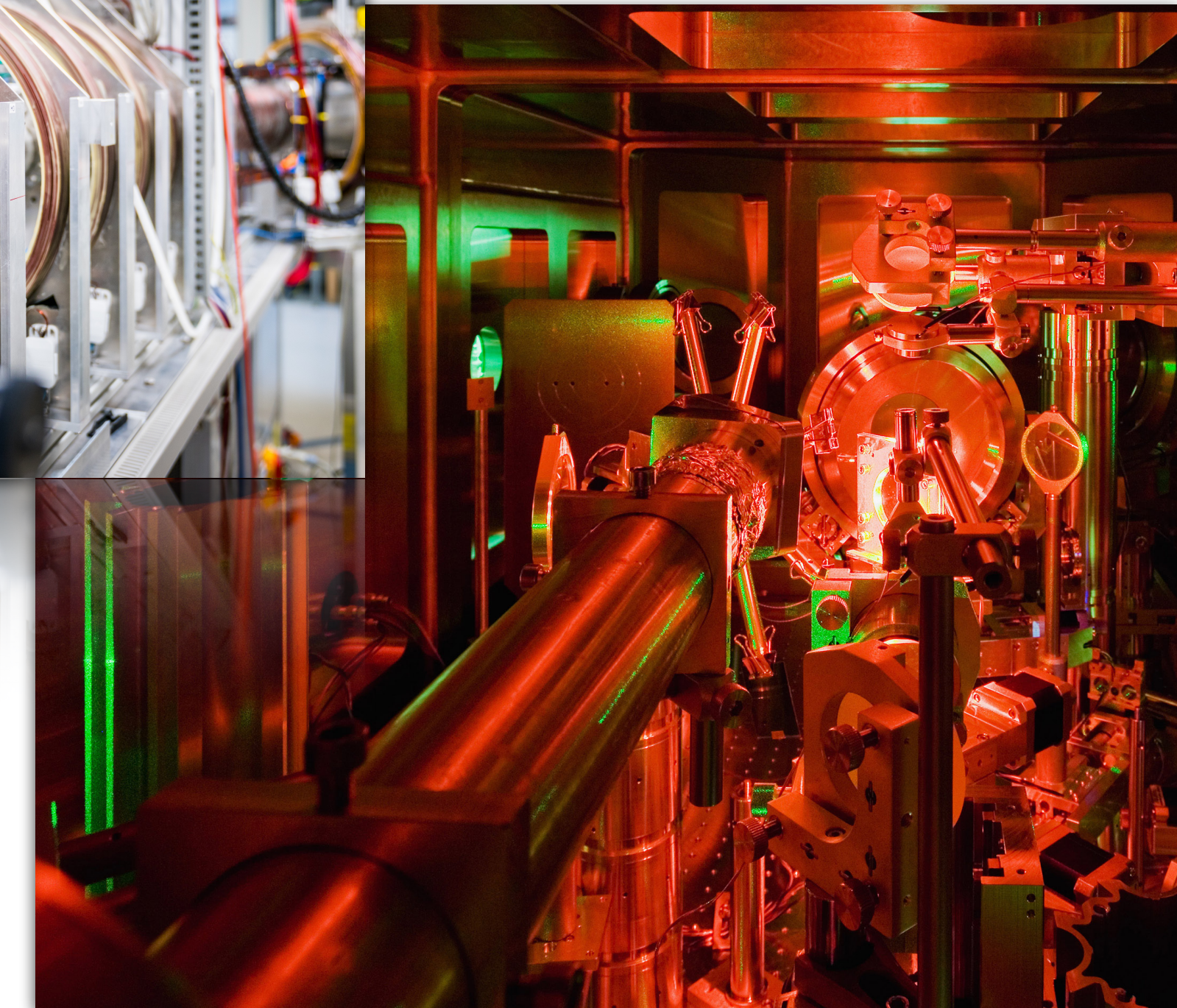
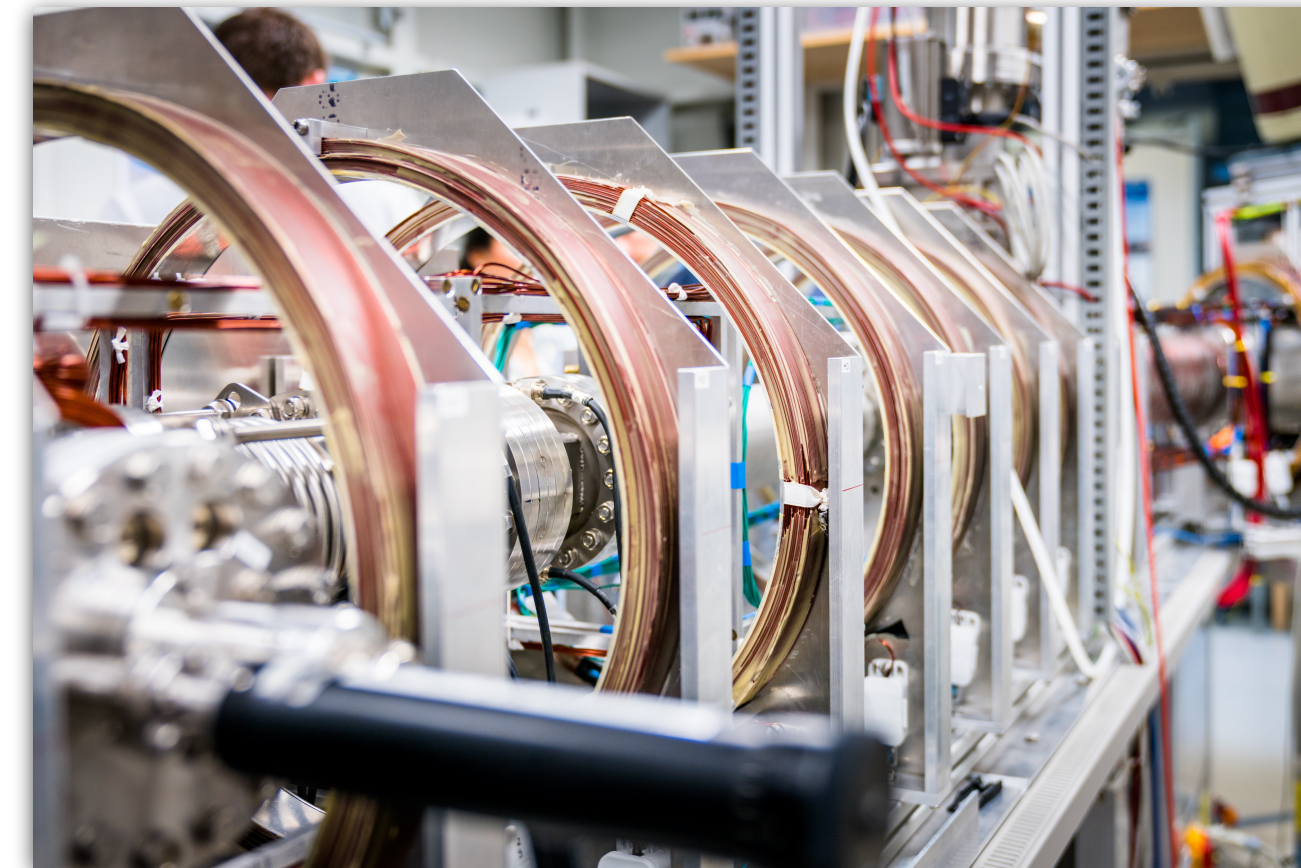
Research Fields

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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.



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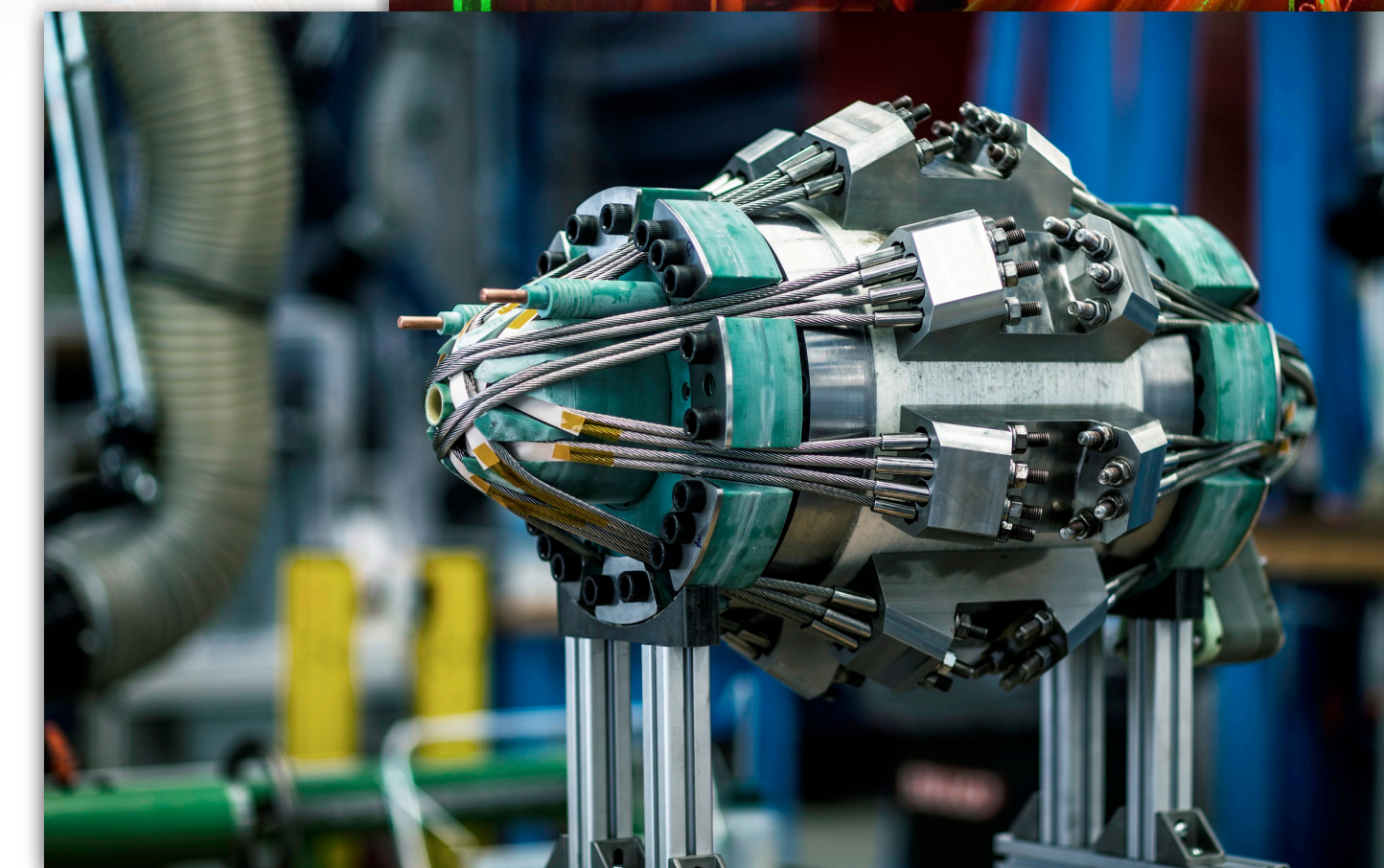
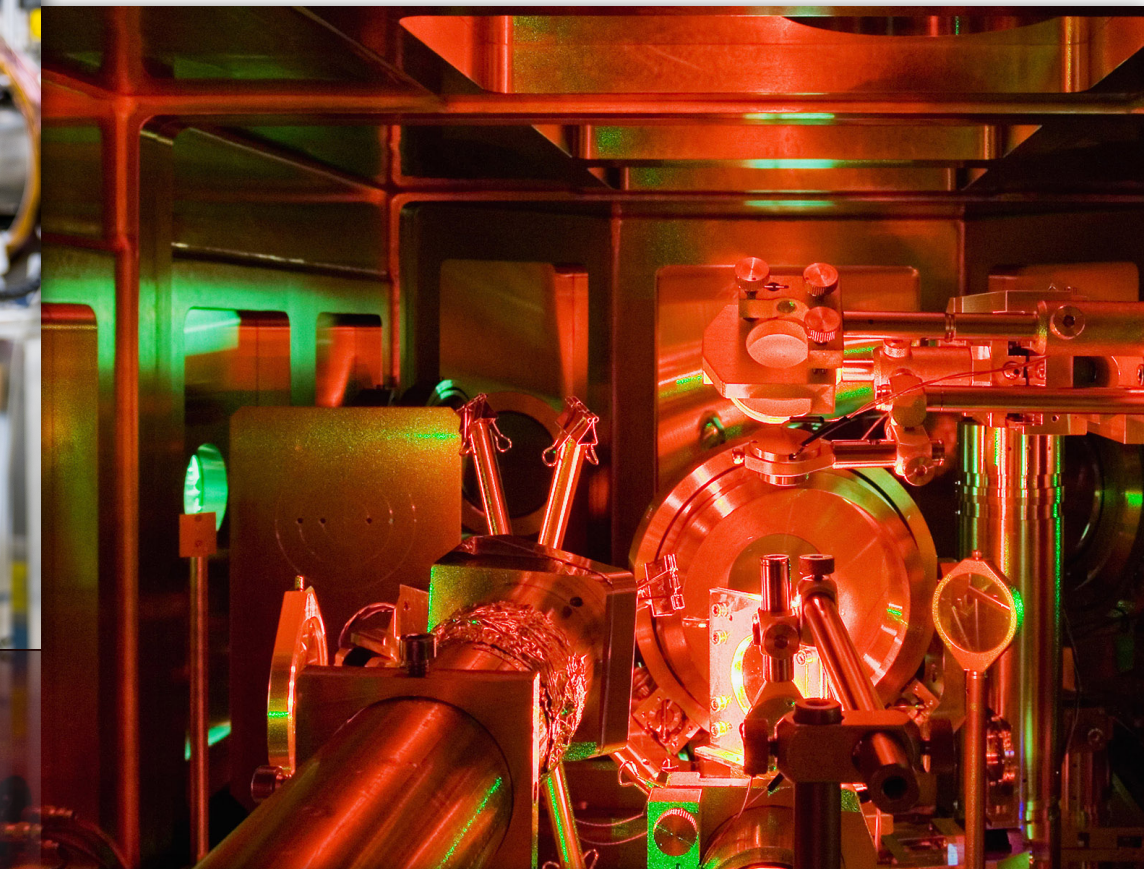
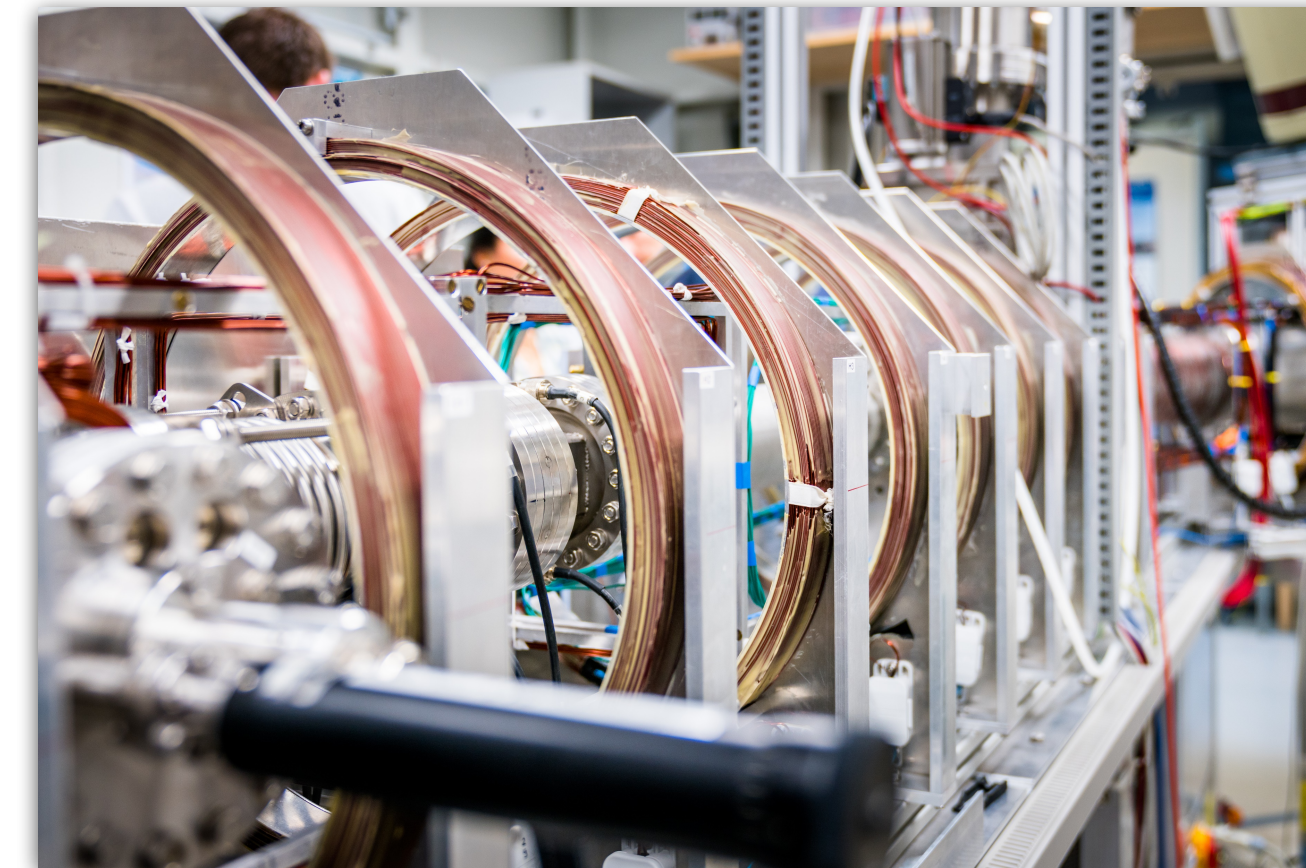
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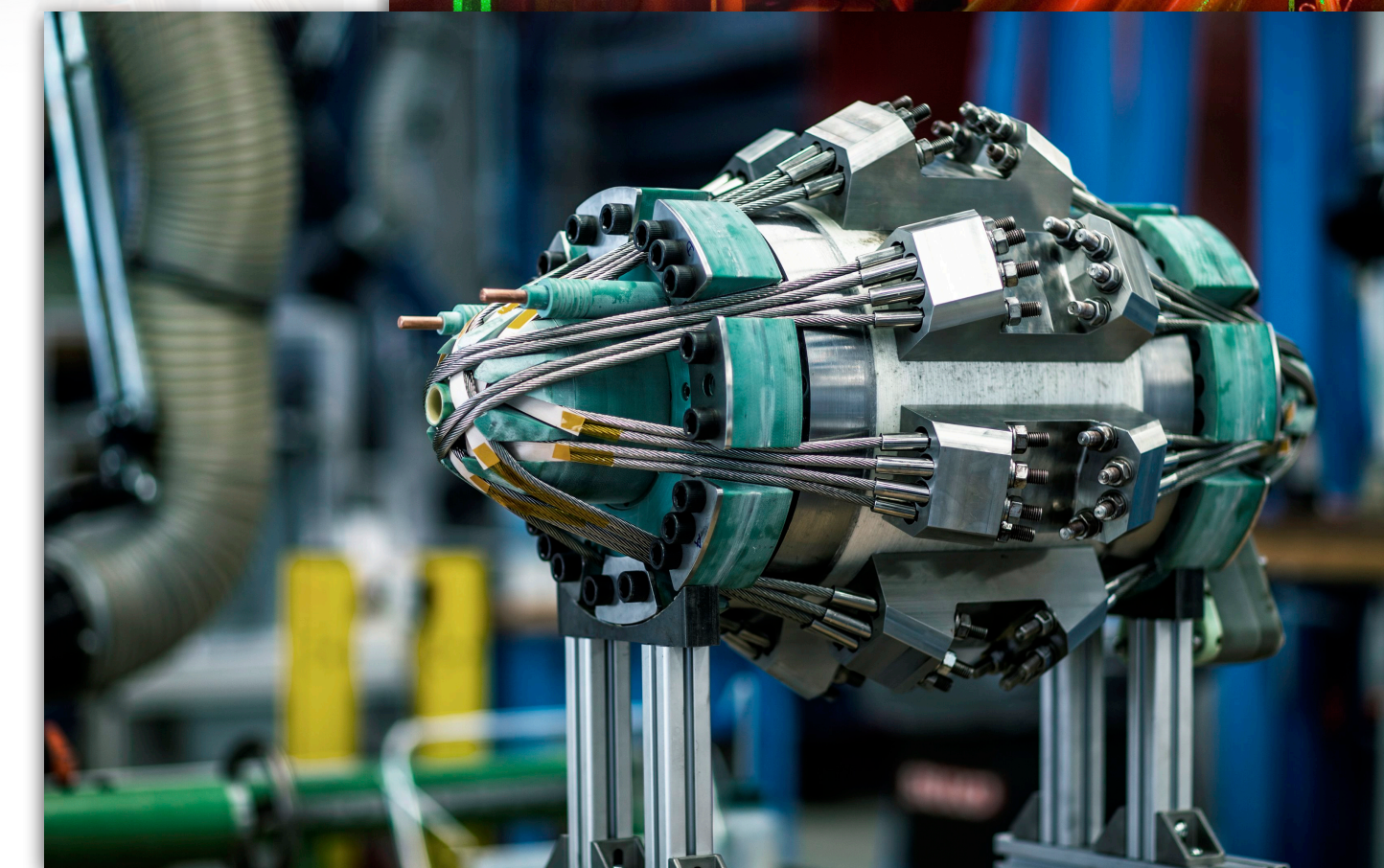
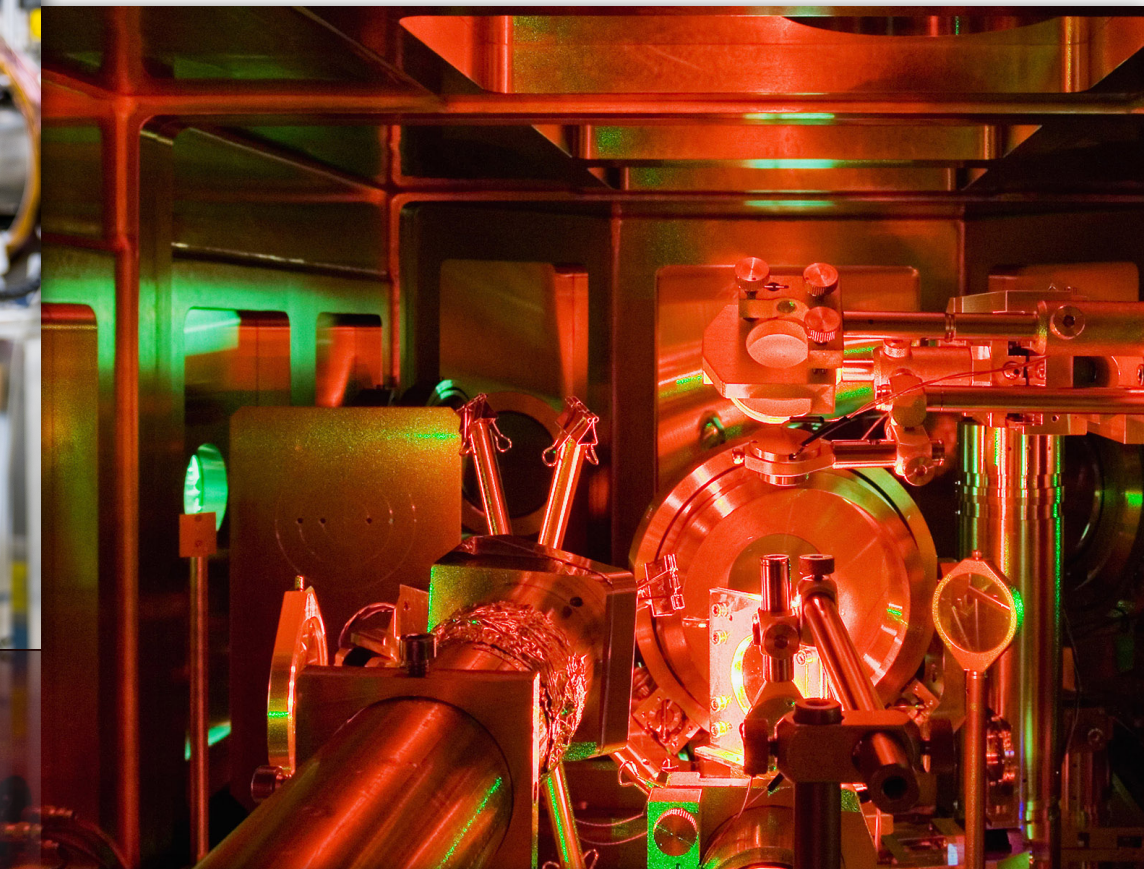
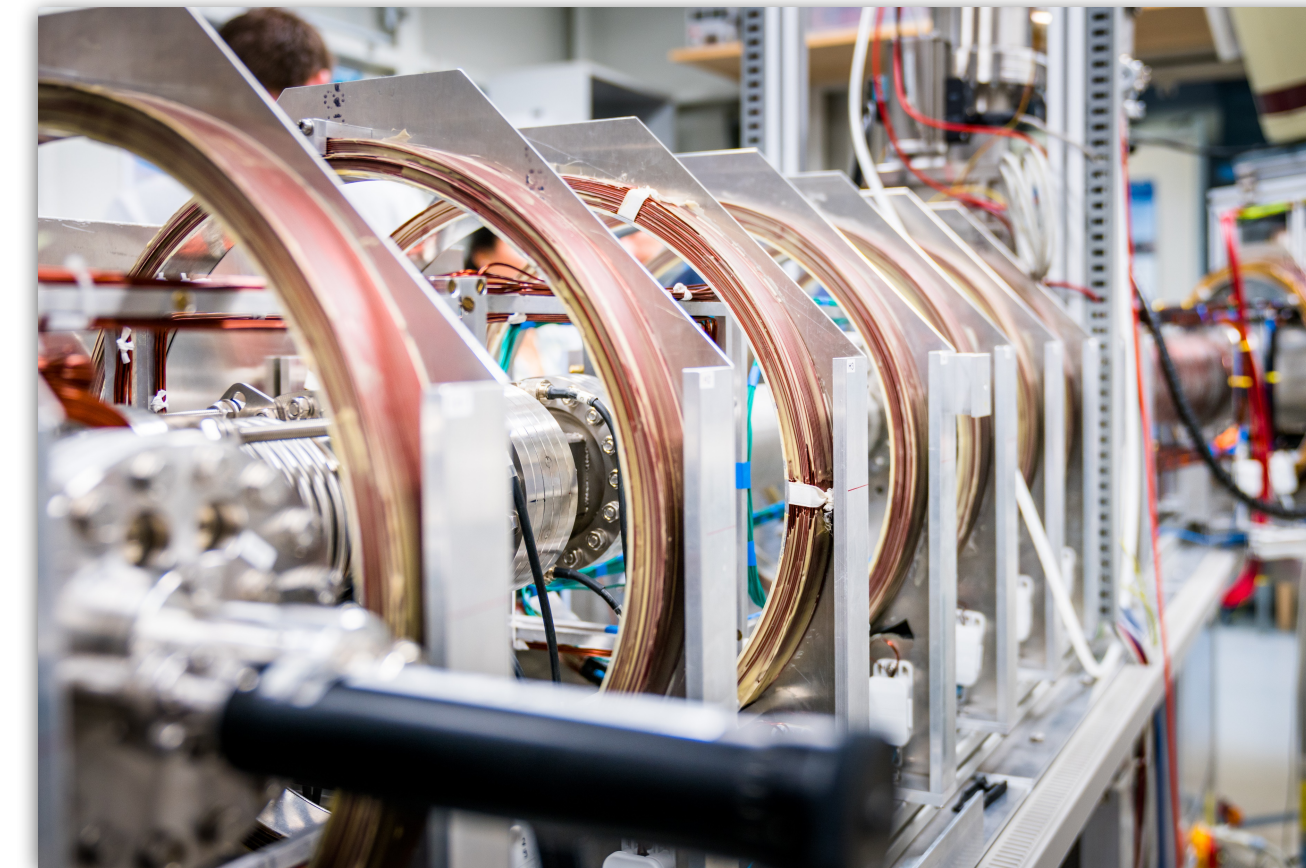
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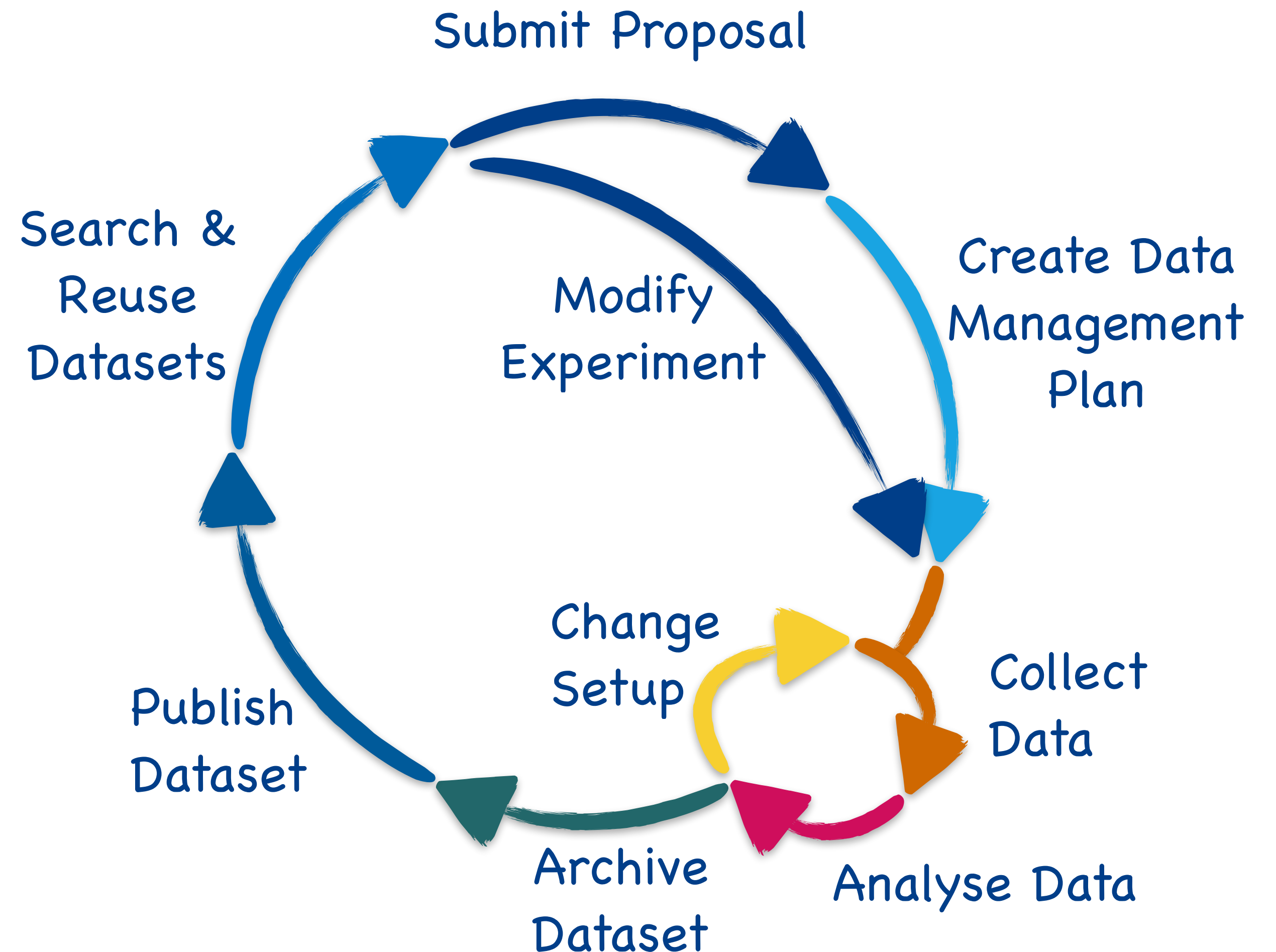
Ion Beam Center (IBC)

— Nanoscale surface analysis and modification.



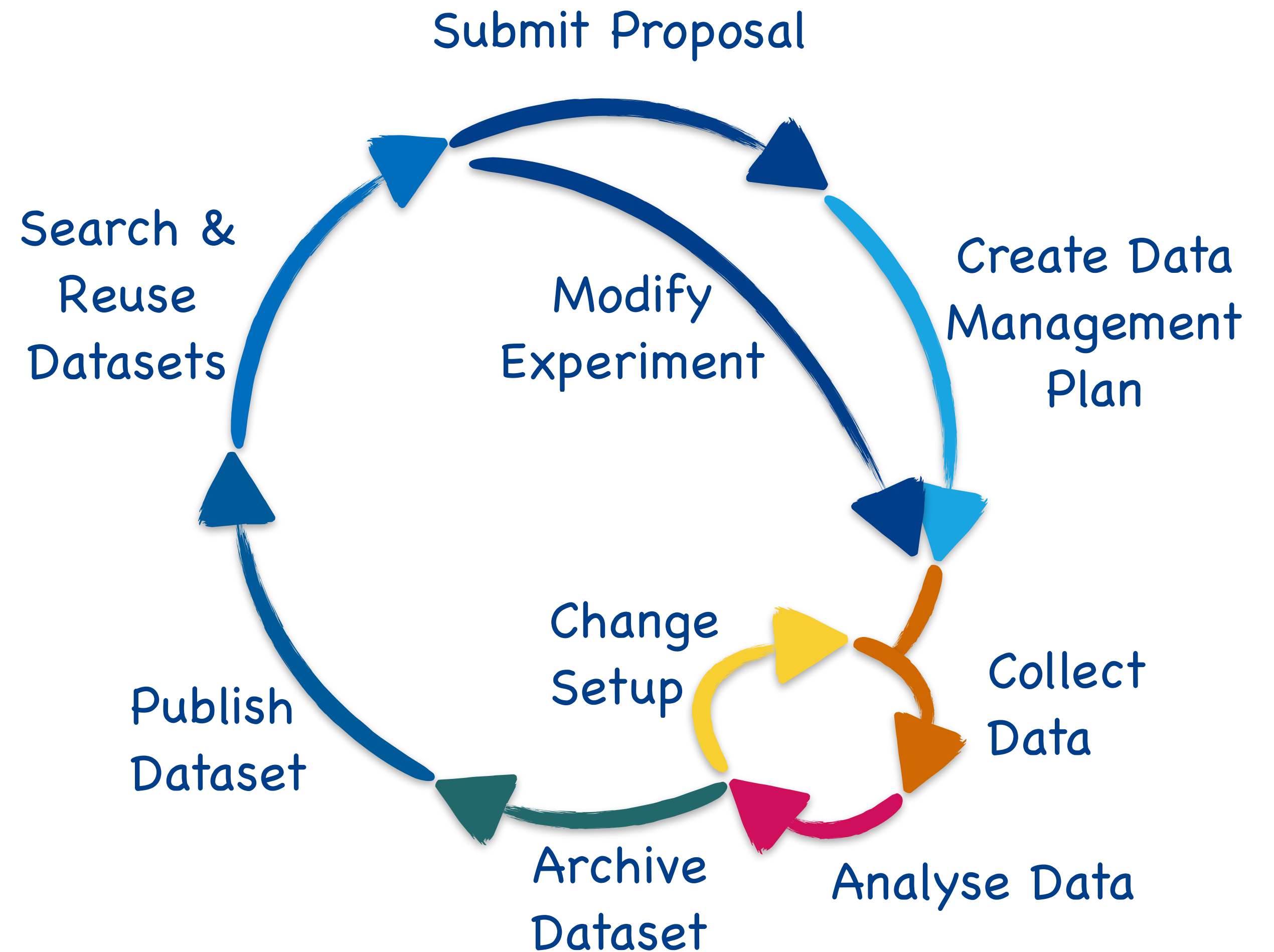
Our Challenge: An End-to-End Digital Data Lifecycle

- We support many steps of our different research experiment (matter, energy and health) with tools:
- electronic lab books,
 - interactive analysis,
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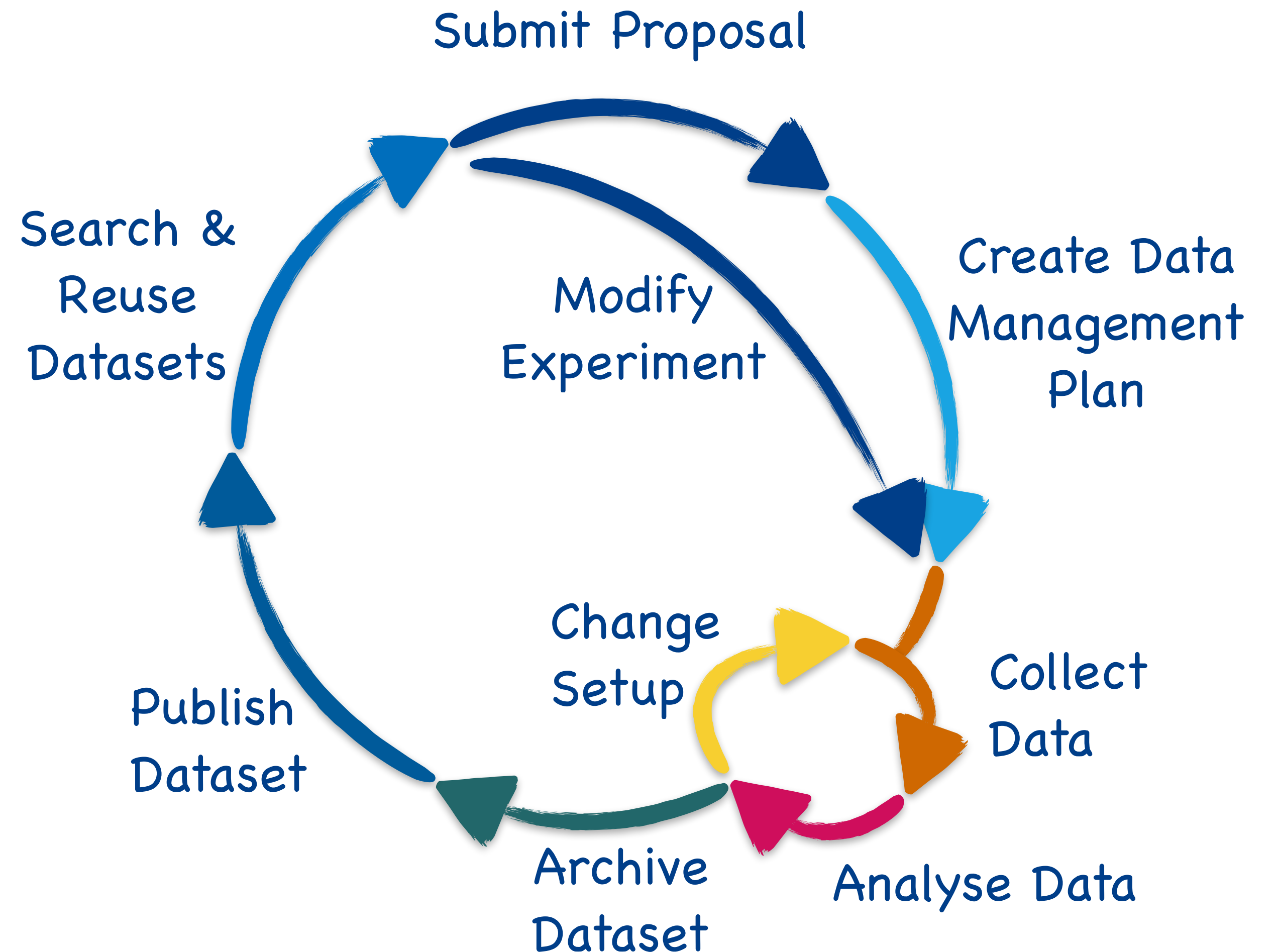
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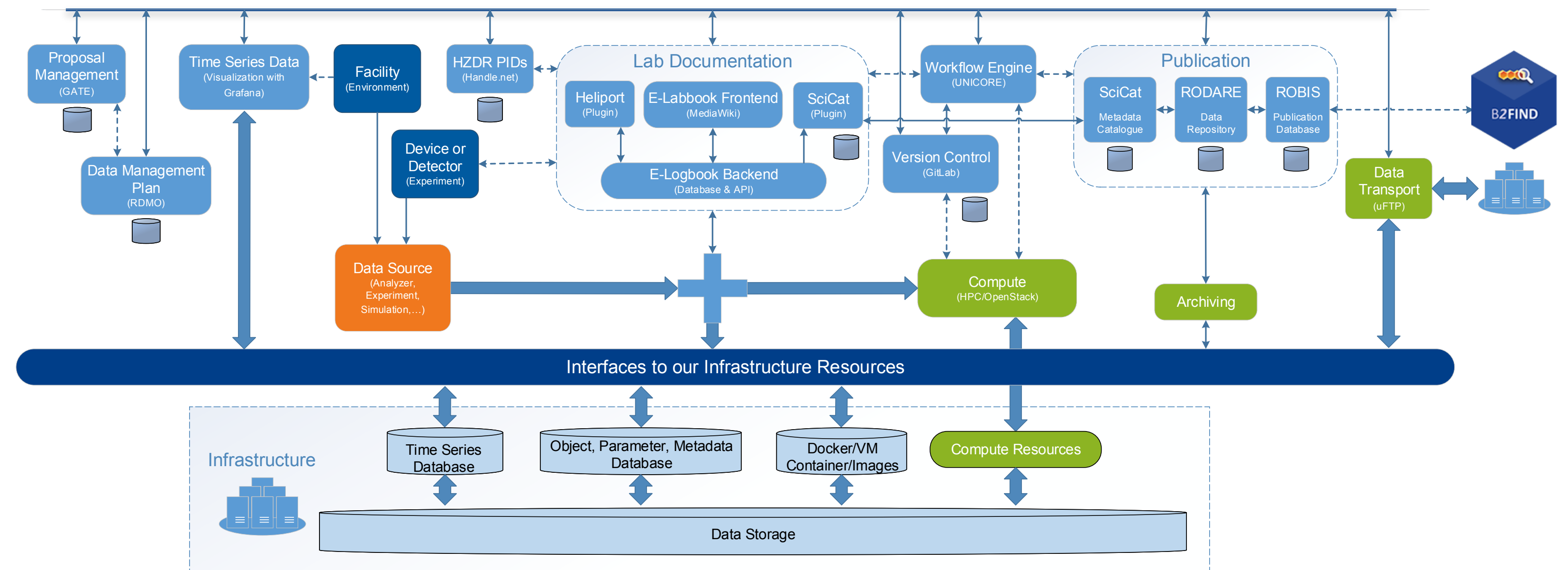
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- The documentation of all these linked resources is essential to create a **comprehensible** and **FAIR** data lifecycle.



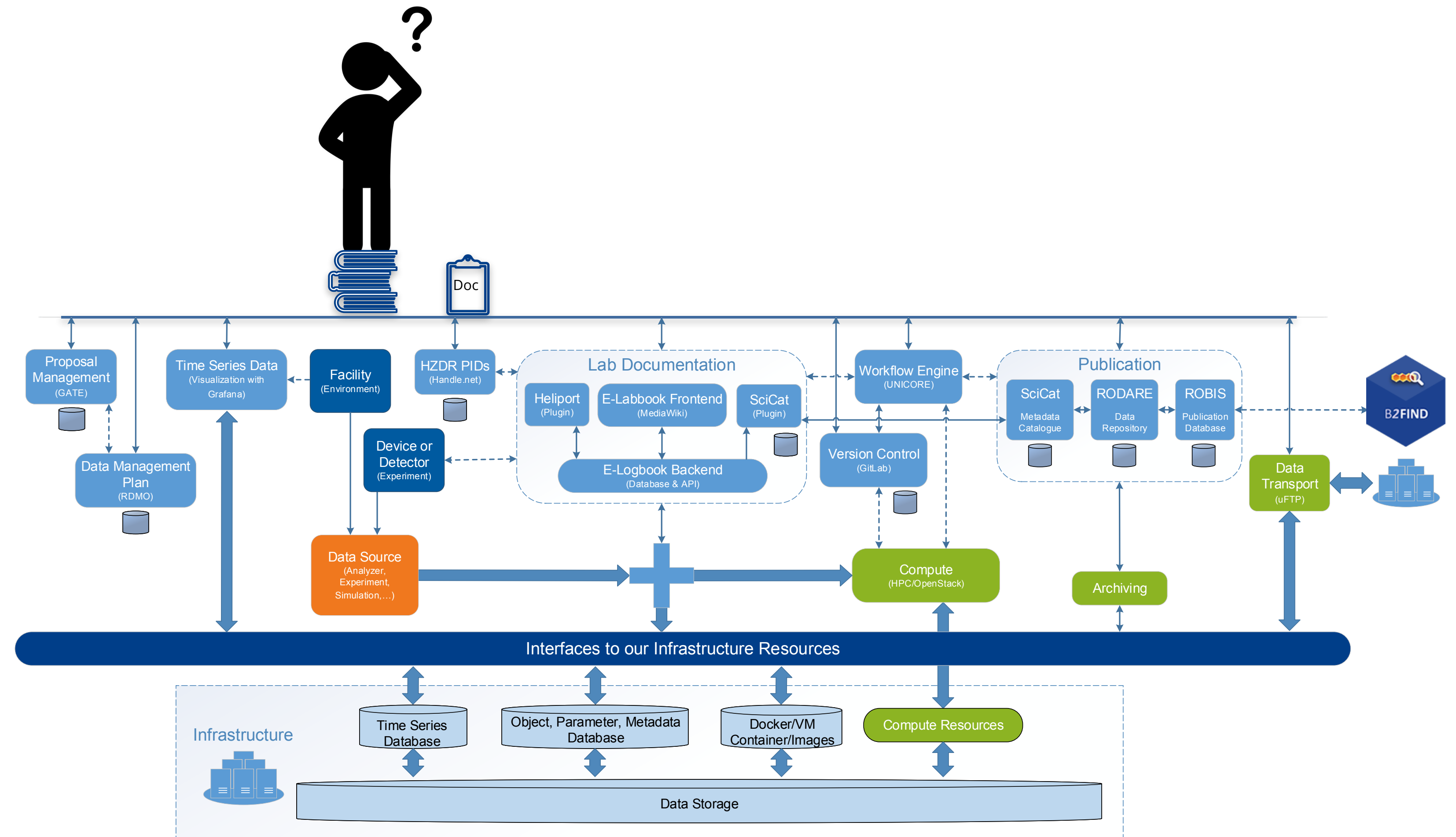
Our Observations and Experiences

- Our IT infrastructures can support various experiments, but they are complex...



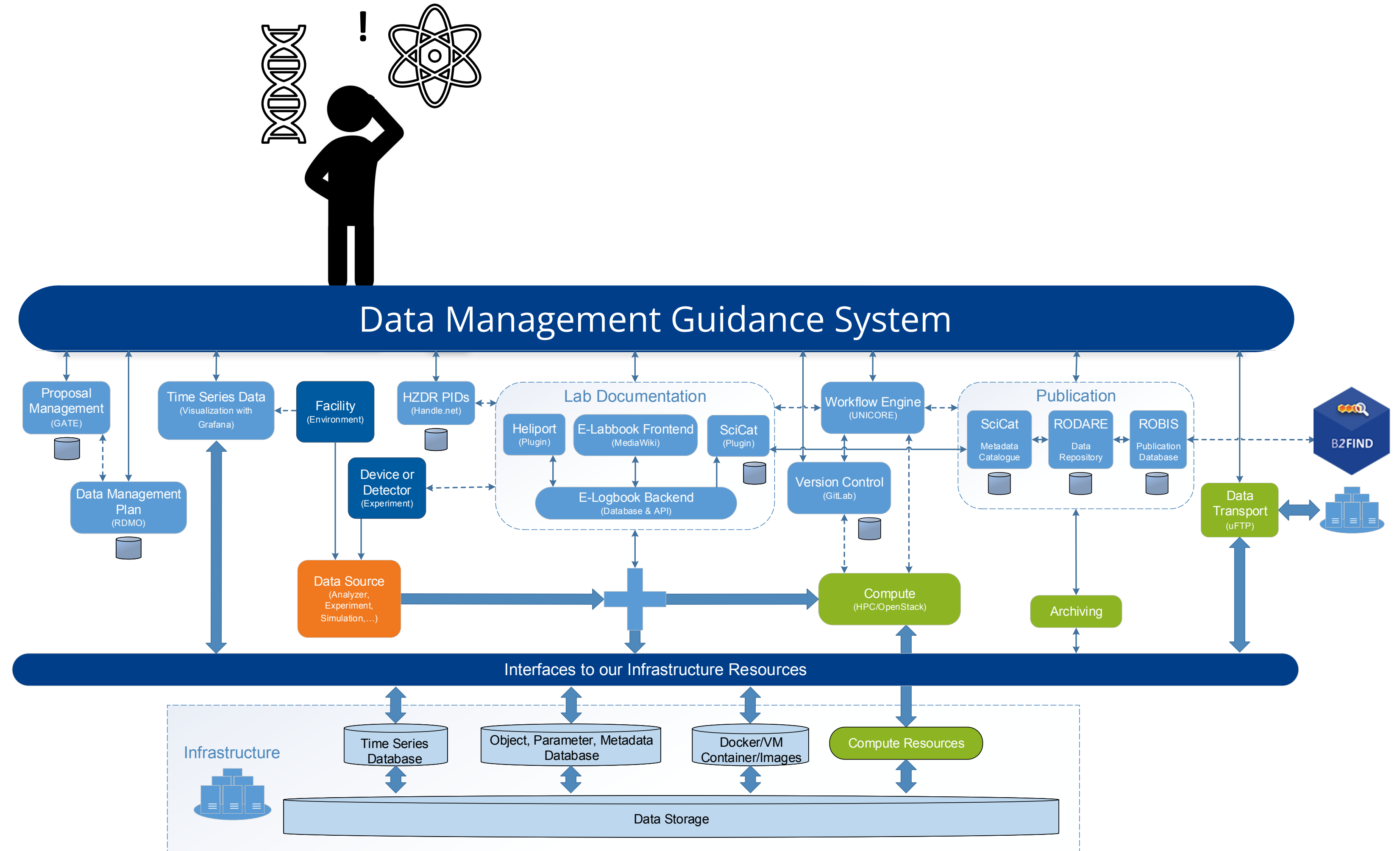
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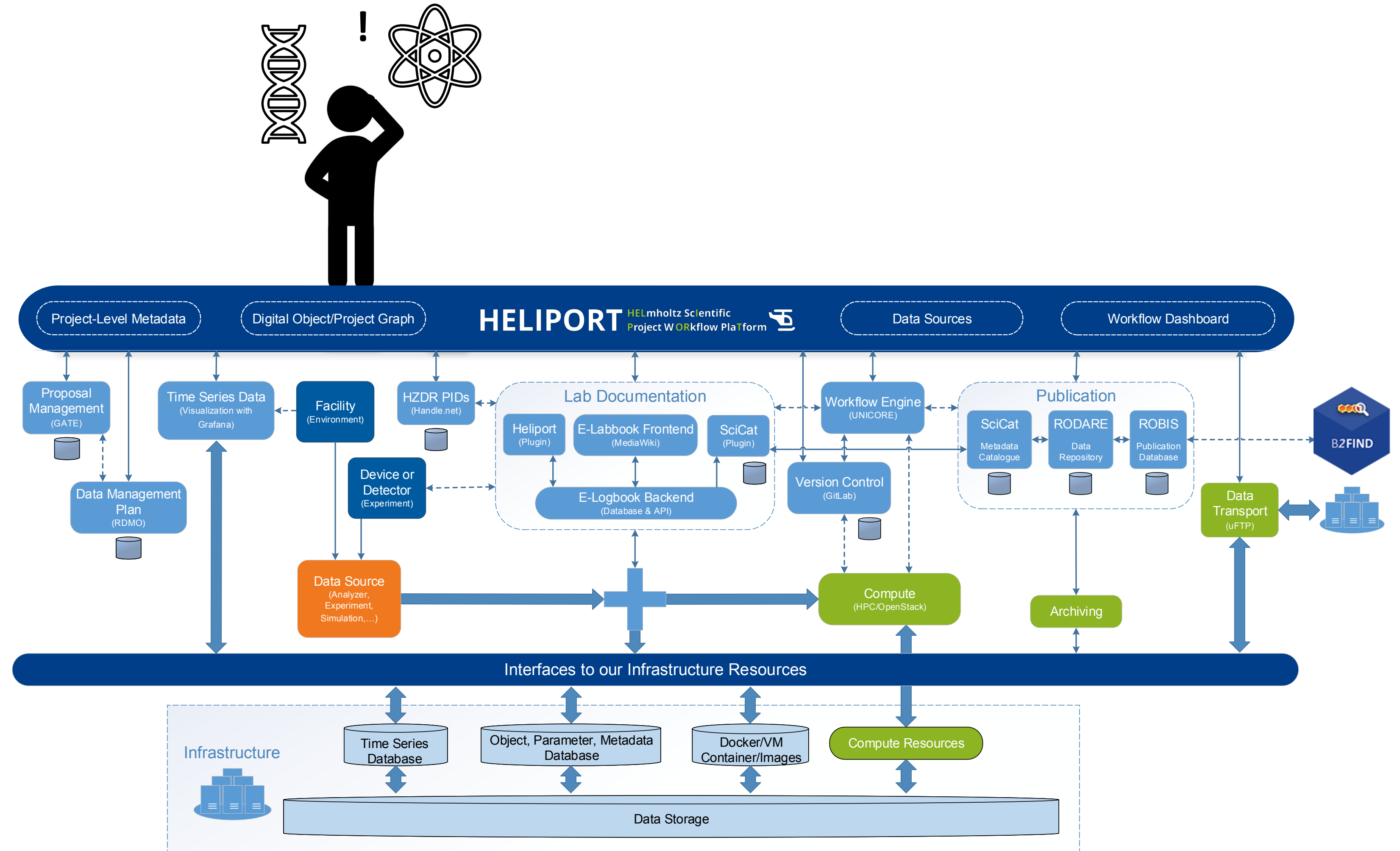
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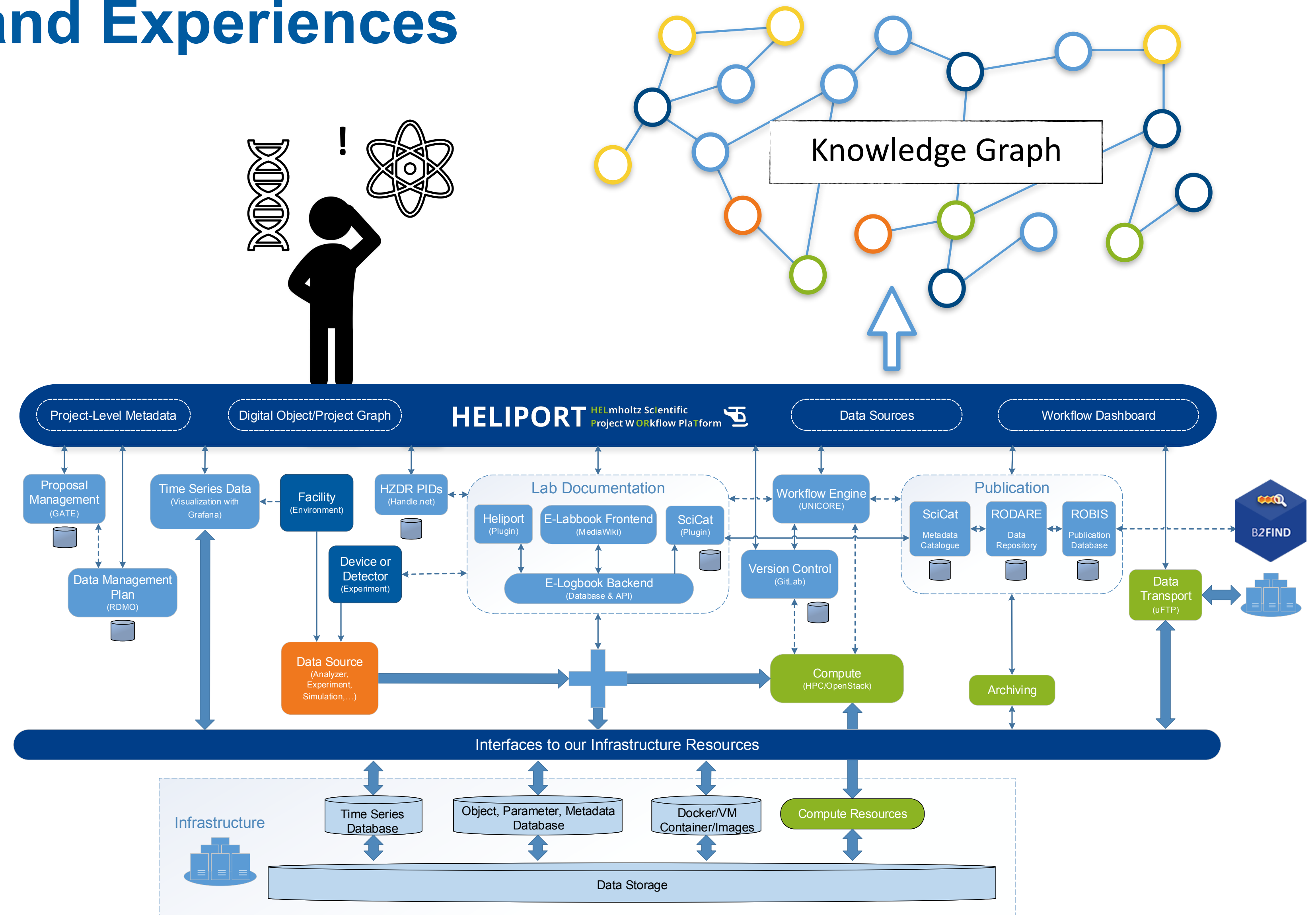
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- In next step we can provide an overall knowledge graph!

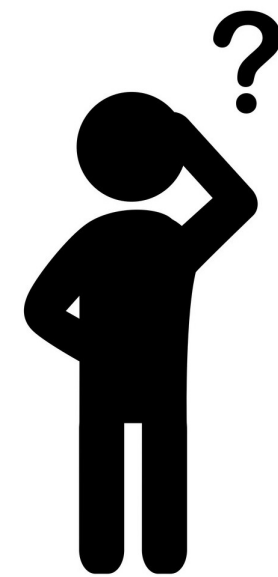


Requirements and Conditions

- HELIPORT was intended to provide only the **proposal's metadata**, from internal and external scientists, to allow the assignment of resources.

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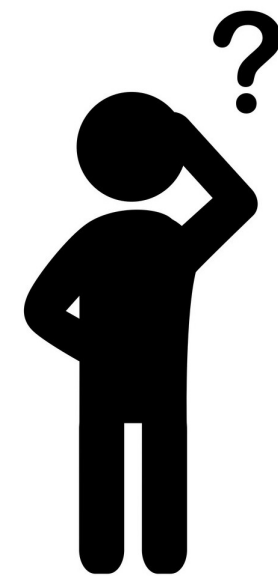
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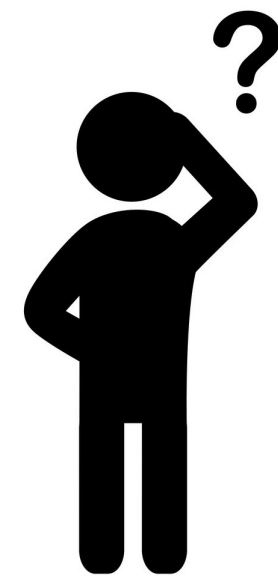
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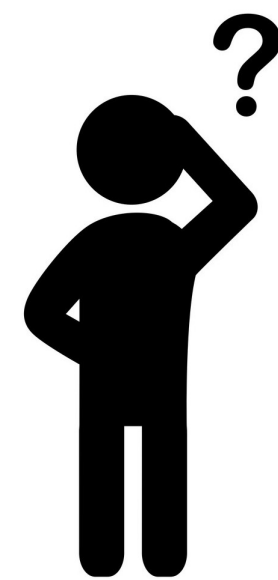


Which datasets or software can be **published** (and how)?

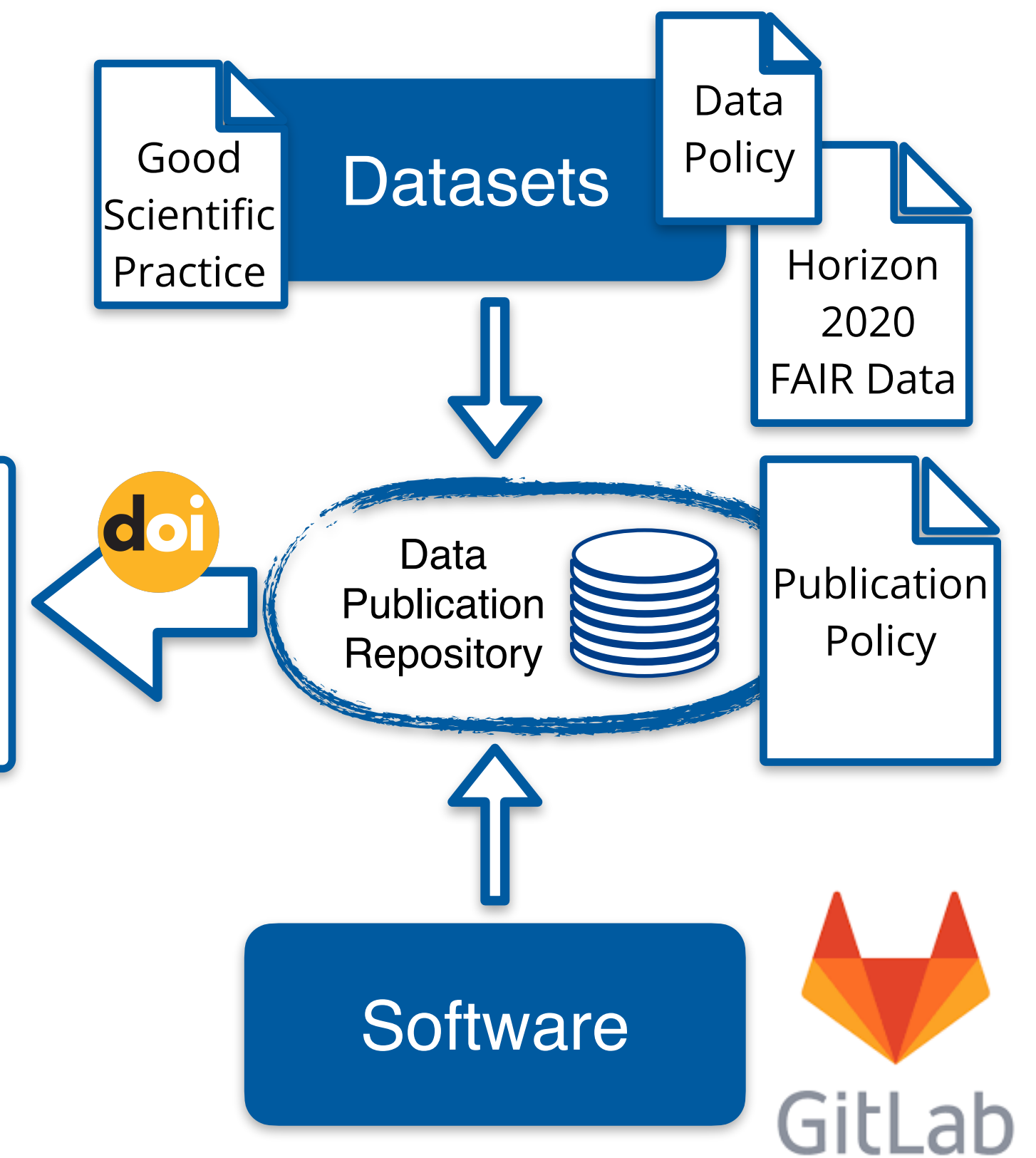
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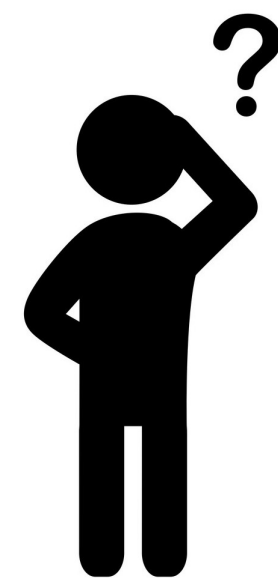
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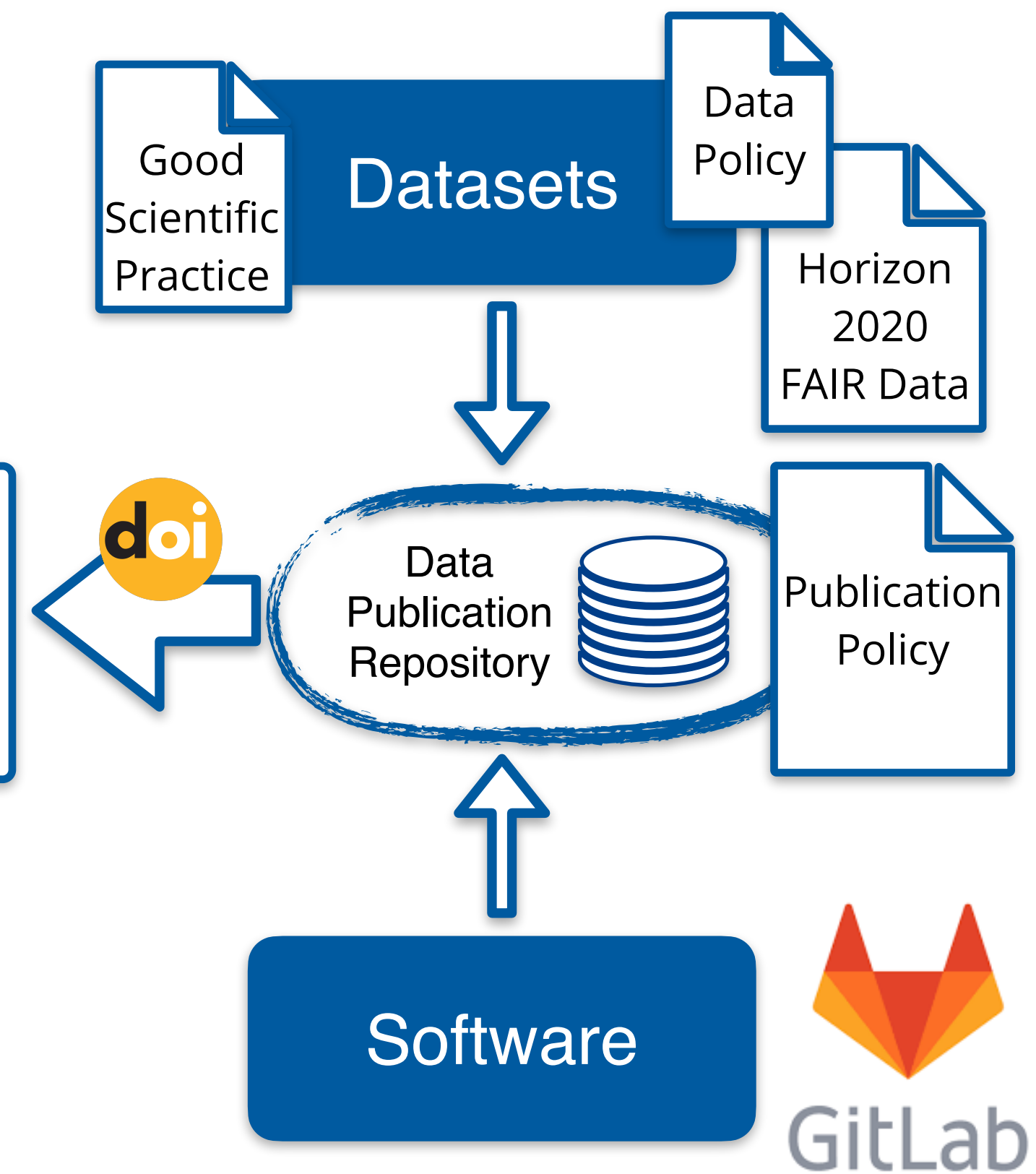
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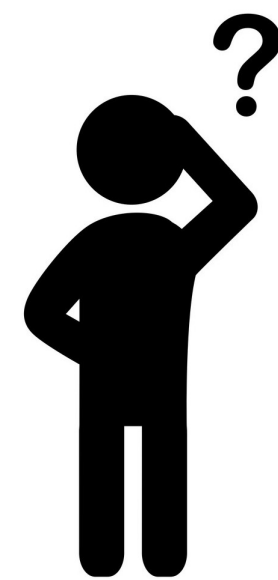


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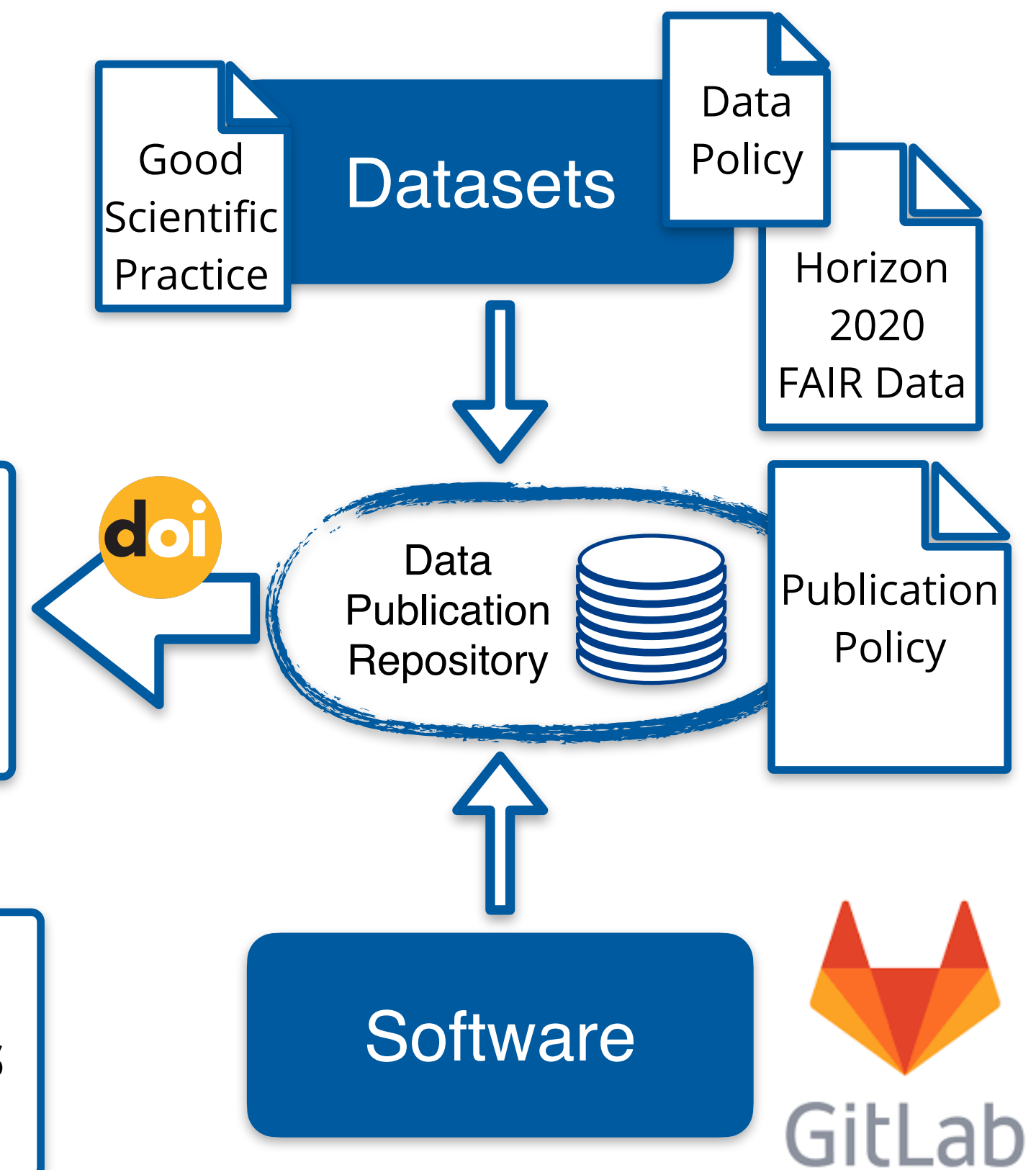
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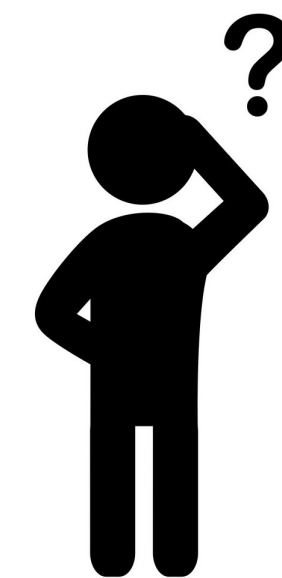
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What are the necessary steps towards a full comprehensible and FAIR research experiment ensuring data provenance?

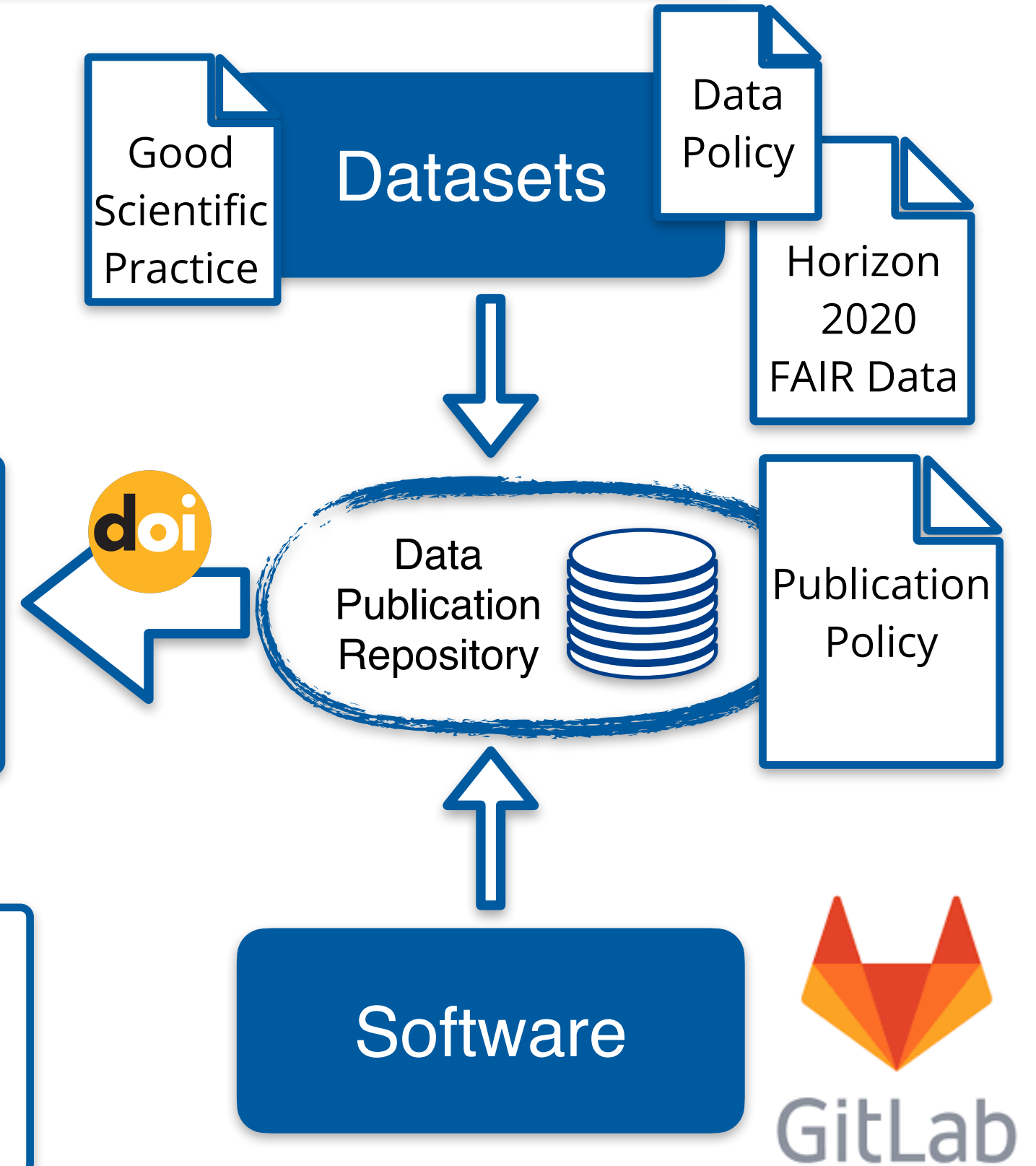
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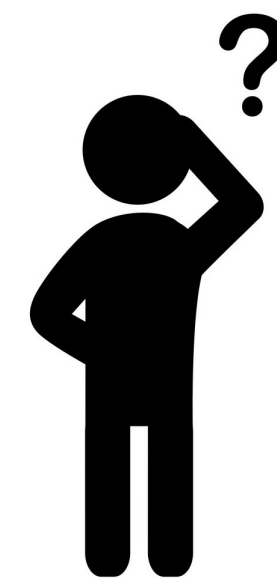


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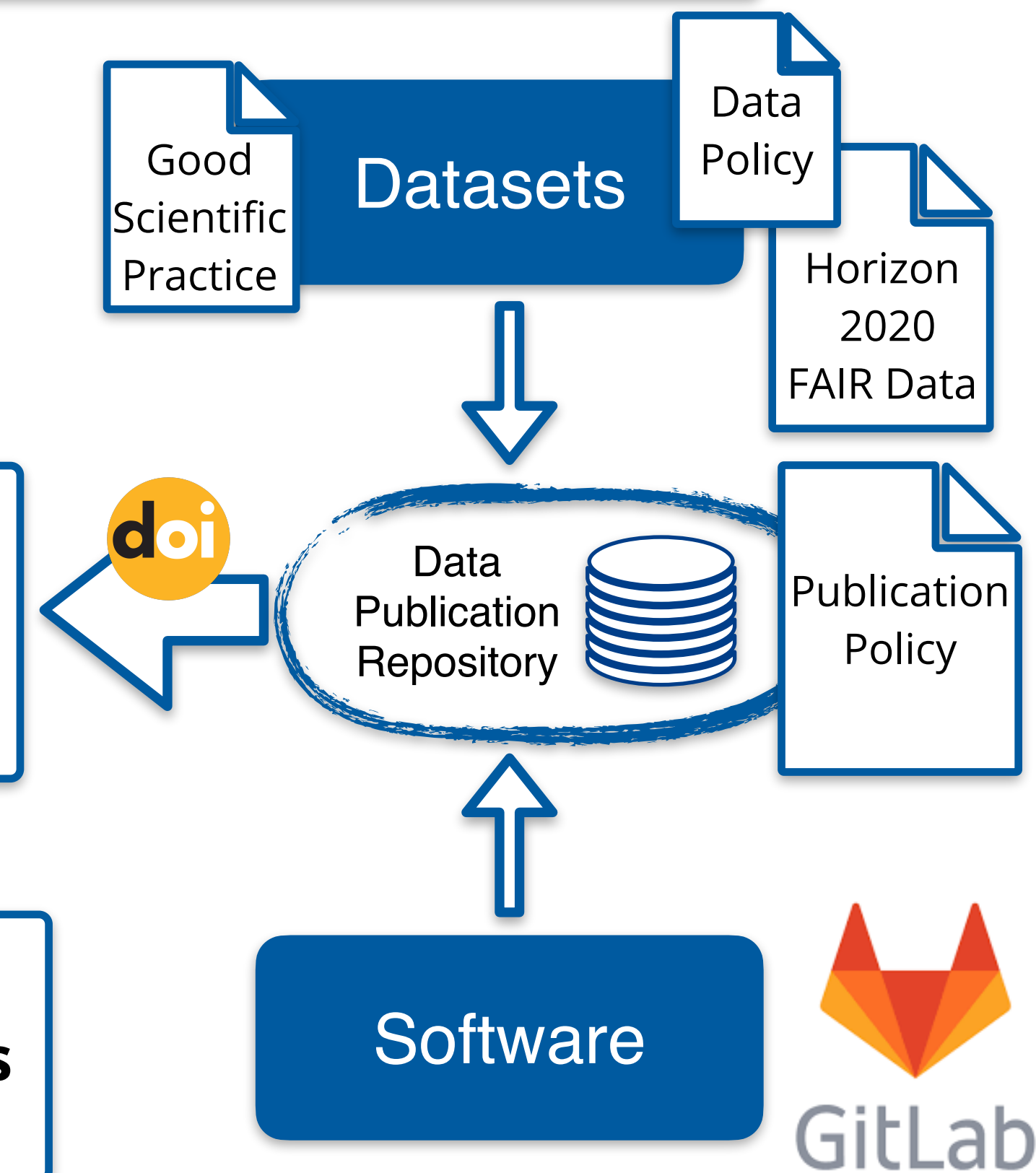


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And how we can support them?!

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HELIPORT HELMholtz Scientific Project WOrkflow PlaTform



“ 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:



HELIPORT About Docs knodel39

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		Publication
Documentation	UNICORE Storages		
Digital Objects			

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```

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Metadata crosswalk to
schema.org
ResearchProject

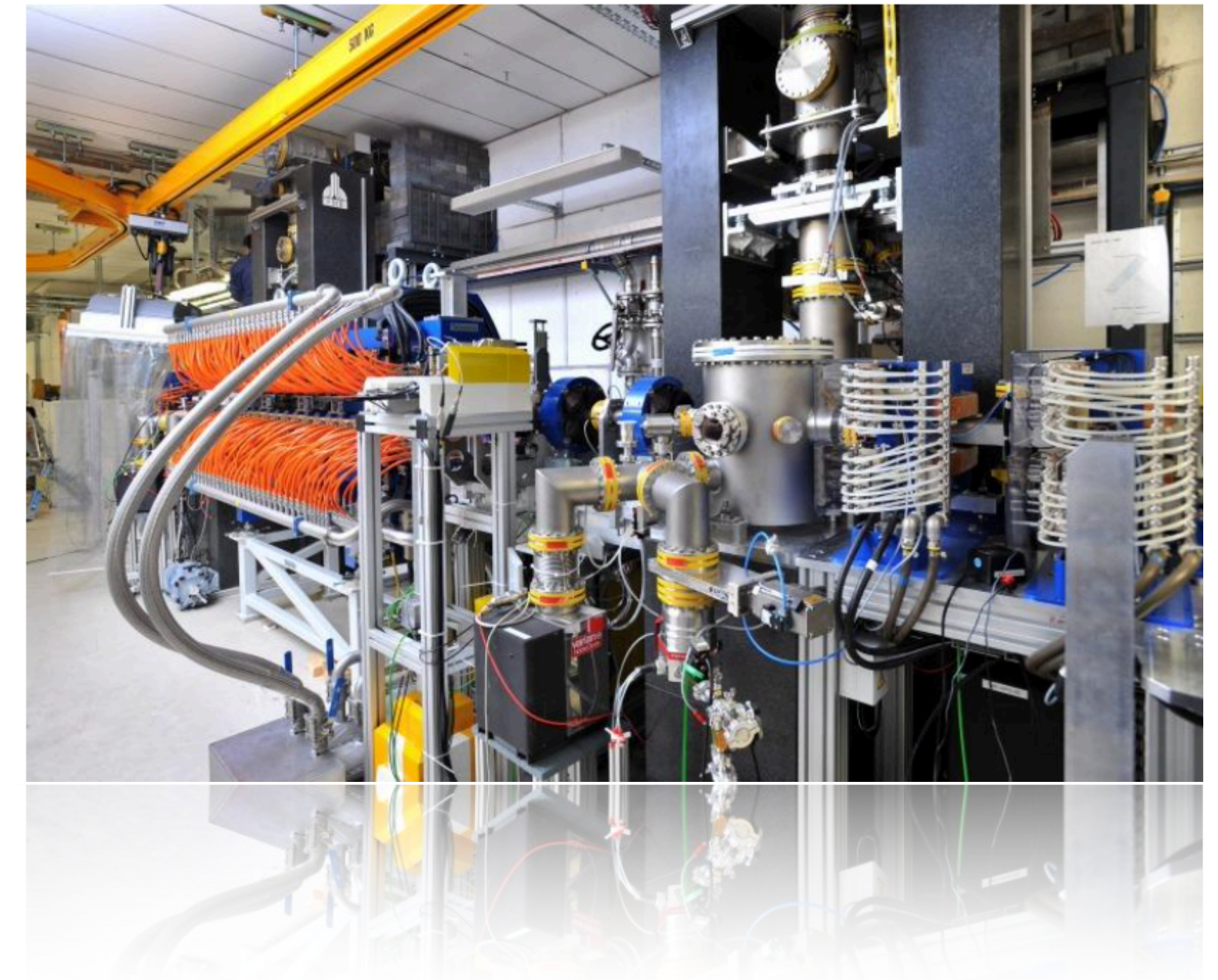
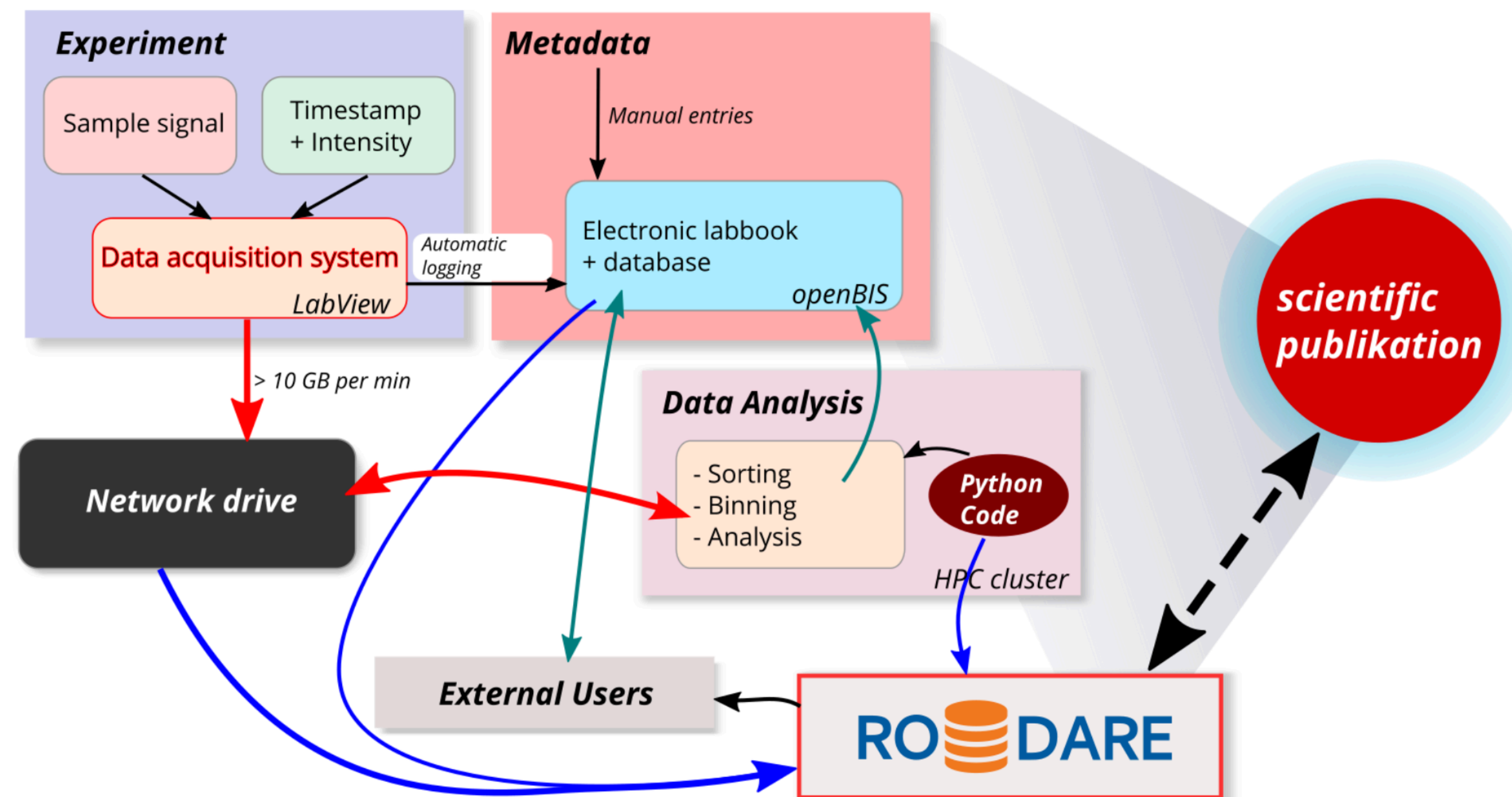


TELBE in HELIPORT



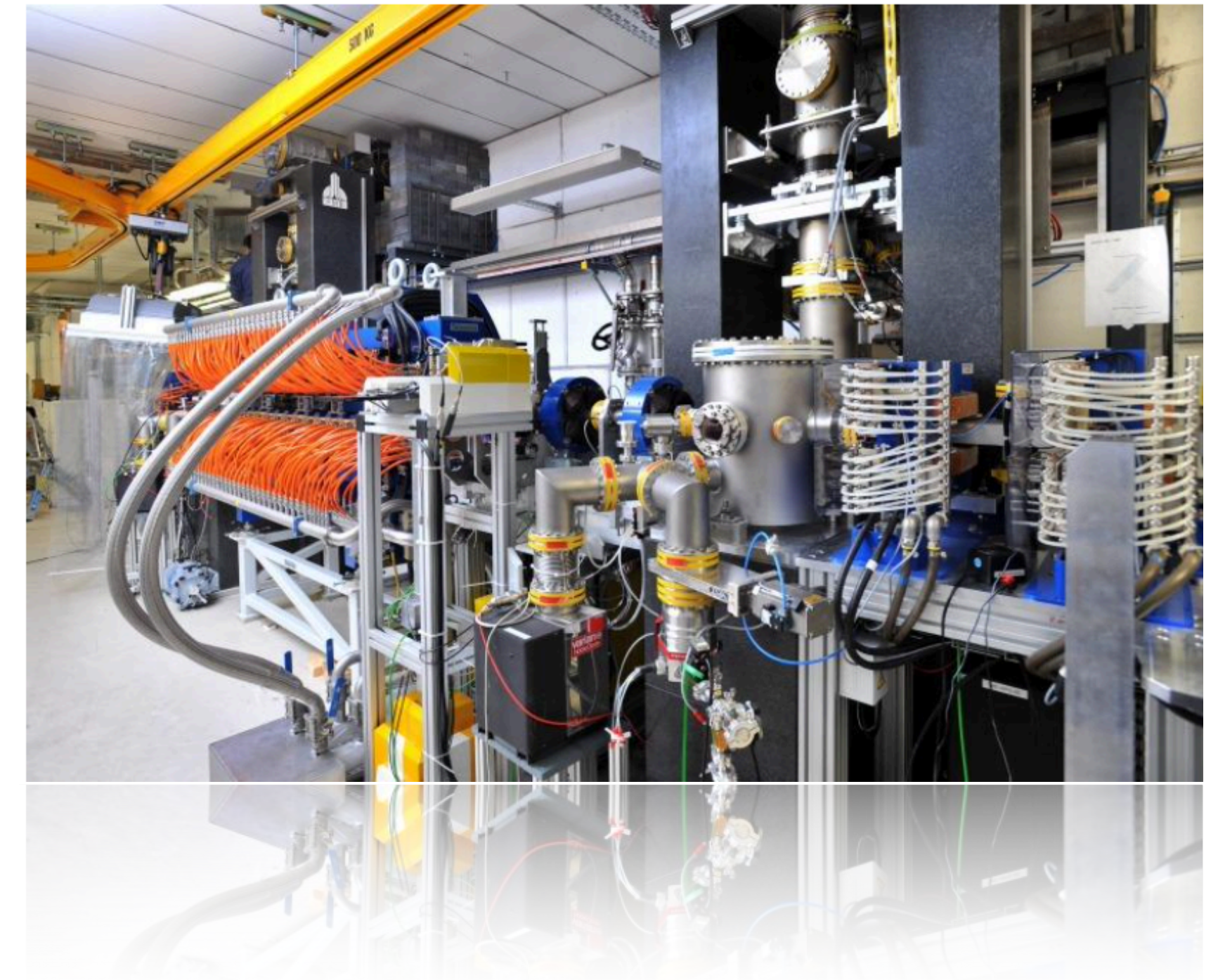
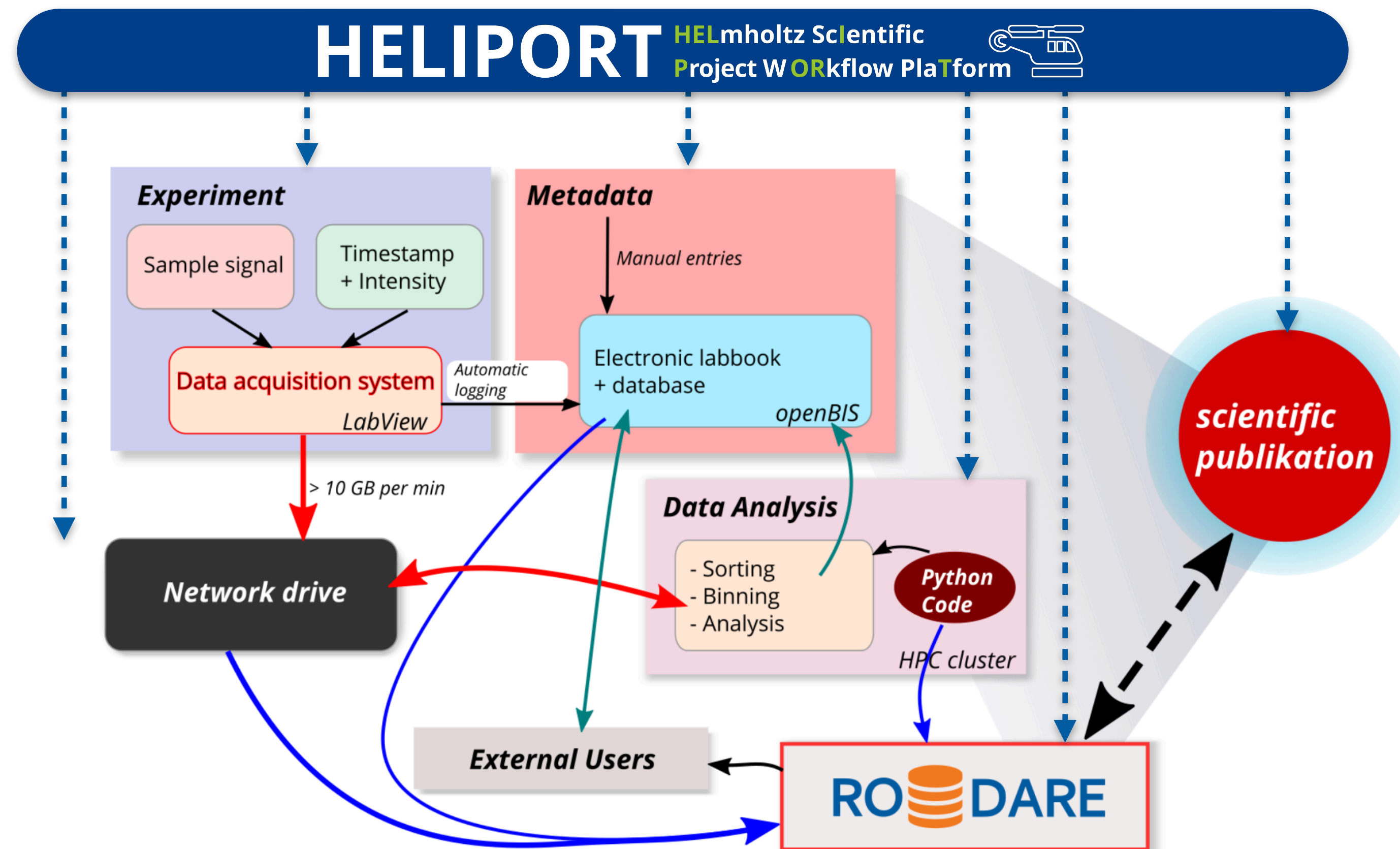
Data Management View of the TELBE Experiment

— Terahertz facility at the ELBE center for High-Power Radiation Sources.



Data Management View of the TELBE Experiment

- Terahertz facility at the ELBE center for High-Power Radiation Sources.
- In the future HELIPORT should guide external scientists through the complete experiment.



Mapping of the TELBE Resources to HELIPORT

Project-Level Metadata

Digital Object/Project Graph

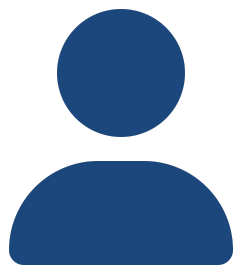
HELIPORT HELmholtz Scientific
Project WOrkflow PlaTform 

Data Sources

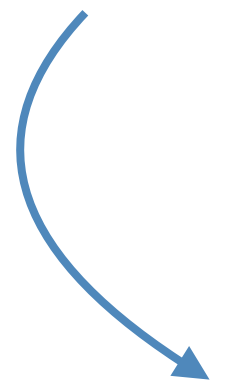
Workflow Dashboard

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Proposer
(Principle
Investigator)



I. Apply



Project-Level Metadata

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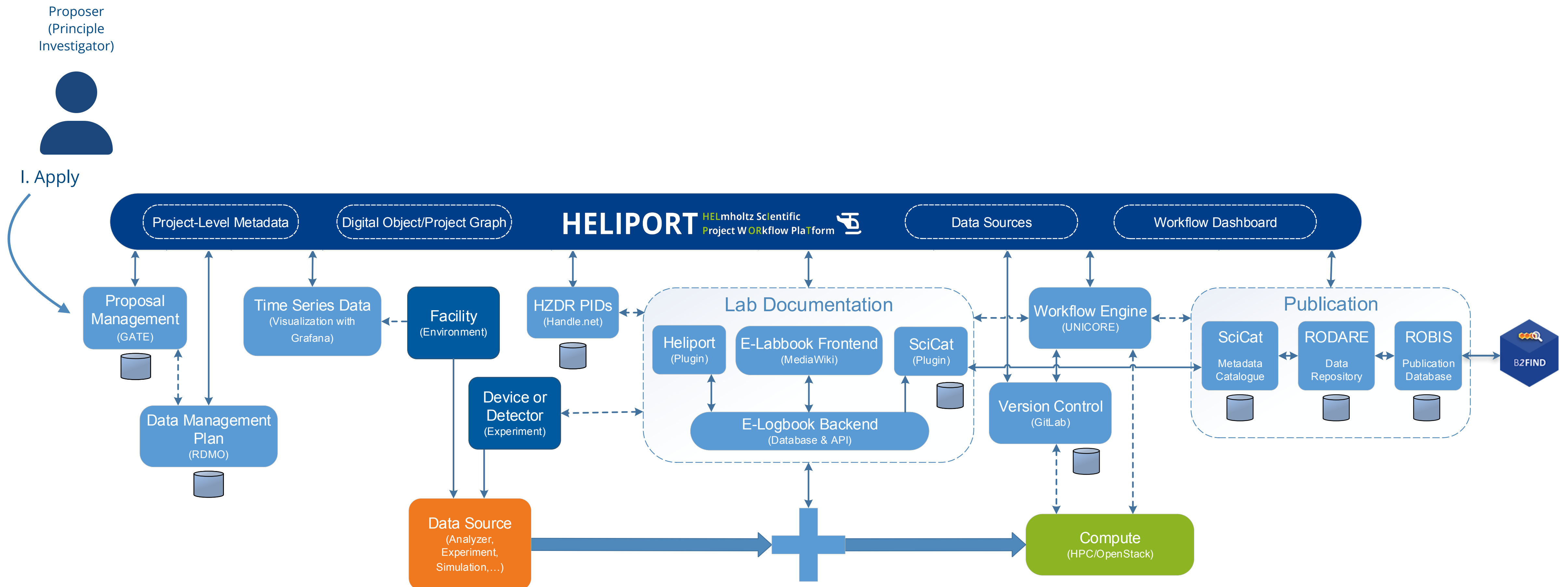
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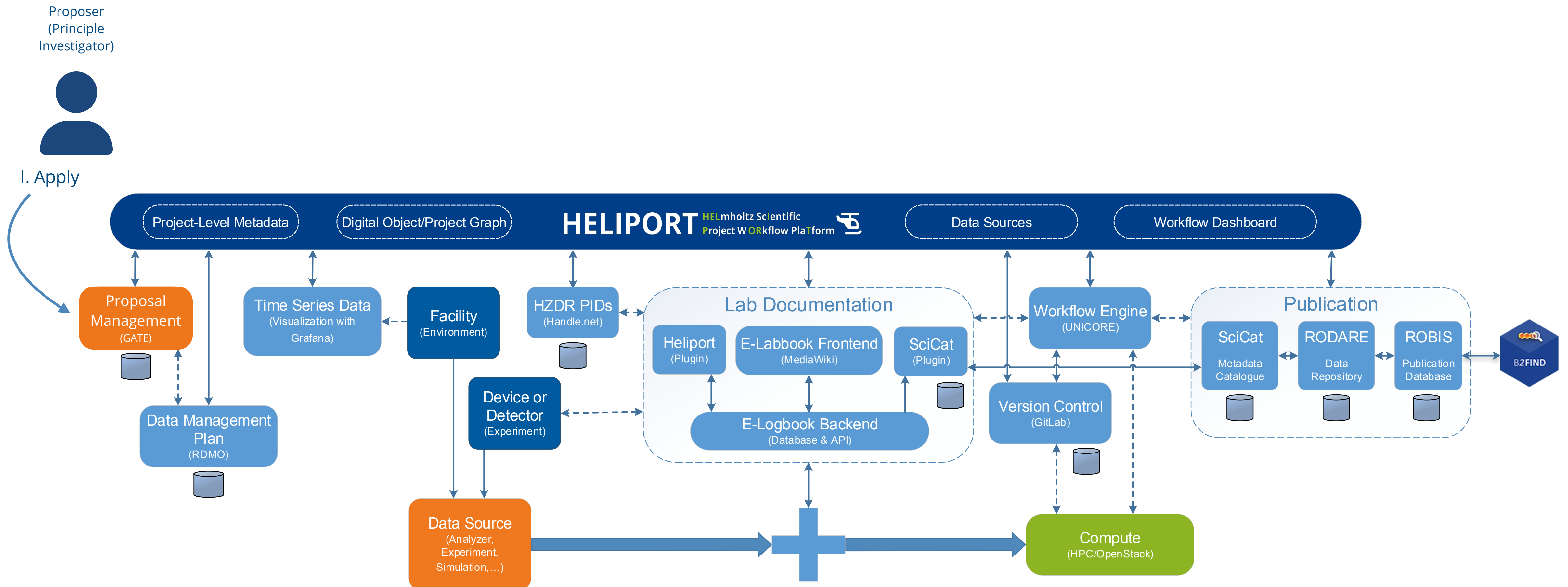
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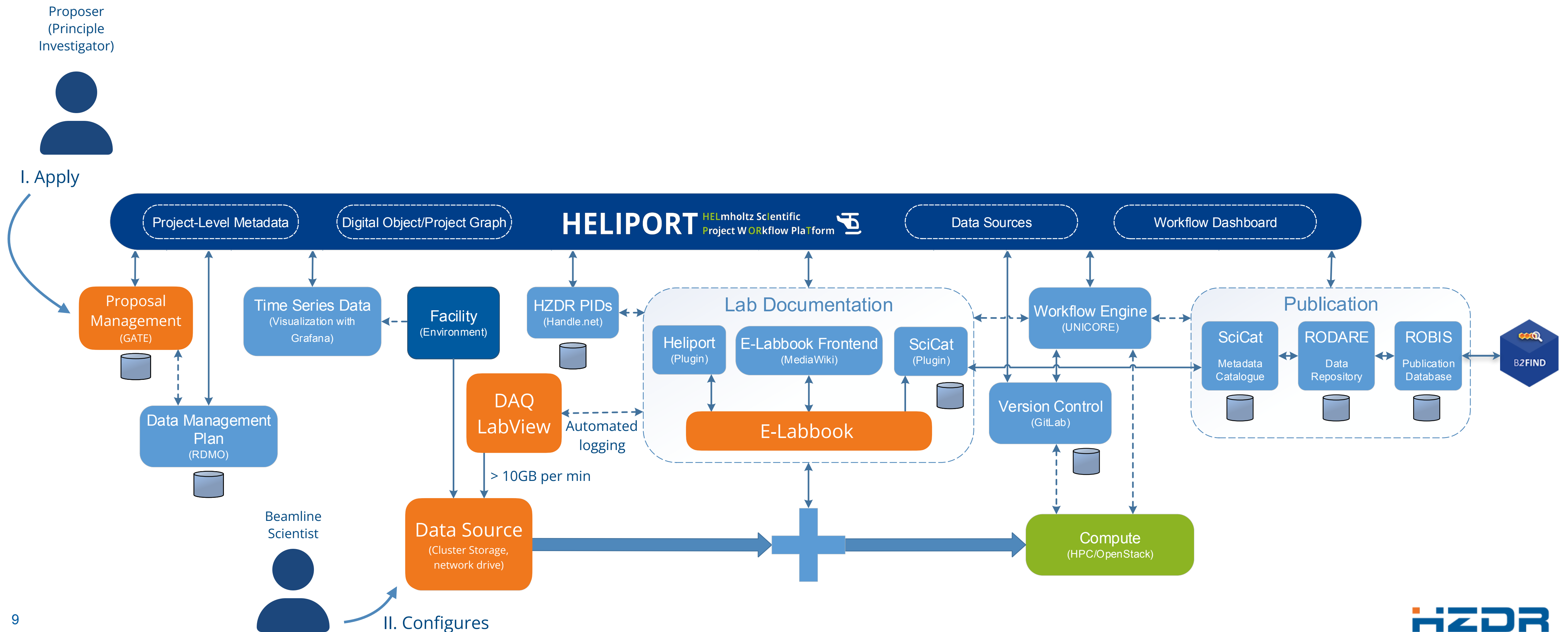
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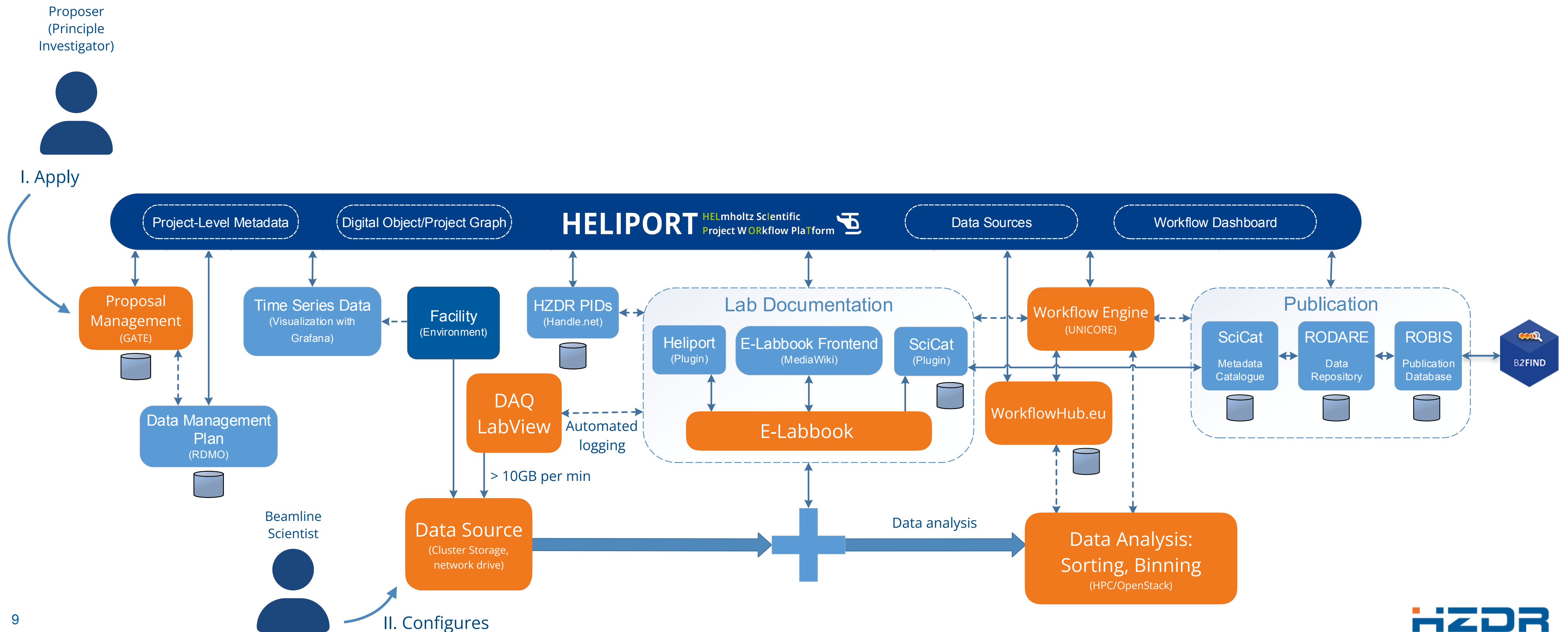
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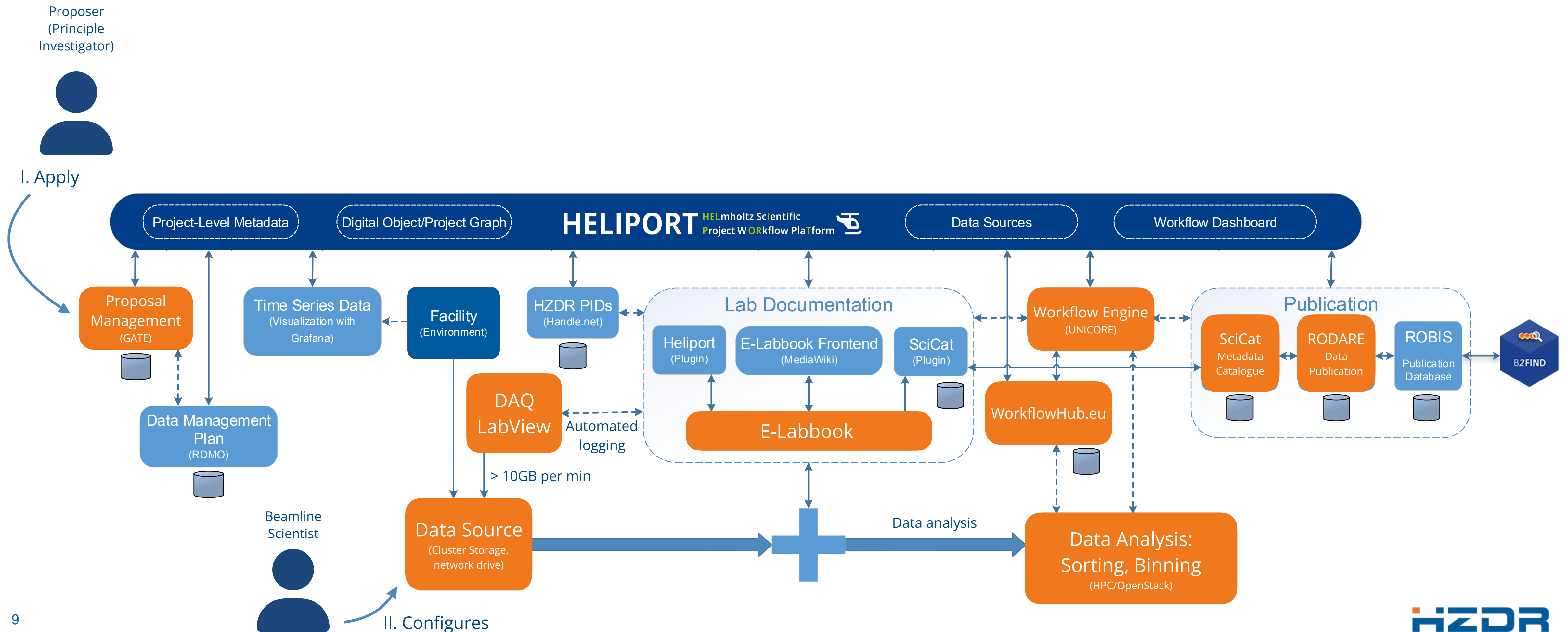
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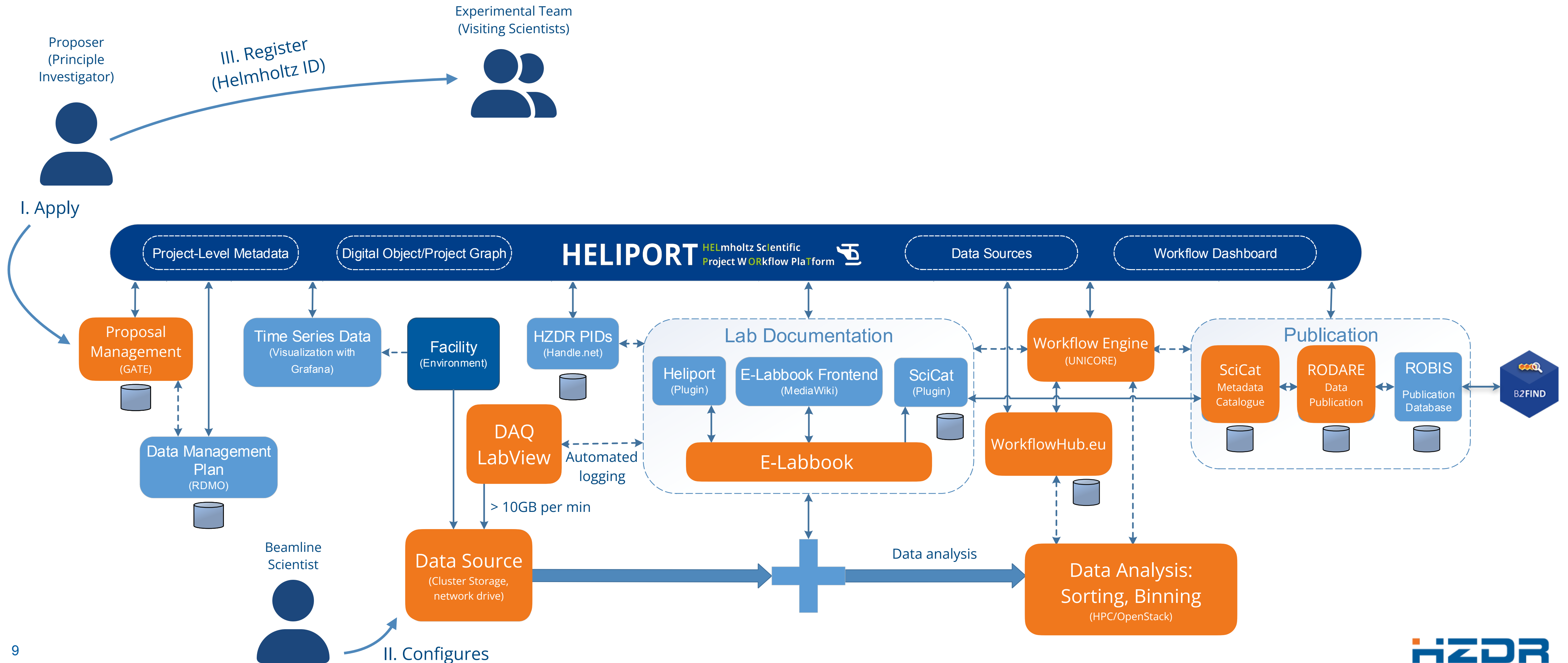
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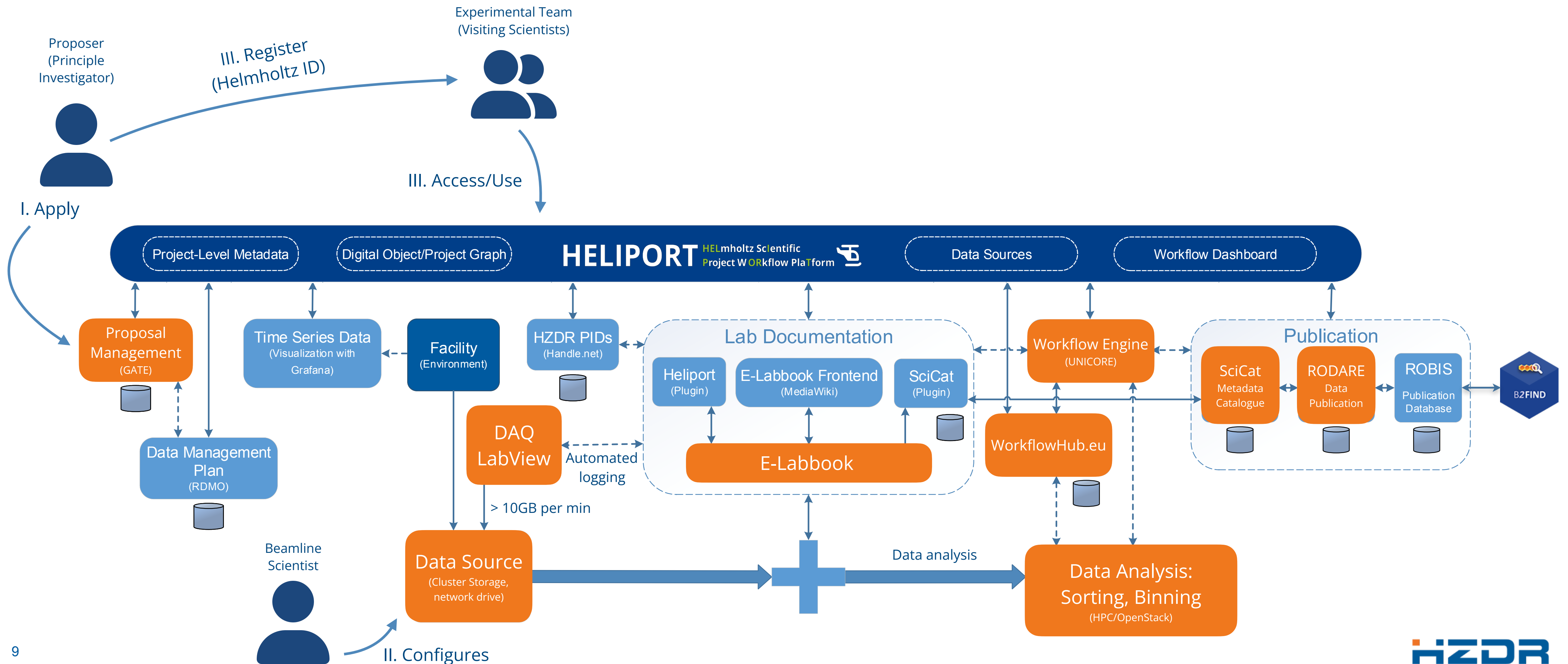
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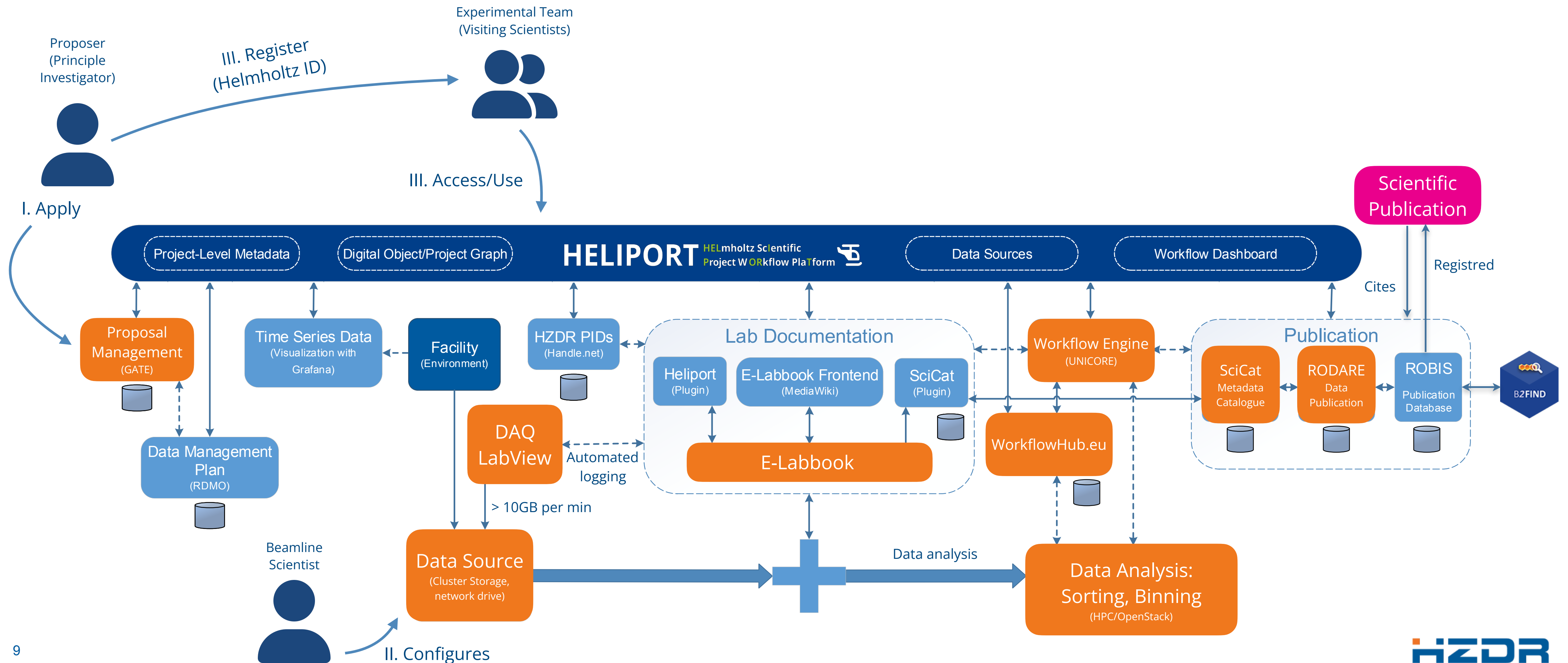
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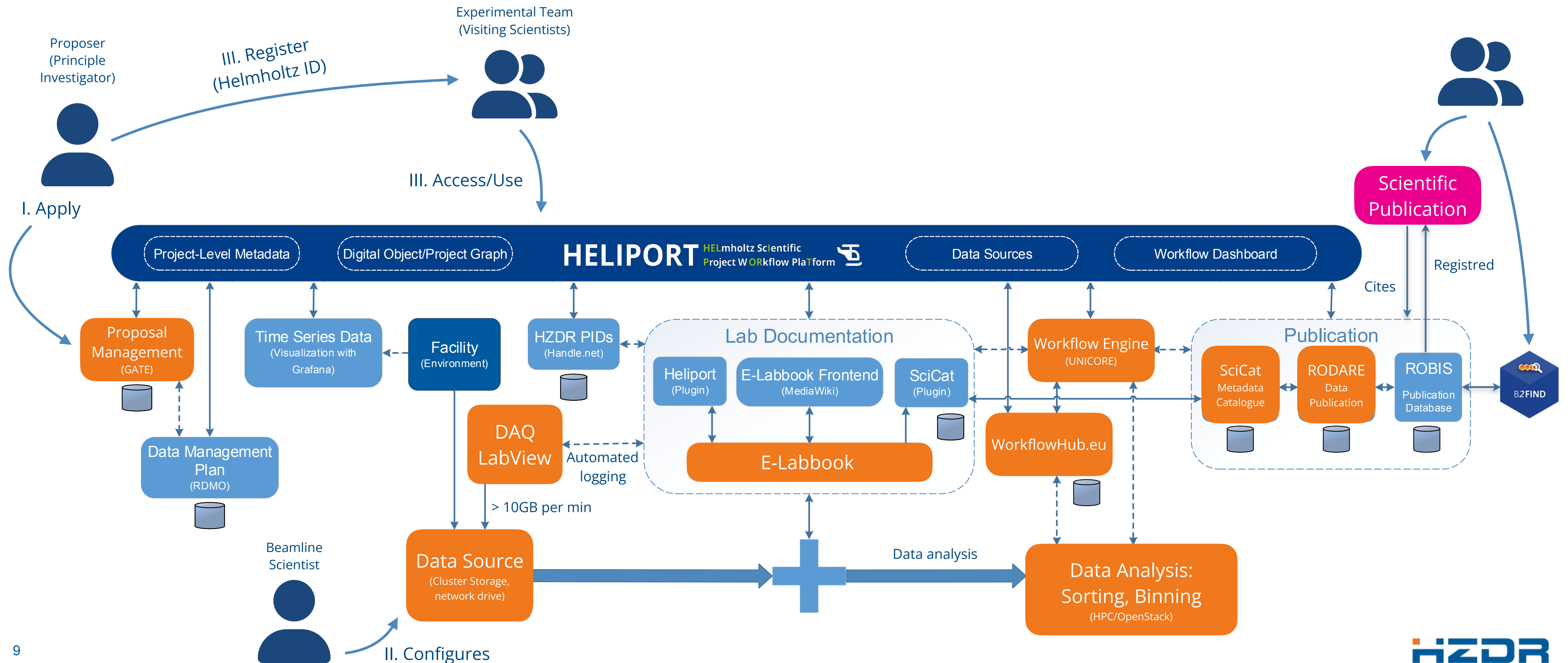
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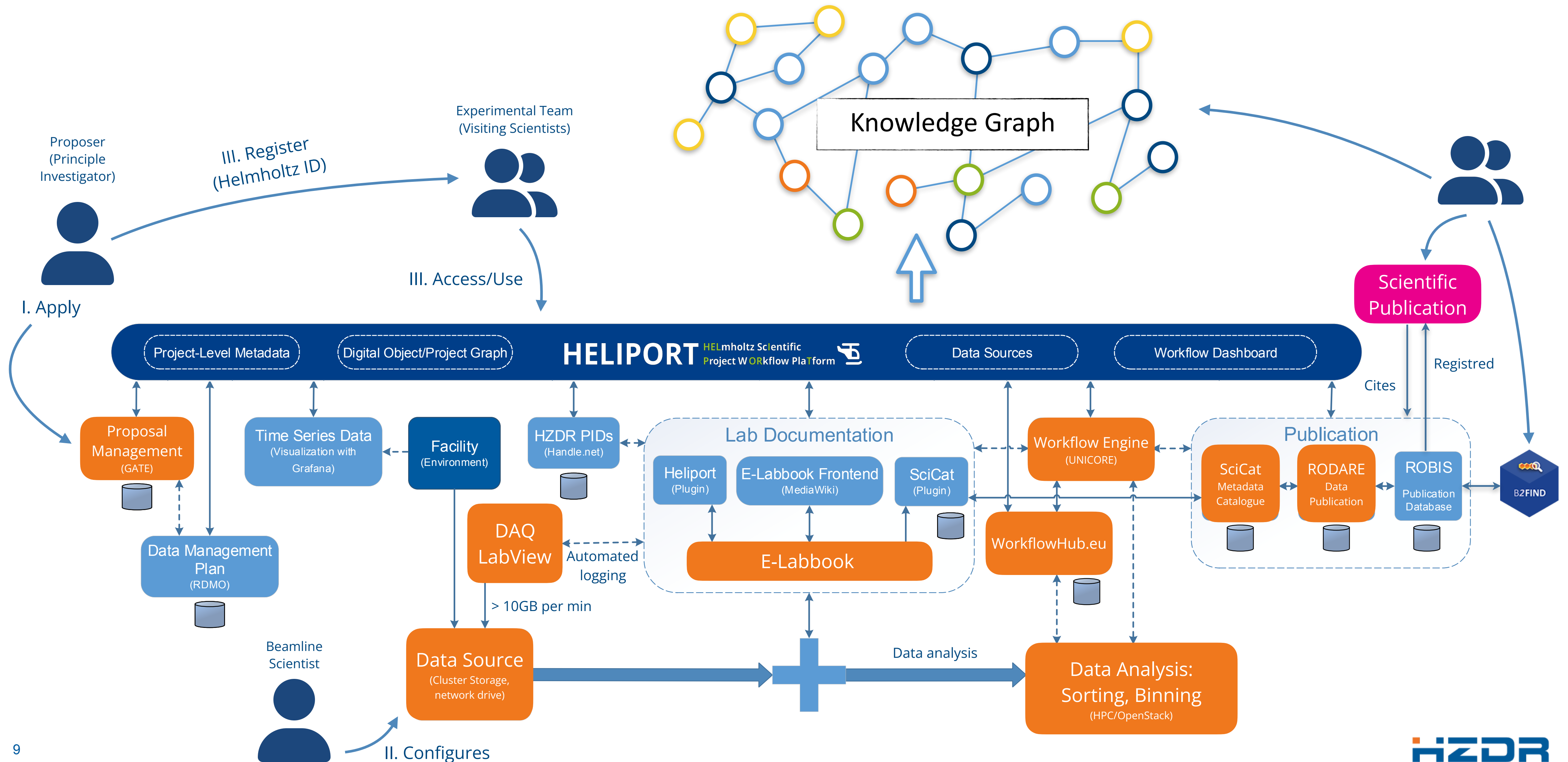
Mapping of the TELBE Resources to HELIPOINT



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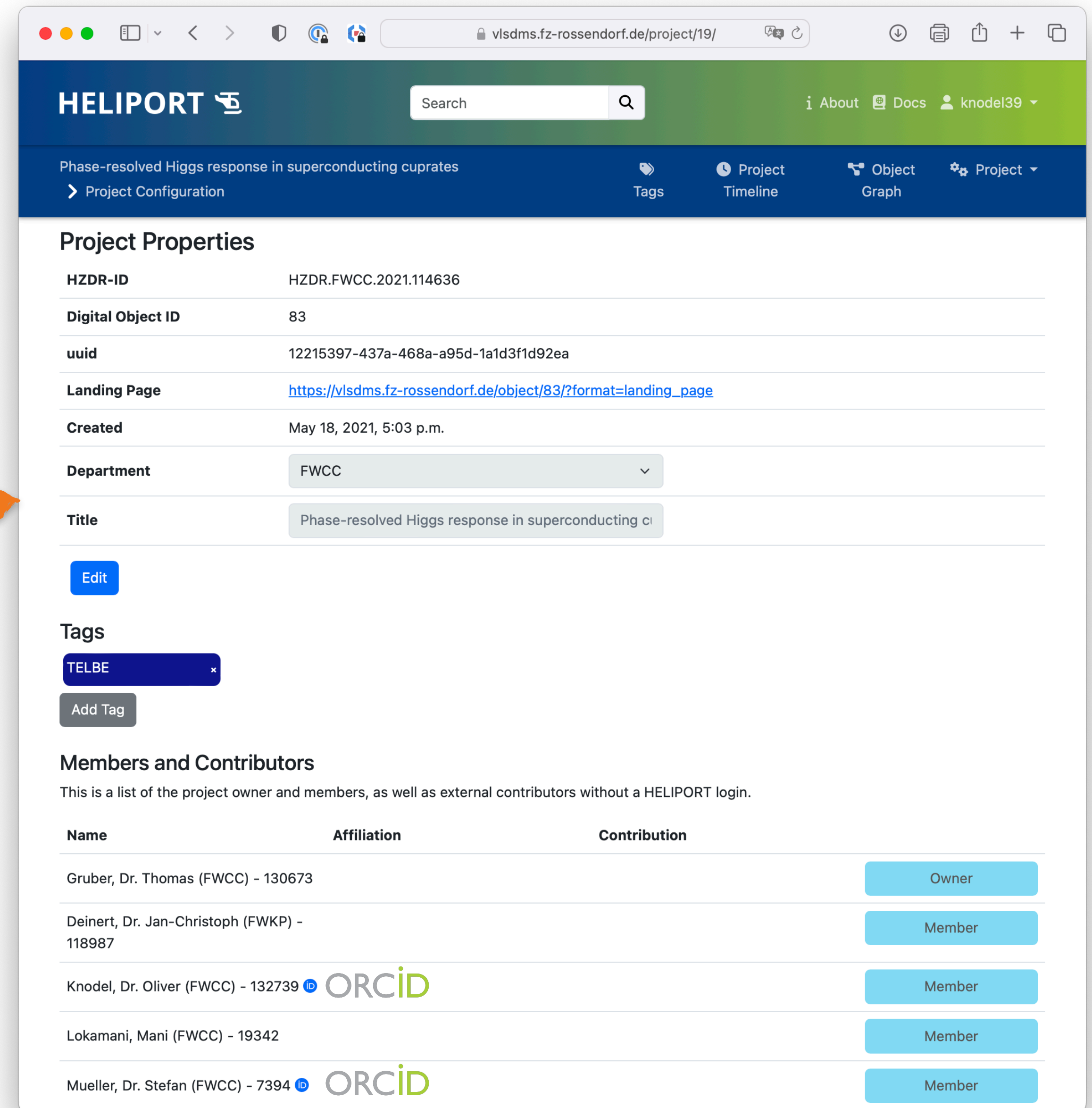
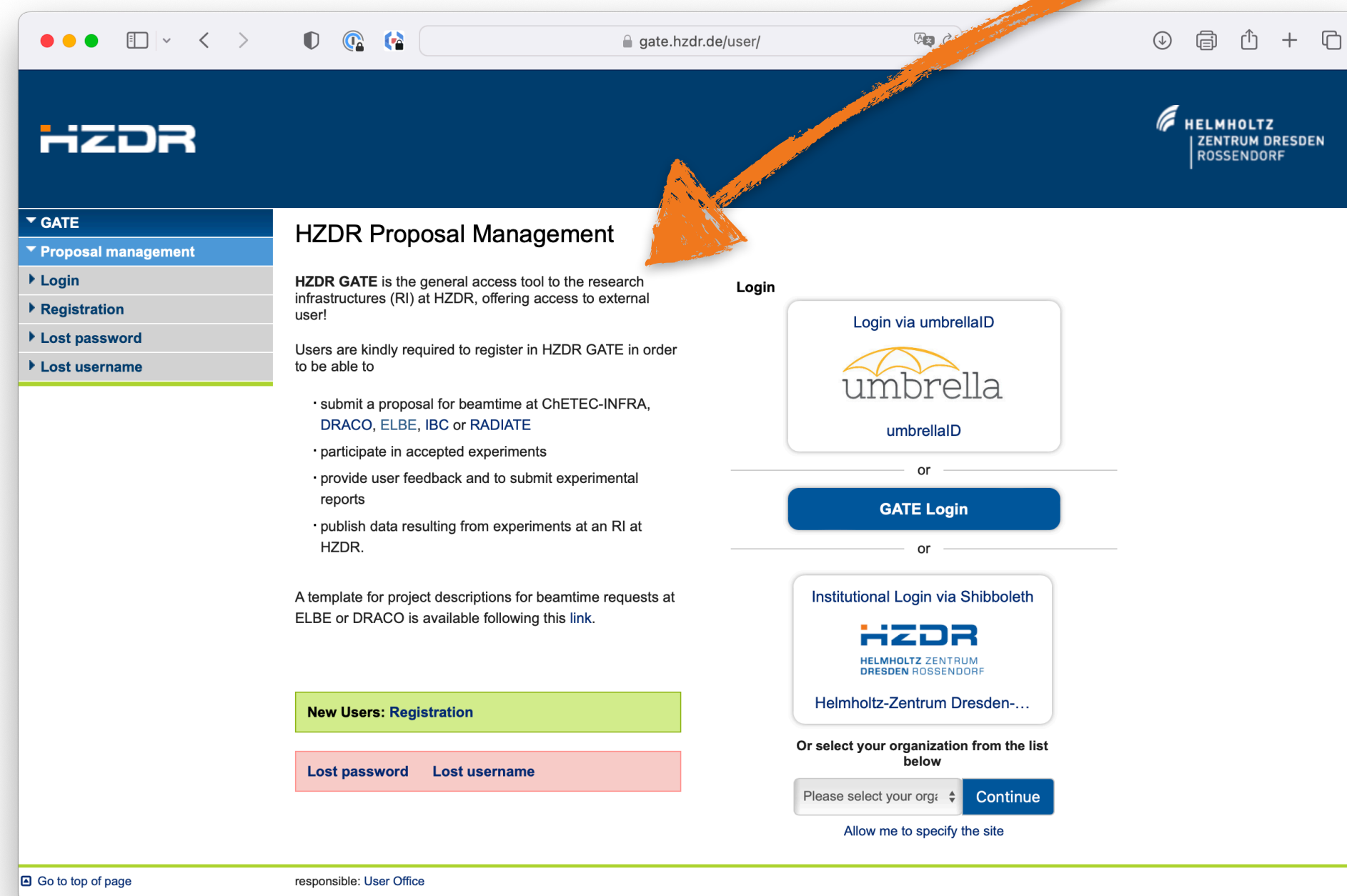
Mapping of the TELBE Resources to HELIPOINT



I. Proposal Submission

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

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



II. Project List and Dashboard

- Typically, a beam line scientist is the owner of a HELIPOINT 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.

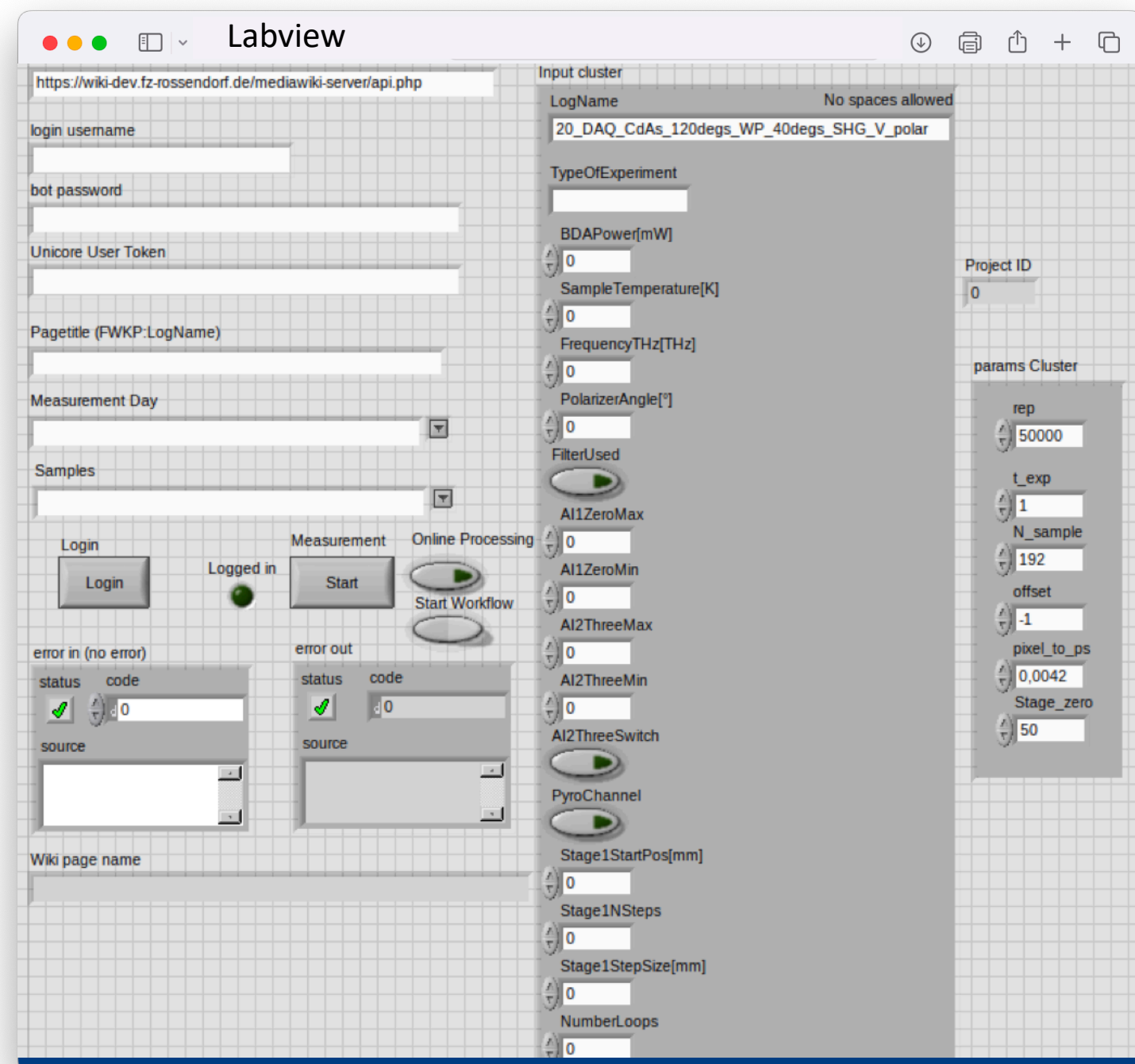
The left screenshot shows the 'Project List' page. It features a table with columns for Project Name, Last Modified, Owner, and an Open button. The projects listed include Semantic x-Lab, gELBE Projects (with sub-projects like gELBE beamtime 21102205-ST and 21202619-ST), Example parent project, ML Ops Project, SOTA on Uncertainties, Phase-resolved Higgs response in superconducting cuprates, Digital Twin Showcase, Beamtime Dashboard Test, and Rodare Data Publication Project. A 'Create Project' button and pagination controls are at the bottom.

Project Name	Last Modified	Owner	Open
Semantic x-Lab	Jul 11, 2023	Voigt, Martin (FWCC-D) - 141575	Open
gELBE Projects	Apr 24, 2023	Mueller, Dr. Stefan (FWCC) - 7394	Open
gELBE beamtime 21102205-ST	Sep 11, 2023	Mueller, Dr. Stefan (FWCC) - 7394	Open
gELBE beamtime 21202619-ST	Sep 11, 2023	Mueller, Dr. Stefan (FWCC) - 7394	Open
Example parent project	Apr 24, 2023	Voigt, Martin (FWCC-D) - 141575	Open
ML Ops Project	Jun 06, 2023	Knodel, Dr. Oliver (FWCC) - 132739	Open
SOTA on Uncertainties	May 23, 2023	Pape, David (FWCC) - 139658	Open
Phase-resolved Higgs response in superconducting cuprates	May 23, 2023	Gruber, Thomas (FWCC-D) - 141575	Open
Digital Twin Showcase	Jun 07, 2023	Voigt, Martin (FWCC-D) - 141575	Open
Beamtime Dashboard Test	May 31, 2022	Voigt, Martin (FWCC-D) - 141575	Open
Rodare Data Publication Project	Aug 09, 2022	Knodel, Dr. Oliver (FWCC) - 132739	Open

The right screenshot shows the 'Project Dashboard' for the project 'Phase-resolved Higgs response in superconducting cuprates'. It features a workflow diagram with four main stages: Systems, Resources, Automation, and Results. Each stage contains several components: Systems (Version Control, Data Management Plan, Documentation, Digital Objects), Resources (Data Source, SSH Files/Directories, UNICORE Storages), Automation (UNICORE Jobs), and Results (Archive, Publication). Plus signs indicate expandable sections.

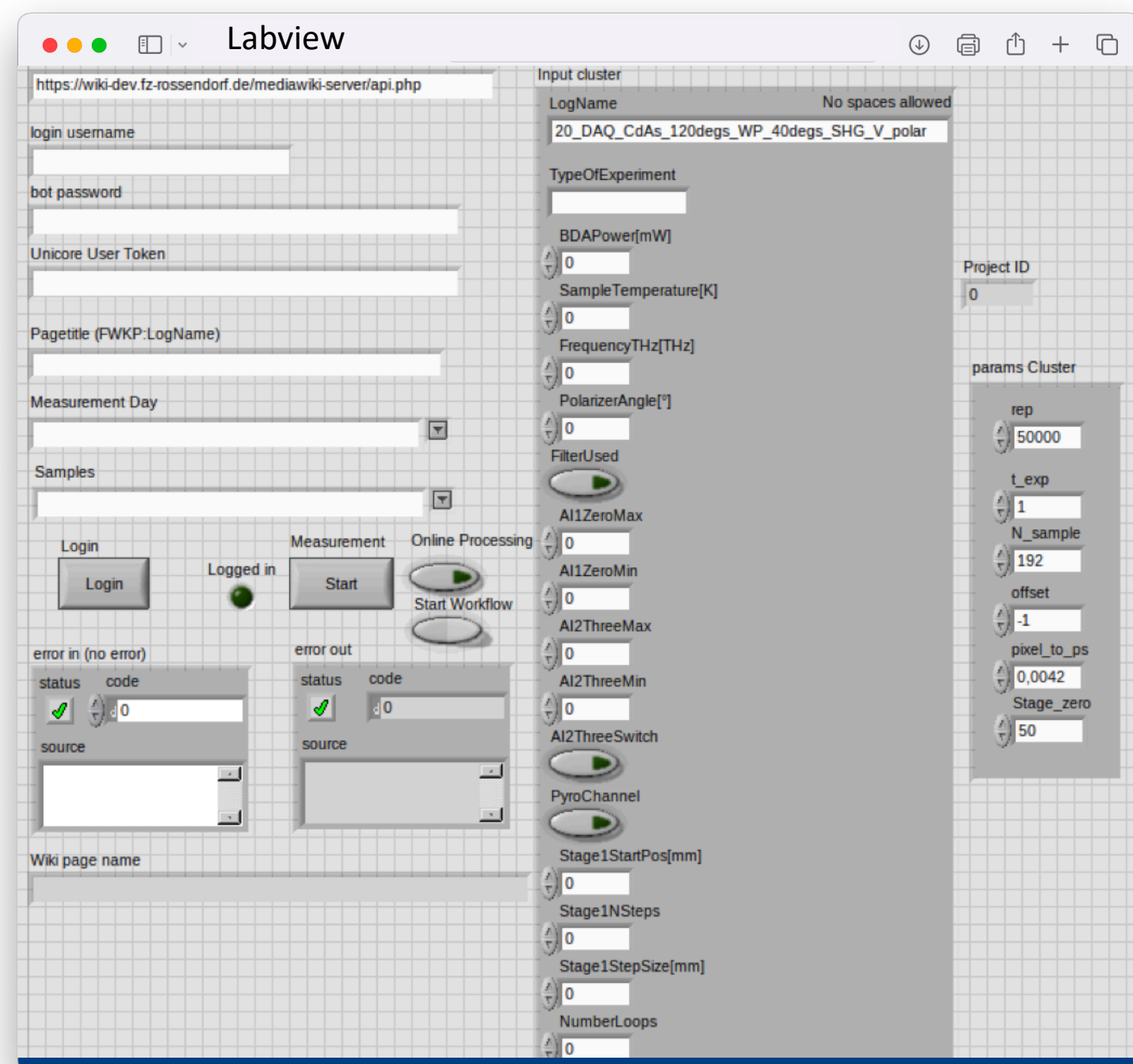
III. Detector Control and Workflows

- The HELIPORT REST-API enables the transfer of metadata between HELIPORT and external systems (e.g. the detector control in LabView).



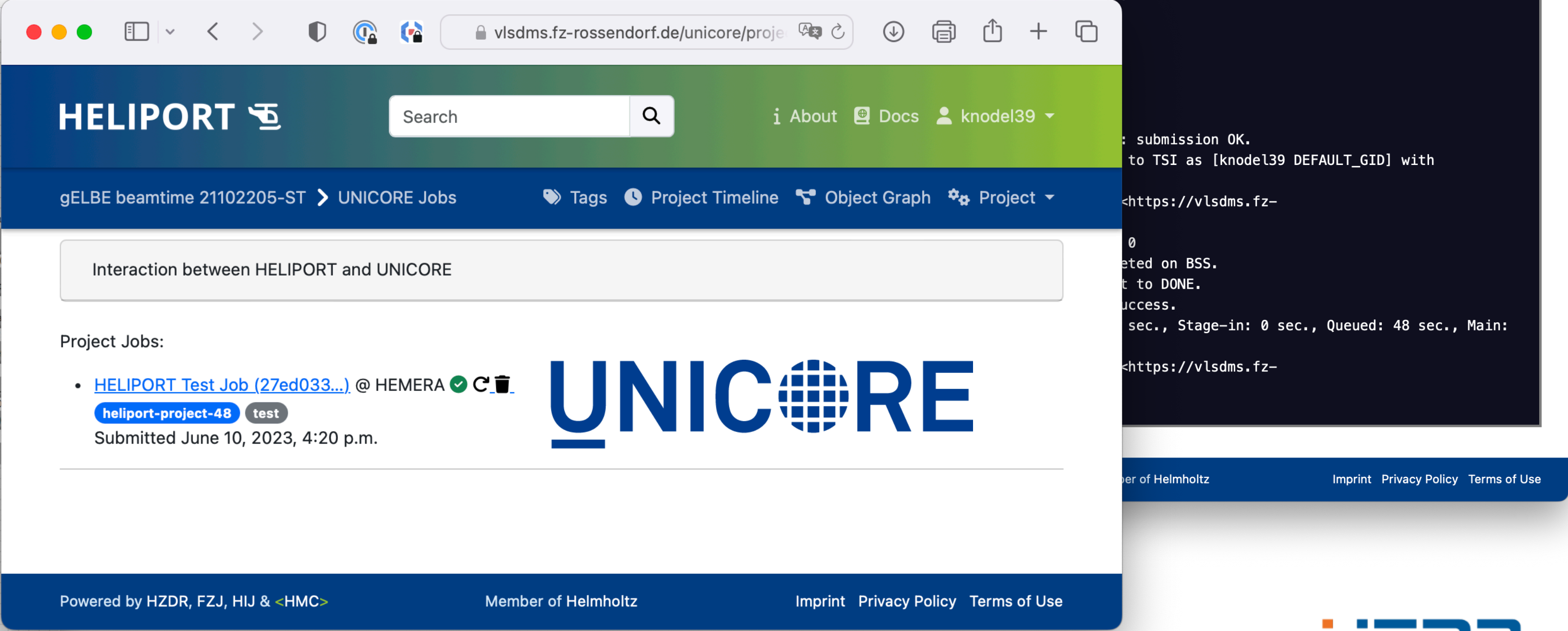
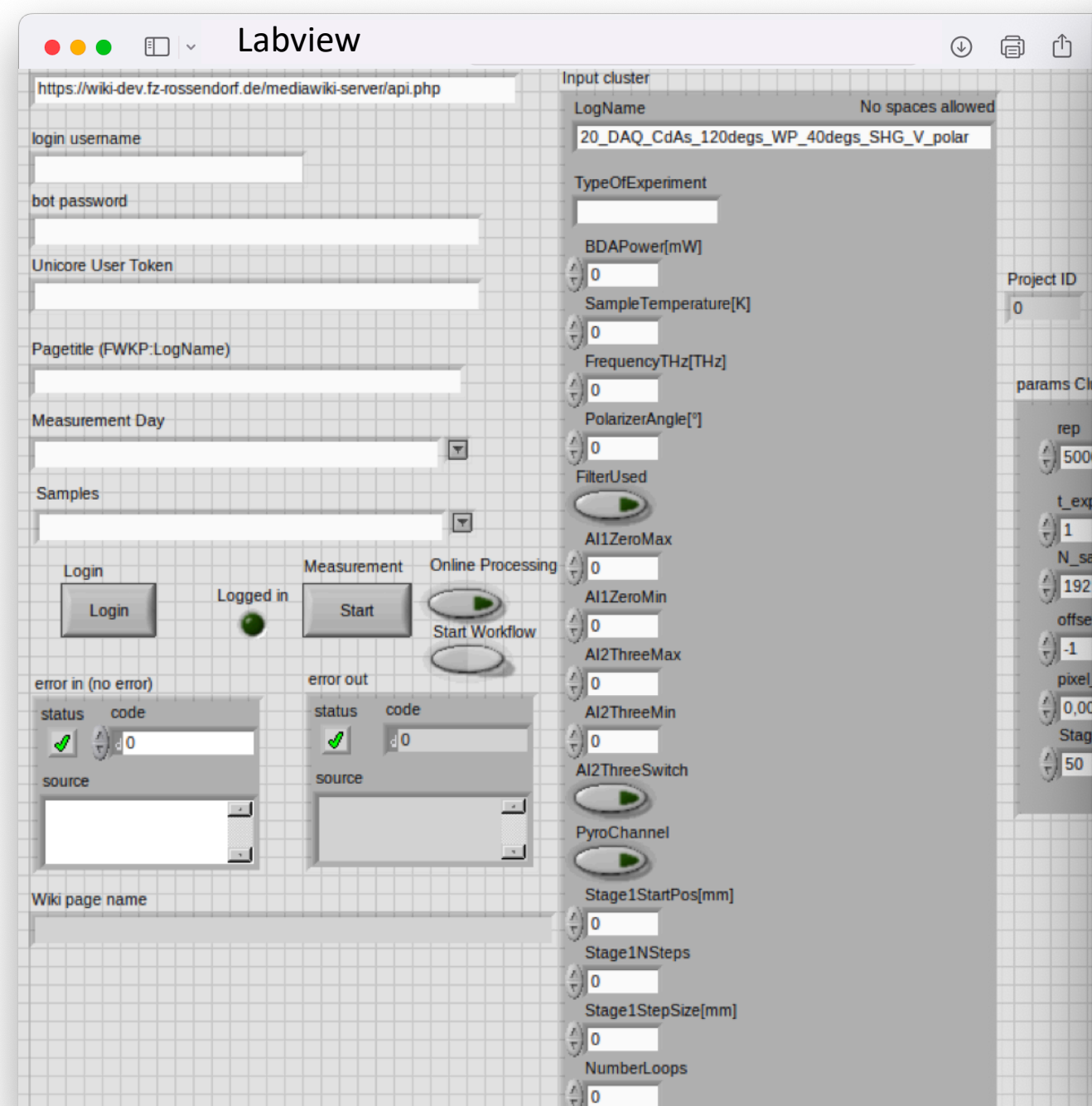
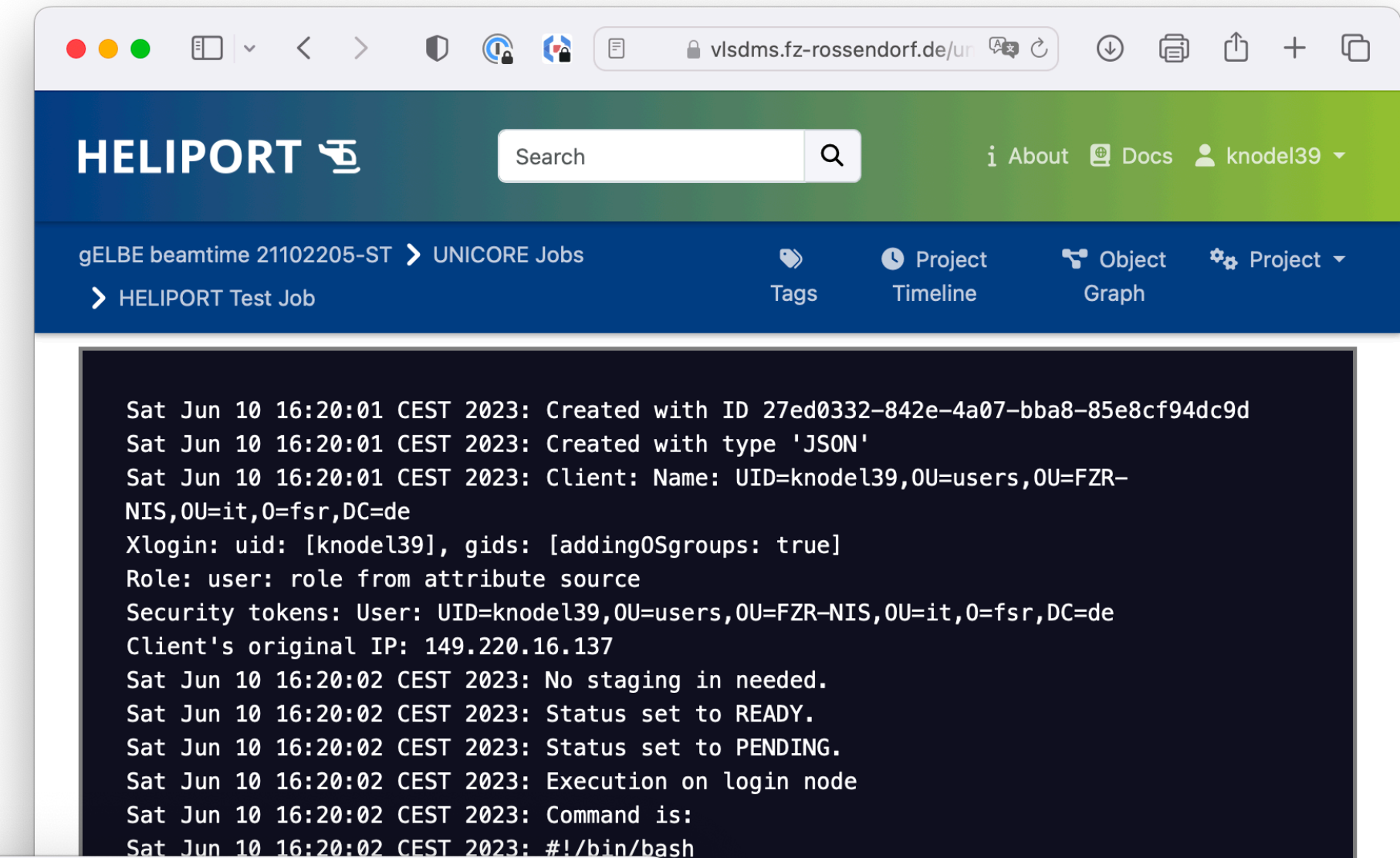
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- The HELIPORT REST-API enables the transfer of metadata between HELIPORT and external systems (e.g. the detector control in LabView).
- Via the API, LabView can control the integrated workflow management (e.g. UNICORE), which provides metadata for provenance information.



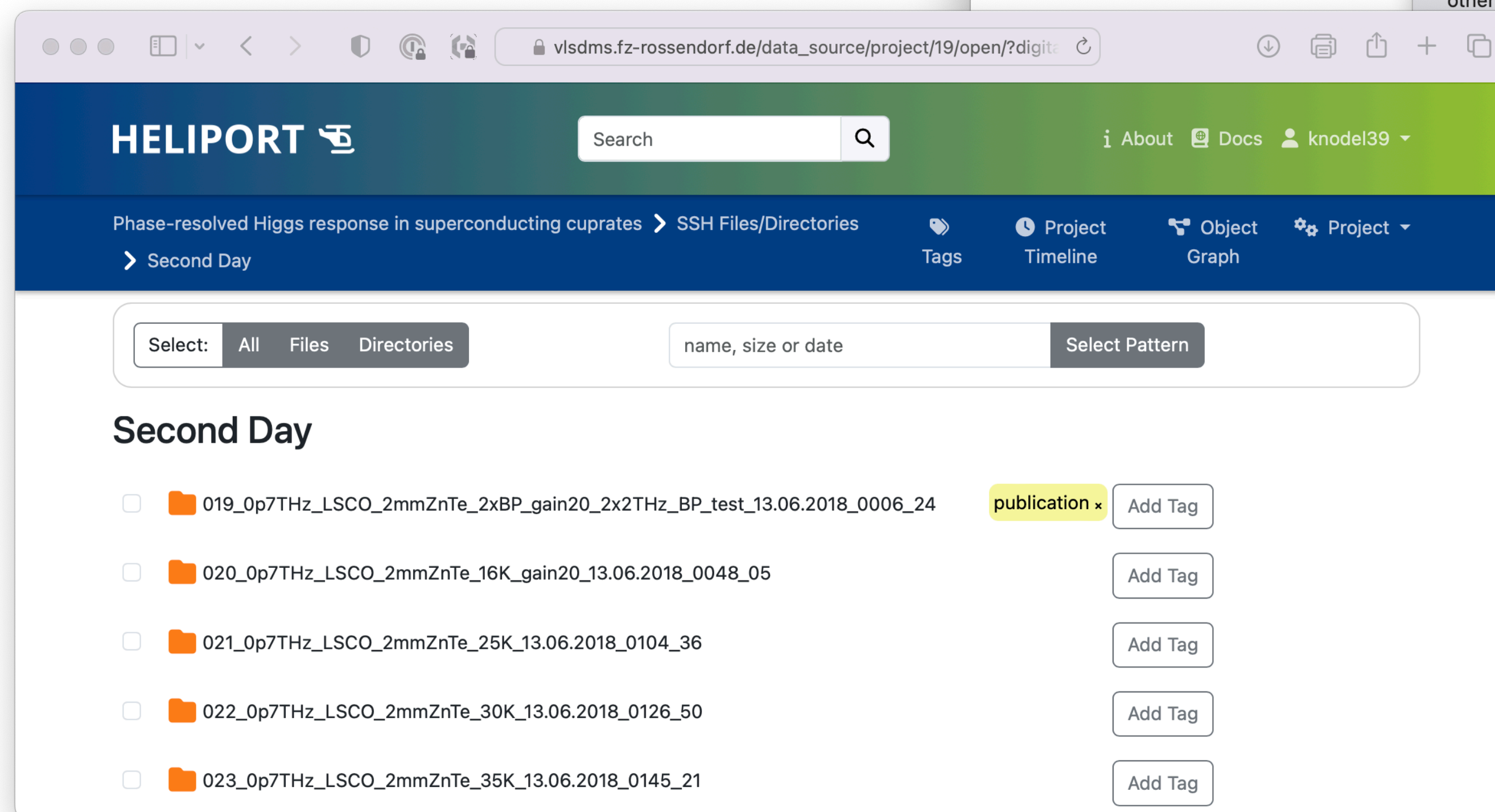
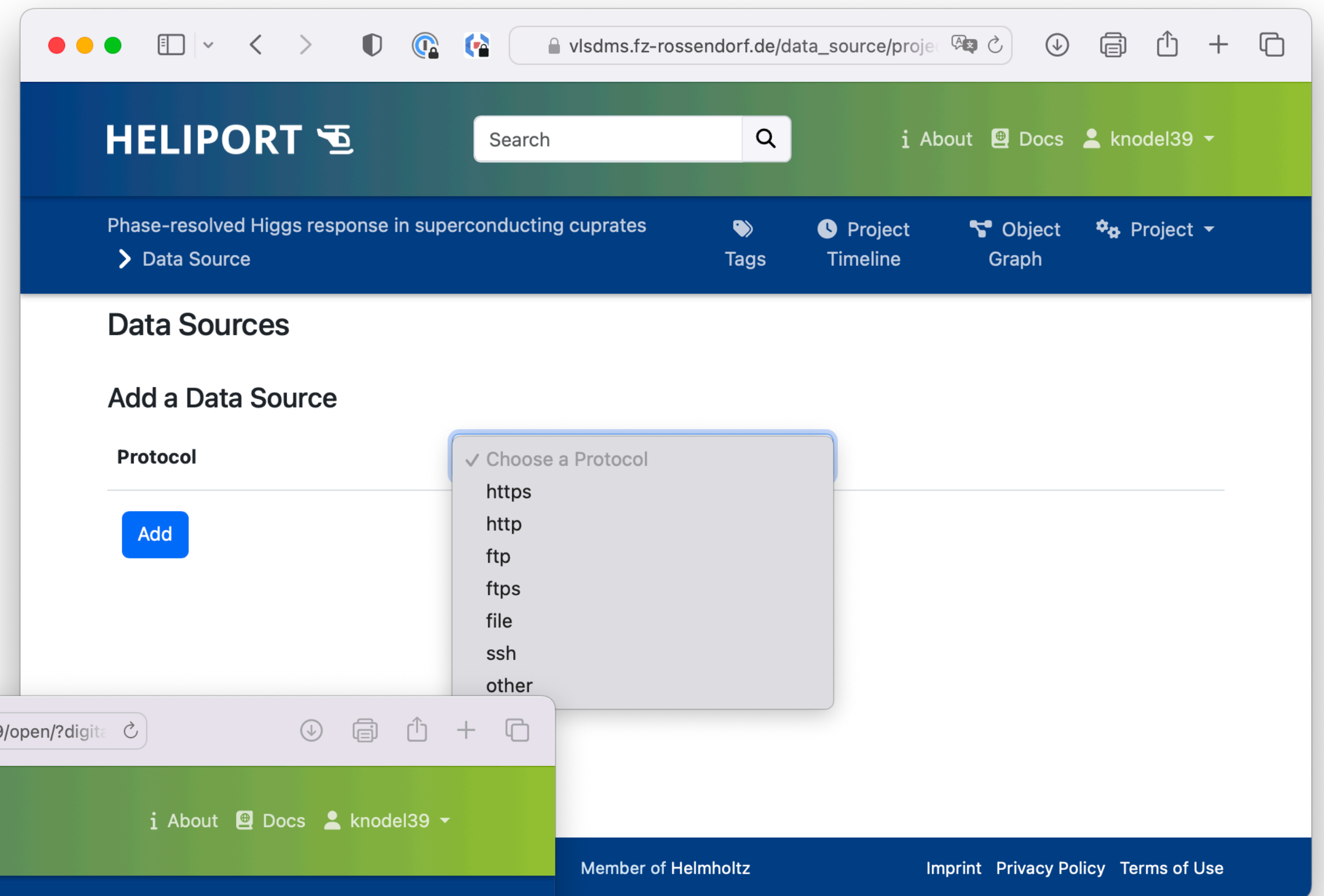
III. Detector Control and Workflows

- The HELIPOINT REST-API enables the transfer of metadata between HELIPOINT and external systems (e.g. the detector control in LabView).
- Via the API, LabView can control the integrated workflow management (e.g. UNICORE), which provides metadata for provenance information.
- The output of workflows (on our HPC cluster) can be accessed by any project member directly in the HELIPOINT web frontend.



IV. Data Sources

- Folders and Files in our internal filesystem can be registered in HELIPOINT as data source.
- Each member of a HELIPOINT project (Login via Helmholtz ID) has access to the files and folders.
- The provenance of the data sets generated from an experiment is entirely comprehensible.



V. Resources: Documentation and Repositories

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

- E-Labbook (Mediawiki),

The image shows two overlapping browser windows. The top window displays the HELIPORT documentation interface, which includes a search bar, navigation links, and a table of documentation entries. The bottom window shows a Mediawiki page for a specific dataset, featuring three plots, a metadata table, and a sidebar with navigation options.

HELIPORT Documentation Table:

ID	Description	System	Open	Edit	Remove
57	Project documentation in Mediawiki	MediaWiki	[Open]	[Edit]	[Remove]

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

Dataset [edit | edit source]

FWKP:direct plot of 22 DAQ CdAs 120degs WP 45degs SHG V polar

FWKP:fft power linscale plot of 22 DAQ CdAs 120degs WP 45degs SHG V polar

FWKP:fft power logscale plot of 22 DAQ CdAs 120degs WP 45degs SHG V polar

Data Files	File:FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar all loops.dat
Workflowhub URL	https://workflowhub.eu/workflows/459/ro_crate?version=1
Workflowhub Version	1
Repetition Rate	50000 Hz
time on single step measurement	1

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

BDA Power mW

Frequency THz

Polarizer

Angle

Filter Used No

AI2 Three Switch

Pyro Channel No

Stage1 Start Pos mm

Stage1 Step Size mm

Path binned /bigdata/telbe/Sorted_data/2022/2022-file March_datasorting/2022-03-13/binned

Scicat Export No

MediaWiki

V. 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, ...

The screenshot shows the WorkflowHub interface for a workflow titled "Sorting and registration of Terahertz ELBE raw data" (Version 1). The page includes a search bar, navigation tabs for Overview, Files, and Related items, and a detailed description of the workflow. It also lists the creator (Thomas Gruber) and the license (Creative Commons Attribution 4.0). A version history section shows the initial commit.

The screenshot shows the HELIPORT documentation page. The header includes the HELIPORT logo, a search bar, and navigation links for About, Docs, and user profile. The main content area displays a table of documentation entries with columns for ID, Description, and System. A table with 3 columns (ID, Description, System) is shown below the header.

ID	Description	System
57	Project documentation in Mediawiki	MediaWiki

The screenshot shows the HELIPORT Version Control page. It features a search bar and navigation links. The main content area displays a table of source code repositories with columns for ID and Name. A table with 2 columns (ID, Name) is shown below the header.

ID	Name
7	Telbe sorting script

The screenshot shows a Mediawiki page for a dataset titled "FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar 01". The page includes a navigation sidebar, a "Dataset" section with three plots, and a metadata table. The plots show data for FWKP:direct plot, FWKP:fft power linscale plot, and FWKP:fft power logscale plot. The metadata table includes fields like Data Files, Workflowhub URL, and Repetition Rate.

Field	Value
Data Files	File:FWKP:22 DAQ CdAs 120degs WP 45degs SHG V polar all loops.dat
Workflowhub URL	https://workflowhub.eu/workflows/459/ro_crate?version=1
Workflowhub Version	1
Repetition Rate	50000 Hz
time on single step measurement	1

VI. Integration in an Overall Data Publication Workflow

The screenshot displays the HELIPORT web interface. On the left, a sidebar shows project details for 'Phase-resolved Higgs response in superconducting cuprates'. The main area features a workflow diagram with four stages: Systems, Resources, Automation, and Results. An orange arrow points from the 'Project Configuration' link in the sidebar to the 'Automation' stage of the workflow.

Project Properties

HZDR-ID	HZDR.FWCC.2021.114636
Digital Object ID	83
uuid	12215397-437a-468a-a95d-1a1d3f1d92ea
Landing Page	https://vlsdms.fz-rossendorf.de/object/83/?format=landing_page
Created	May 18, 2021, 5:03 p.m.
Department	FWCC
Title	Phase-resolved Higgs response in superconducting ci

Tags

TELBE

Add Tag

Members and Contributors

This is a list of the project owner and members, as well as external contributors without a HELIPORT login.

Name	Affiliation	Contribution
Gruber, Dr. Thomas (FWCC) - 130673		Owner
Deinert, Dr. Jan-Christoph (FWKP) - 118987		Member
Knodel, Dr. Oliver (FWCC) - 132739		Member
Lokamani, Mani (FWCC) - 19342		Member
Mueller, Dr. Stefan (FWCC) - 7394		Member

Workflow Diagram:

- Systems:** Version Control, Data Management Plan, Documentation, Digital Objects
- Resources:** Data Source, SSH Files/Directories, UNICORE Storages
- Automation:** UNICORE Jobs
- Results:** Archive, Publication

Automated data publication with:

- Metadata from Proposal System,

VI. Integration in an Overall Data Publication Workflow

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Systems

- Version Control
- Data Management Plan
- Documentation
- Digital Objects

Resources

- Data Source
- SSH Files/Directories
- UNICORE Storages

RODARE Record

December 16, 2021

Phase-resolved Higgs response in superconducting cuprates

2,980 views | 10,619 downloads

Publication date: December 16, 2021

DOI: [10.14278/rodare.1289](https://doi.org/10.14278/rodare.1289)

Keyword(s): Superconductors, terahertz, Higgs, Nonlinear dynamics, ultrafast

Related identifiers: Identical to: <https://www.hzdr.de/publications/Publ-30902>

Referenced by: <https://www.hzdr.de/publications/Publ-29647>, [10.1038/s41467-020-15613-1](https://www.hzdr.de/publications/Publ-101038)

Communities: Research field: Matter, RODARE

License (for files): Creative Commons Attribution 4.0 International

Versions

Version	Date
Version 2	Dec 16, 2021
10.14278/rodare.1289	

Second Day

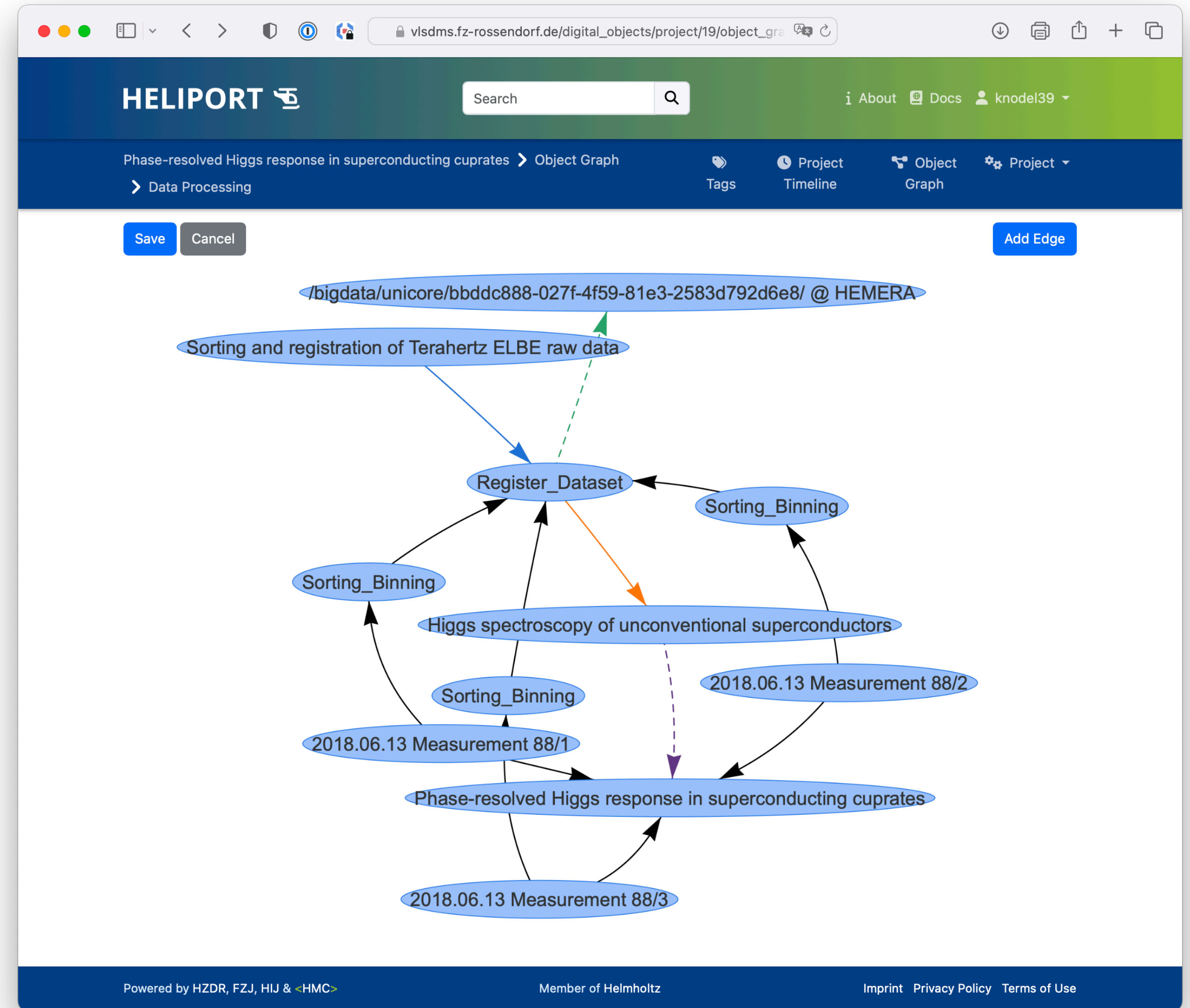
- 019_0p7THz_LSCO_2mmZnTe_2xBP_gain20_2x2THz_BP_test_13.06.2018_0006_24 **publication** Add Tag
- 020_0p7THz_LSCO_2mmZnTe_16K_gain20_13.06.2018_0048_05 Add Tag
- 021_0p7THz_LSCO_2mmZnTe_25K_13.06.2018_0104_36 Add Tag
- 022_0p7THz_LSCO_2mmZnTe_30K_13.06.2018_0126_50 Add Tag
- 023_0p7THz_LSCO_2mmZnTe_35K_13.06.2018_0145_21 Add Tag

Automated data publication with:

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

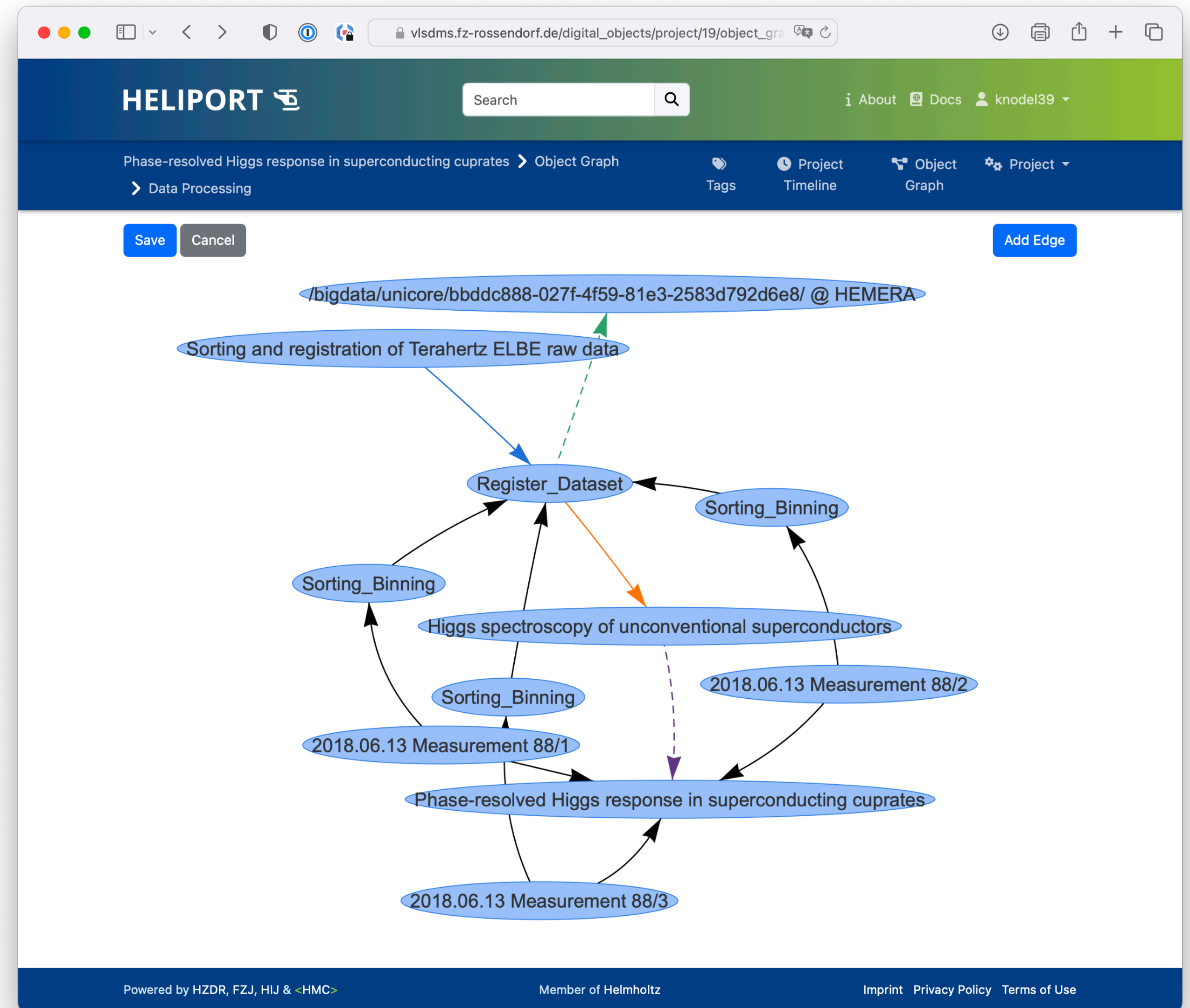
VII. Relations Between Digital Objects and

- Relations between digital objects are visualised to provide a top-level view on the project.



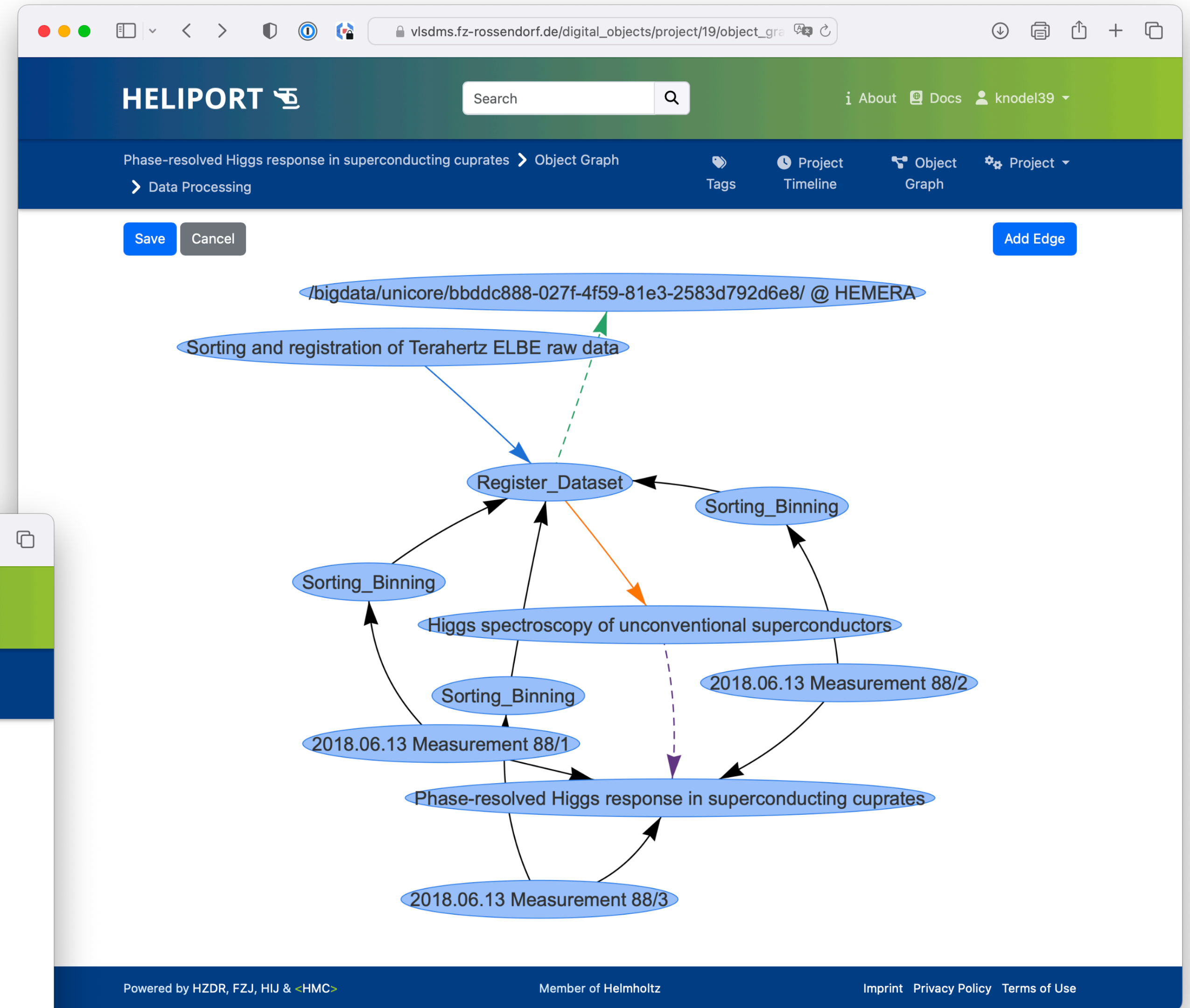
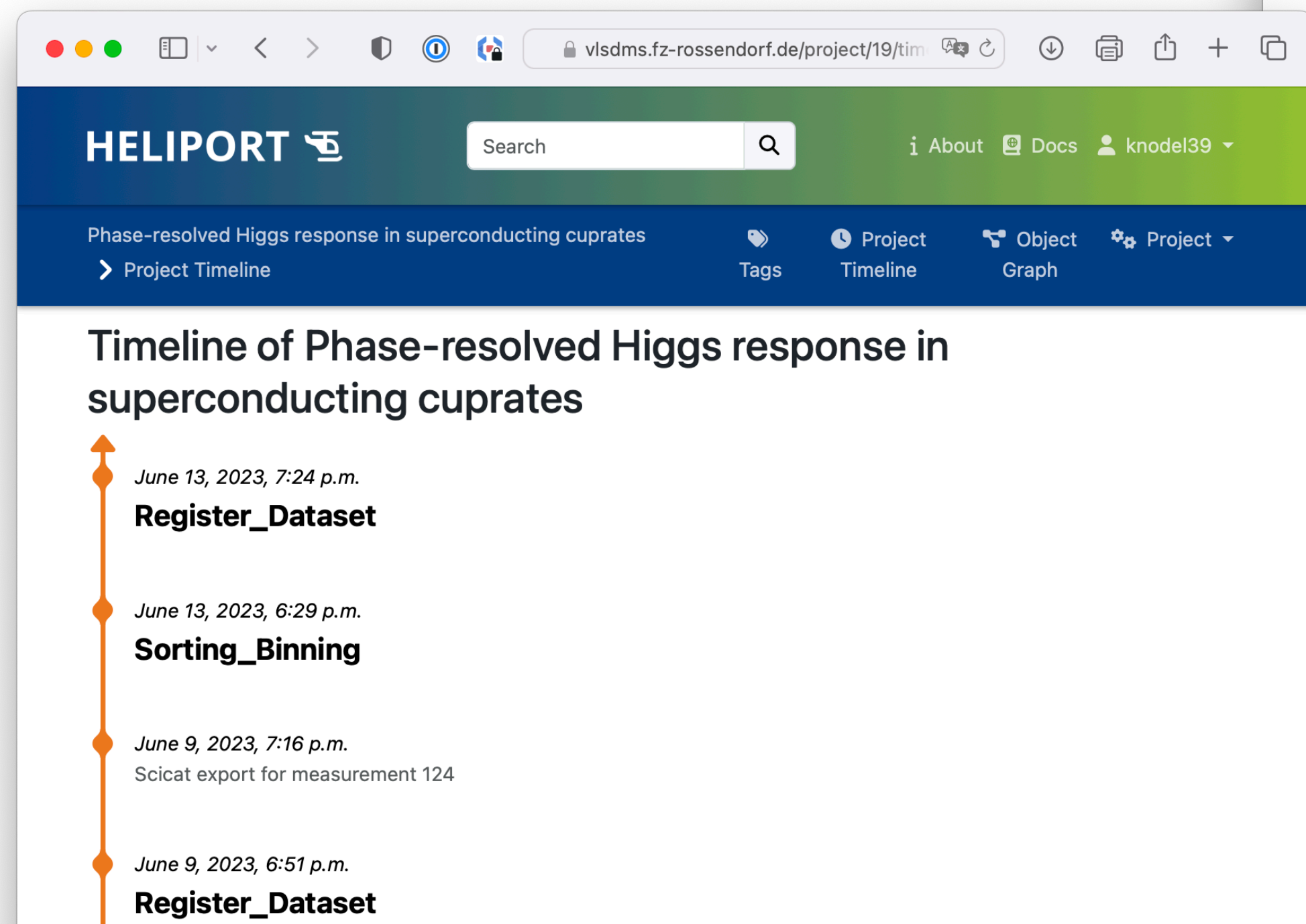
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- The relationships between simulation (surrogate model) and experiment can also be illustrated.



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



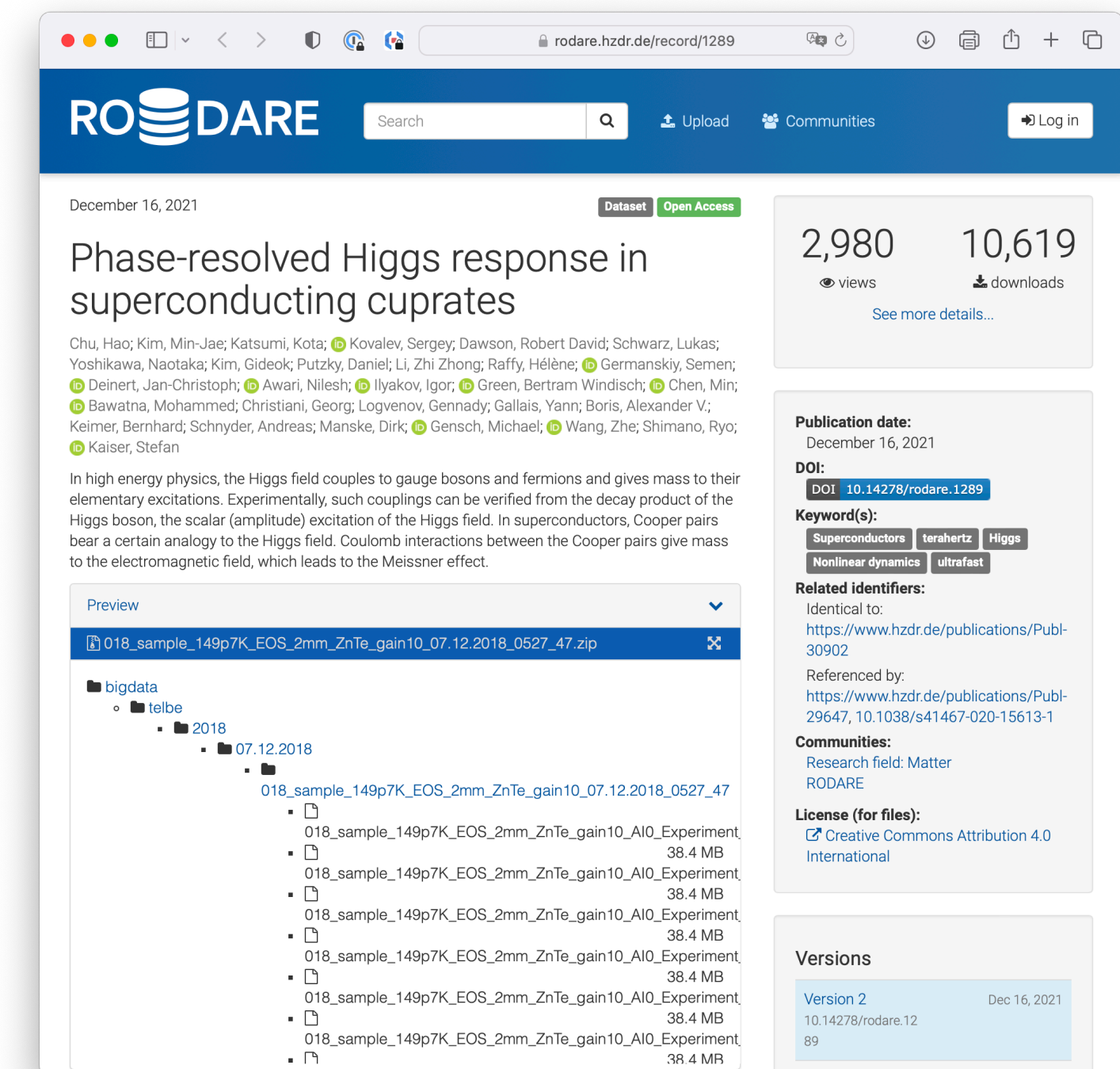
Additional Systems/Services: Grafana & RDMO



The screenshot shows the RDMO web application interface. The header includes 'HZDR RDMO' and 'Language Login'. The main content area features a large banner with the text 'RDMO A tool to support the planning, implementation, and organisation of research data management.' Below the banner, there is a 'Welcome to RDMO' section with a description of the project's aim and a link to the GitHub repository. On the right side, there is a 'Login' form with fields for 'Username' and 'Password', a 'Remember Me' checkbox, and a 'Login' button. Below the login form, there is a note about logging in via Helmholtz AAI with the Helmholtz logo and the text 'SPITZENFORSCHUNG FÜR GROSSE HERAUSFORDERUNGEN'.

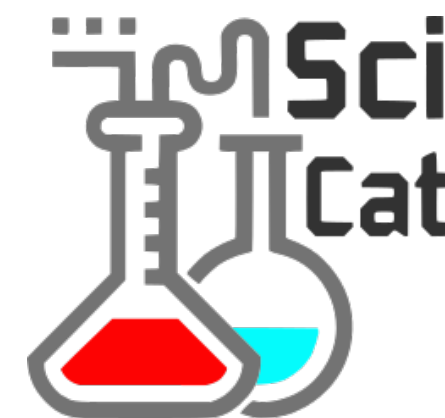
Next Steps: Integration of an Additional Metadata Catalogue

- With our data publication repository RODARE (based on InvenioRDM) we provide a platform for publishing datasets.
- In RODARE, bibliographic metadata is based on DataCite.



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- With our data publication repository RODARE (based on InvenioRDM) 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.



The SciCat interface displays the following information for 'Raw Dataset Example 380':

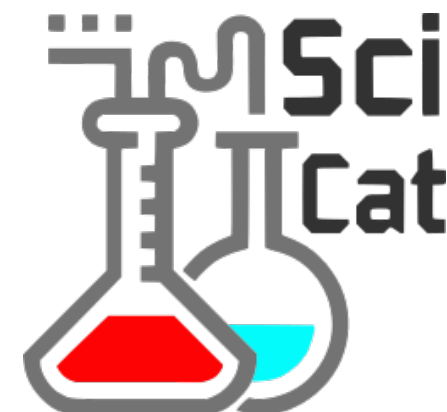
- Name:** Raw Dataset Example 380
- Description:** This input file was created to study aluminum oxide film on rough aluminum surface with high spatial resolution. Load the datafile folder with happi to do analysis.
- PID:** HZDR/73da2dfa-176f-4c6c-853a-b3ffbf4e3d7
- Type:** raw
- Creation Time:** 2022-12-13 17:47
- Keywords:** Rough surface, aluminum oxide film, Smilei simulation

The RODARE interface displays the following information for 'Phase-resolved Higgs response in superconducting cuprates':

- Publication date:** December 16, 2021
- Views:** 2,980
- Downloads:** 10,619
- DOI:** 10.14278/rodare.1289
- Keywords:** Superconductors, terahertz, Higgs, Nonlinear dynamics, ultrafast
- Related identifiers:** Identical to: <https://www.hzdr.de/publications/Publ-30902>; Referenced by: <https://www.hzdr.de/publications/Publ-29647>, <https://www.hzdr.de/publications/Publ-101038>, <https://www.hzdr.de/publications/Publ-101467>
- Communities:** Research field: Matter; RODARE
- License (for files):** Creative Commons Attribution 4.0 International
- Versions:** Version 2 (10.14278/rodare.1289) - Dec 16, 2021

Next Steps: Integration of an Additional Metadata Catalogue

- With our data publication repository RODARE (based on InvenioRDM) 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.
- Within the DAPHNE4NFDI project, we want to establish such an approach for the photon and neutron community.



The image displays two overlapping web browser windows. The top window is the SciCat interface, showing a dataset page for 'Raw Dataset Example 380'. It includes sections for General Information (Name, Description, PID, Type, Creation Time, Keywords), Creator Information (Owner, Principal Investigator, OrCID, Contact Email, Owner Group, Access Groups), File Information (Source Folder, Size, Data Format), Related Documents (Creation Location, Techniques), and Scientific Metadata (a table of parameters like DiagParticleBinningNo, E_to_a0, etc.). The bottom window is the RODARE interface, showing a record for 'Phase-resolved Higgs response in superconducting cuprates'. It features a search bar, upload button, and login link. The record includes the publication date (December 16, 2021), DOI (10.14278/rodare.1289), keyword tags (Superconductors, terahertz, Higgs, Nonlinear dynamics, ultrafast), related identifiers, and a file preview tree showing a directory structure with subfolders like 'bigdata' and 'telbe' containing various data files.

Future: Providing Metadata for UnHIDE (Unified Helmholtz Information and Data Exchange)

The screenshot shows a web browser window with the URL `search.unhide.helmholtz-metadaten.de`. The page features the UnHIDE logo on the left and a search bar on the right containing the text "Helmholz Association (HGF)" and "AWI". Below the search bar, there are navigation links: "Try: Pangaea →", "Forschungszentrum Jülich →", "AWI →", and "DESY →".

A quote is displayed: *"Meaningfully combining data from heterogeneous sources is a knowledge graph's main value proposition."* attributed to - Andreas Blumaür, The Knowledge Graph Cookbook.

The main text states: "The **Unified Helmholtz Information and Data Exchange (UnHIDE)** Project aims to build a sustainable, interoperable, and inclusive digital ecosystem for all stakeholders. Existing and emerging data systems are linked, with the ultimate goal of coordinating action and capacity to improve access to scientific publications, software, data and knowledge. The Project is funded by the centers of the Helmholtz Association and implemented by the Helmholtz Metadata Collaboration (HMC)."

Below the text is a link: [To learn more about this project - click here](#)

The "Categories" section contains two rows of navigation items, each with an icon and a right-pointing arrow:

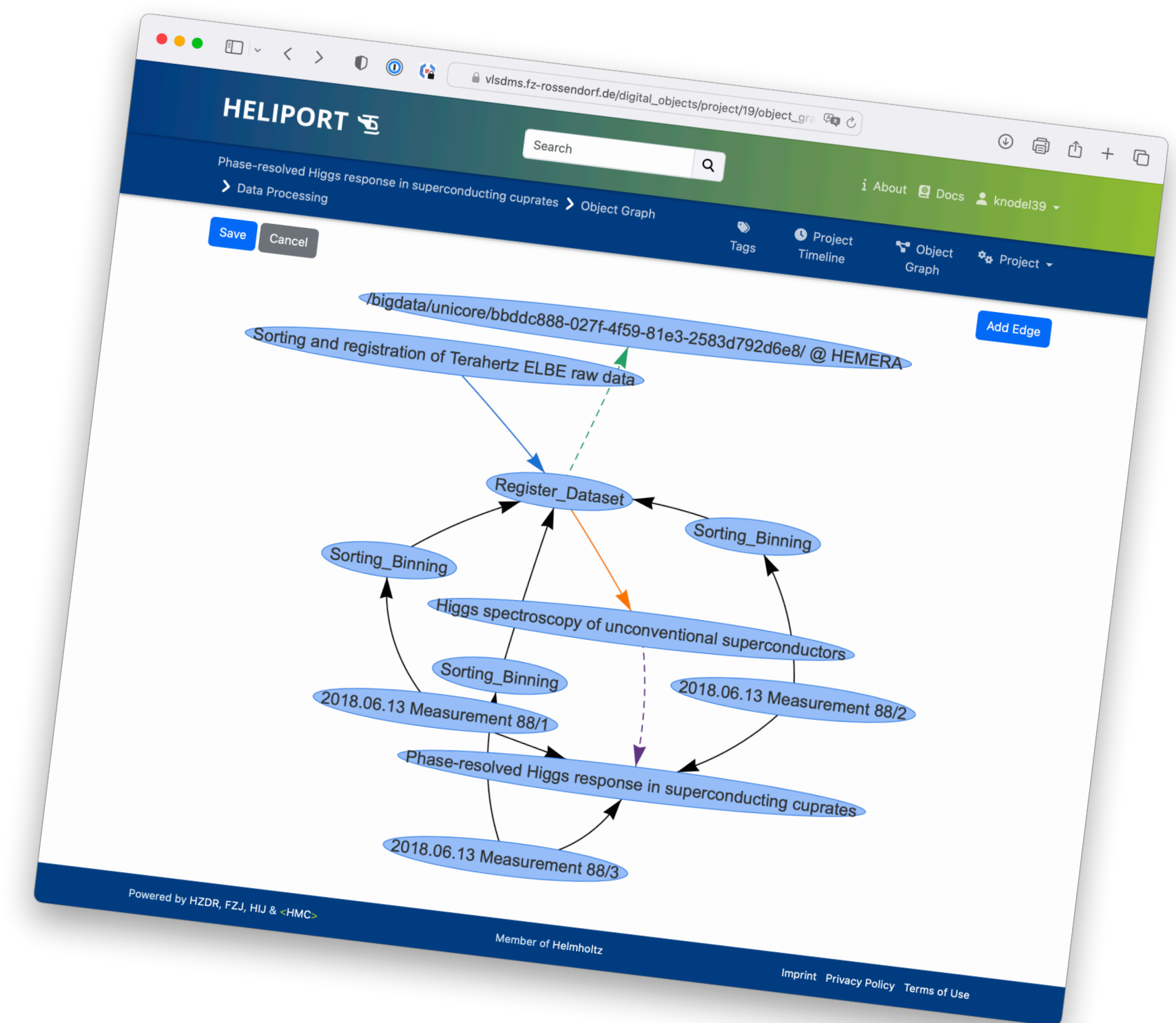
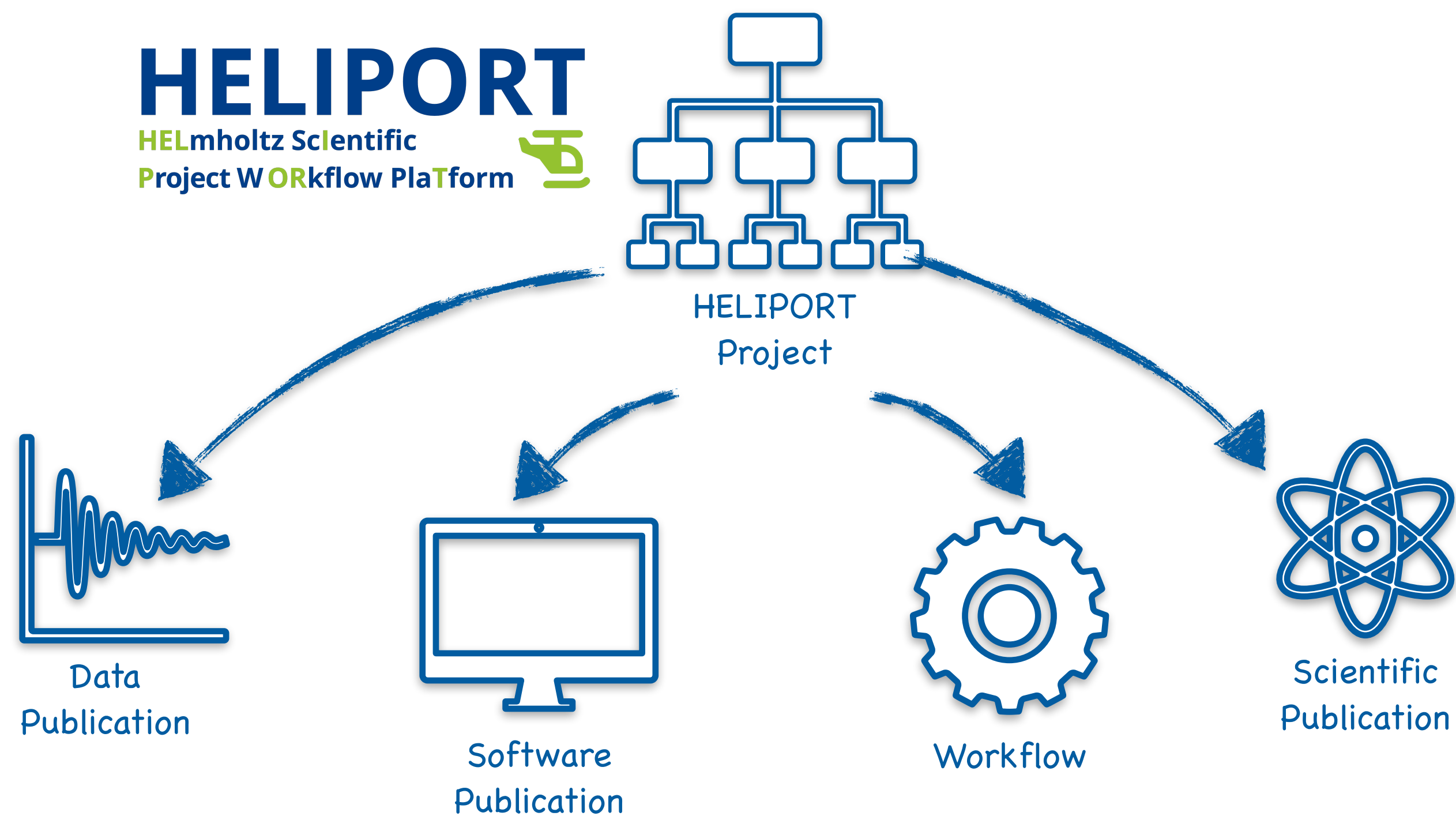
- Row 1: Experts → Documents → Trainings → Datasets → (with a '0' in a circle)
- Row 2: Software → Projects → Institutions → Instruments → (with a '0' in a circle)

The footer includes the Helmholtz logo with the tagline "Research for grand challenges." and the HMC logo with the text "HELMHOLTZ Metadata Collaboration".



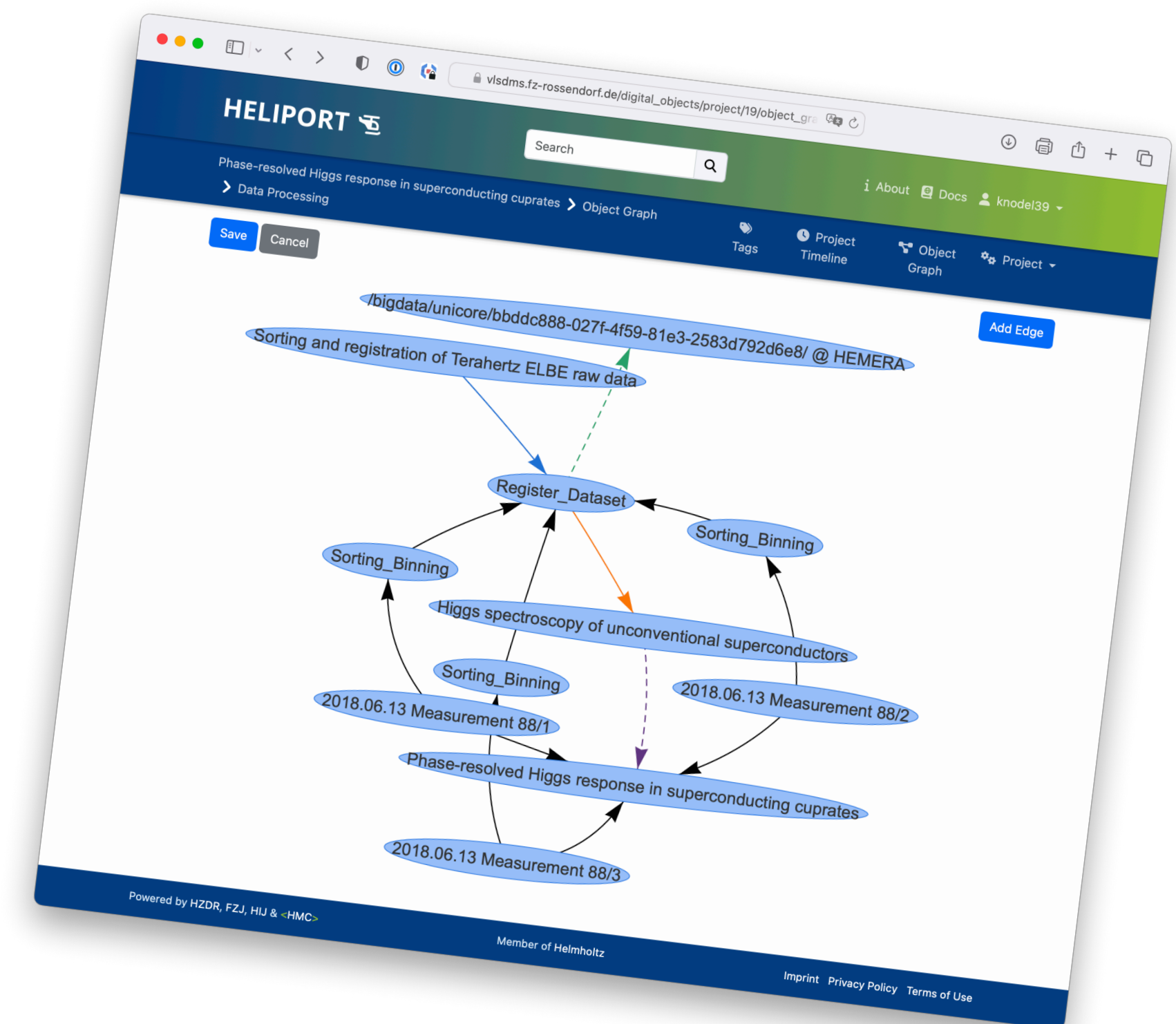
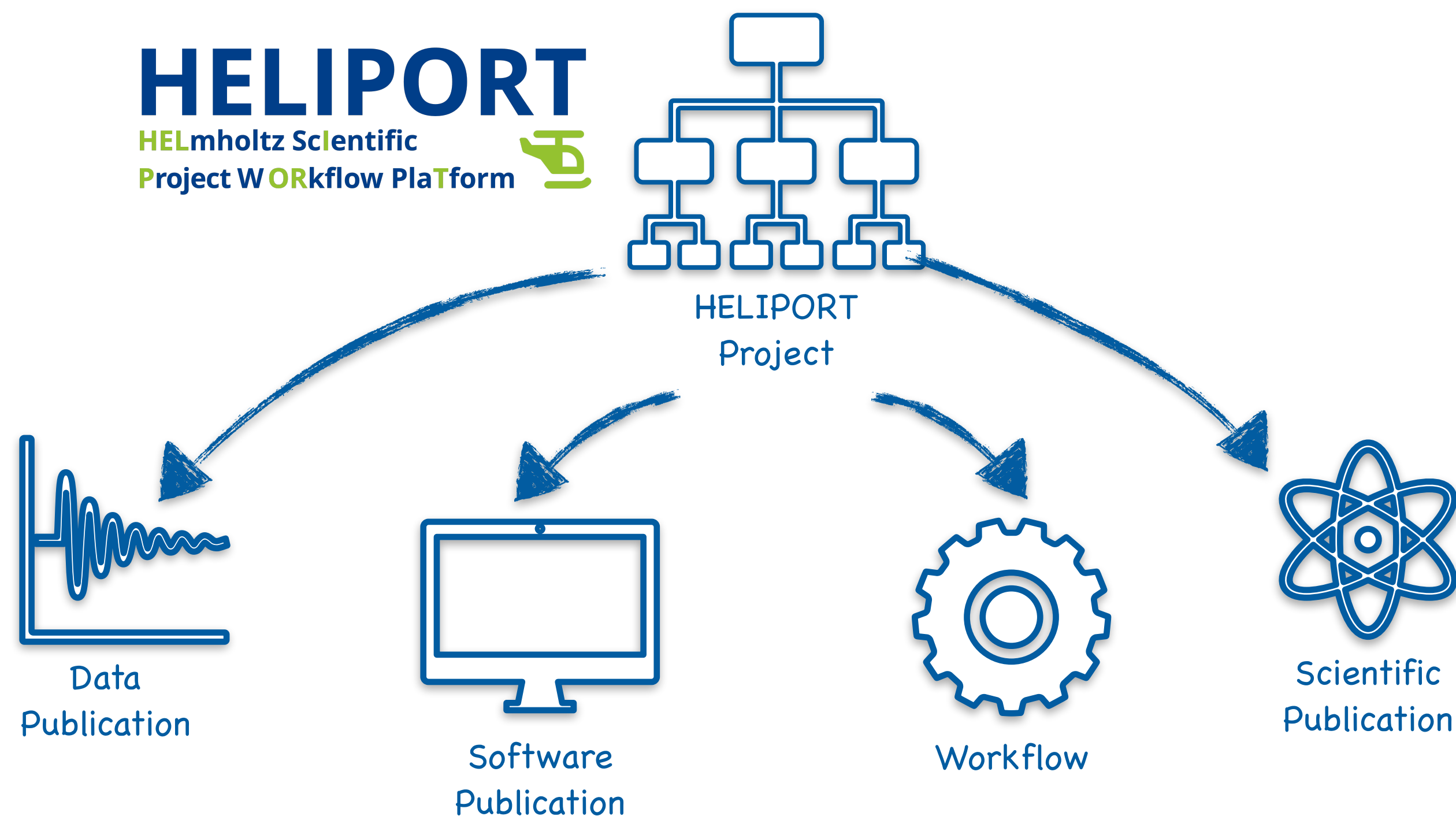
Conclusions

- HELIPORT describes and collects all metadata from all services and systems involved in an scientific experiment.



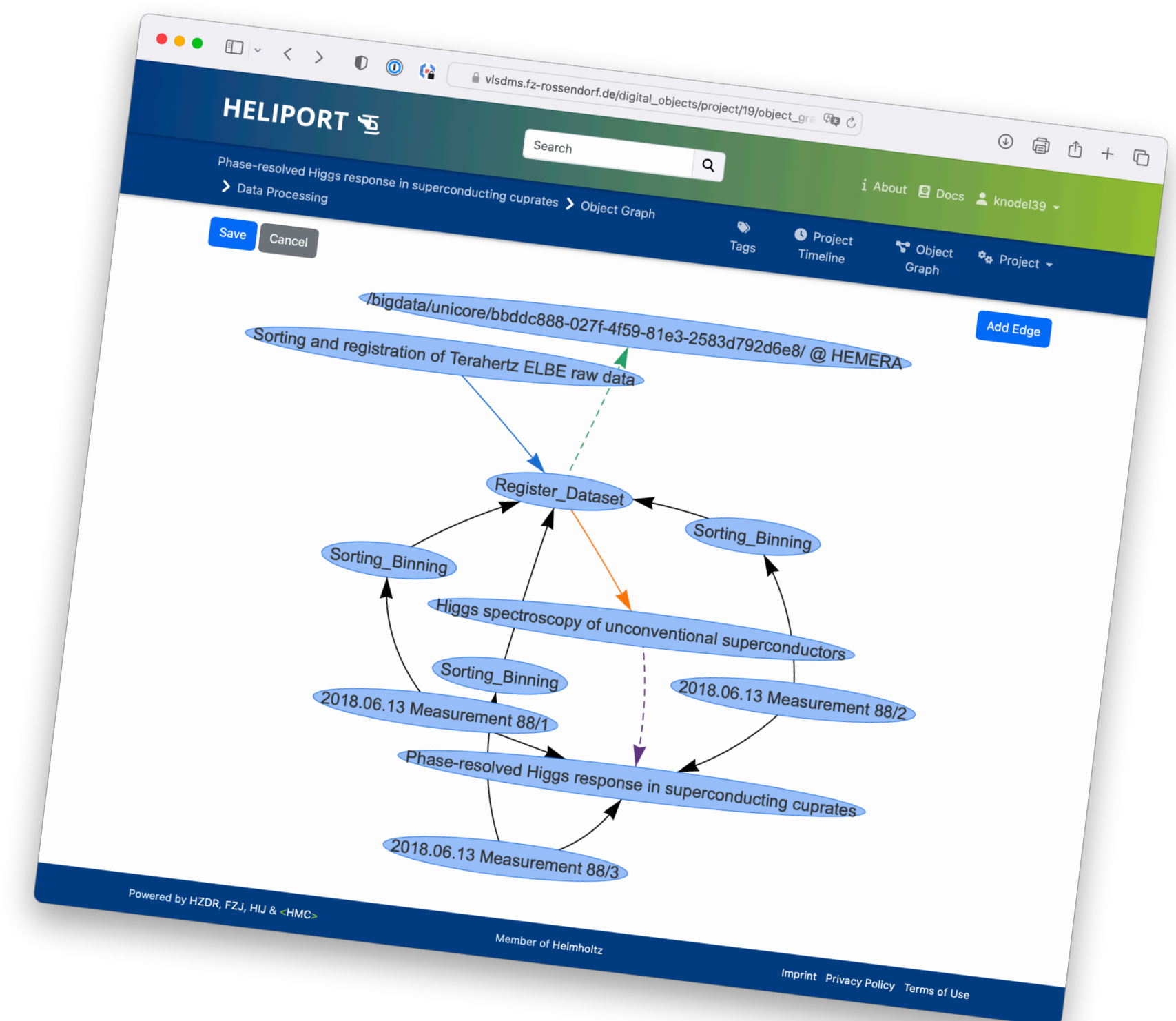
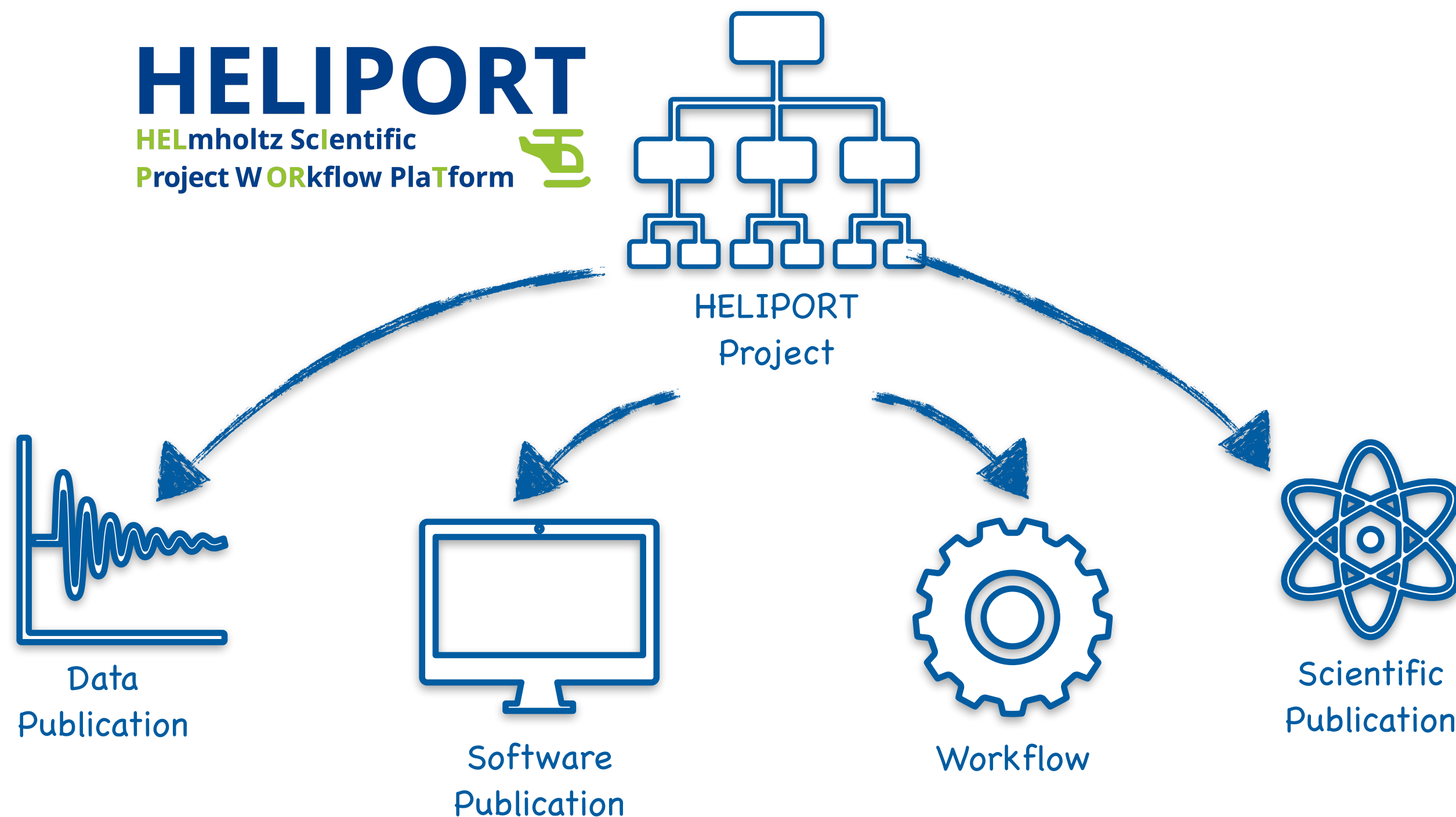
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- Such an approach is desirable and leads us to a fully **FAIR** and **comprehensible** research project.



Conclusions

- HELIPOINT describes and collects all metadata from all services and systems involved in an scientific experiment.
- Such an approach is desirable and leads us to a fully **FAIR** and **comprehensible** research project.
- The computational workflows are essential to keep track of everything what happened during the experiment.



Resources

Website: heliport.hzdr.de

Repository: [codebase.helmholtz.cloud/heliport](https://codebase.helmholtz.cloud/heliport/heliport)

The screenshot shows the HELIPOINT website's 'About' page. The main heading is 'HELIPORT HELmholtz Science Project WORKflow'. Below it, a paragraph describes the system's goal: 'The guidance system HELIPOINT aims to make the entire life cycle of a project at the interoperable and reusable according to the FAIR principles, mentioned below. In particular, it deals with the areas from the generation of the data to the publication of primary research data and the actual research results. For this purpose, a concept was developed which shows the various components and their connections. Descriptions of the individual components can be found in our HZDR Documentation.' A large QR code is overlaid on the right side of the page. Below the text, there is a diagram titled 'Project Graph: gELBE beamtime 21102205-ST' showing a flow from 'Project' to 'Systems', 'Resources', 'Automation', and 'Results'. A sidebar on the left lists various components like 'api', 'gate-connection', 'version-control', etc.

The screenshot shows the HELIPOINT repository page on codebase.helmholtz.cloud. The repository name is 'HELIPORT' with Project ID: 1287. It has 1,941 Commits, 5 Branches, 2 Tags, and 3.4 GiB Project Storage. The current version is 0.6.0, with a pipeline that passed, coverage of 61.00%, and a lifecycle of experimental. The code style is black and the license is GPL-3.0-or-later. A recent commit titled 'Bump django from 4.2.4 to 4.2.5' is shown, authored by HIFIS Bot 40 minutes ago. The repository has 9 stars and 2 forks. Navigation options include 'History', 'Find file', 'Edit', 'Clone', and 'Add Wiki'.

The screenshot shows a workshop presentation slide. The title is 'HELIPORT: A Portable Platform for FAIR {Workflow | Metadata | Scientific Project Lifecycle} Management and Everything'. The authors are Oliver Knodel, Martin Voigt, Robert Ufer, David Pape, Mani Lokamani, Stefan E. Müller, Thomas Gruber, and Guido Juckeland, from Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. The DOI is 10.1145/3456287.3465477. The abstract discusses the challenges of modern scientific collaborations and projects (MSCPs) and the role of HELIPORT in addressing these challenges. The slide also includes an introduction section.