

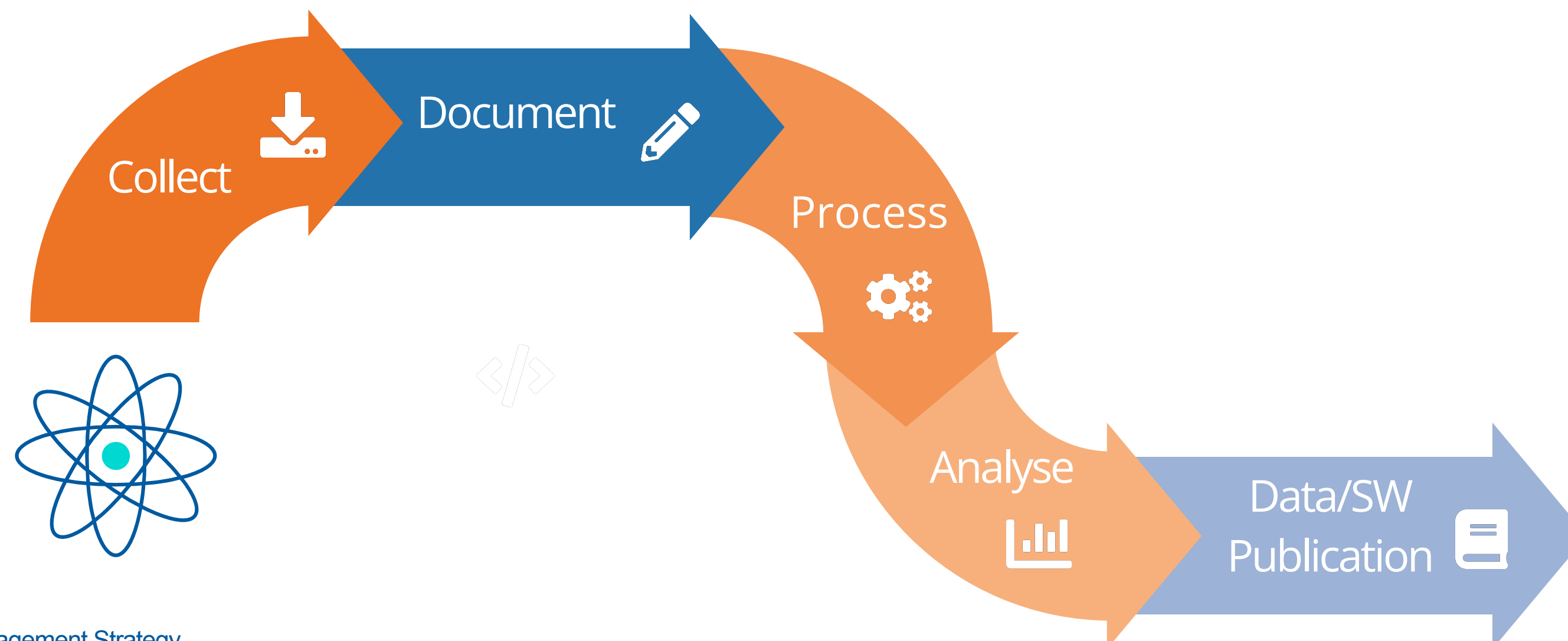
The (emerging) HZDR Data Management Strategy

Data and Software Management Days, October, 2024
Oliver Knodel // contact: o.knodel@hzdr.de



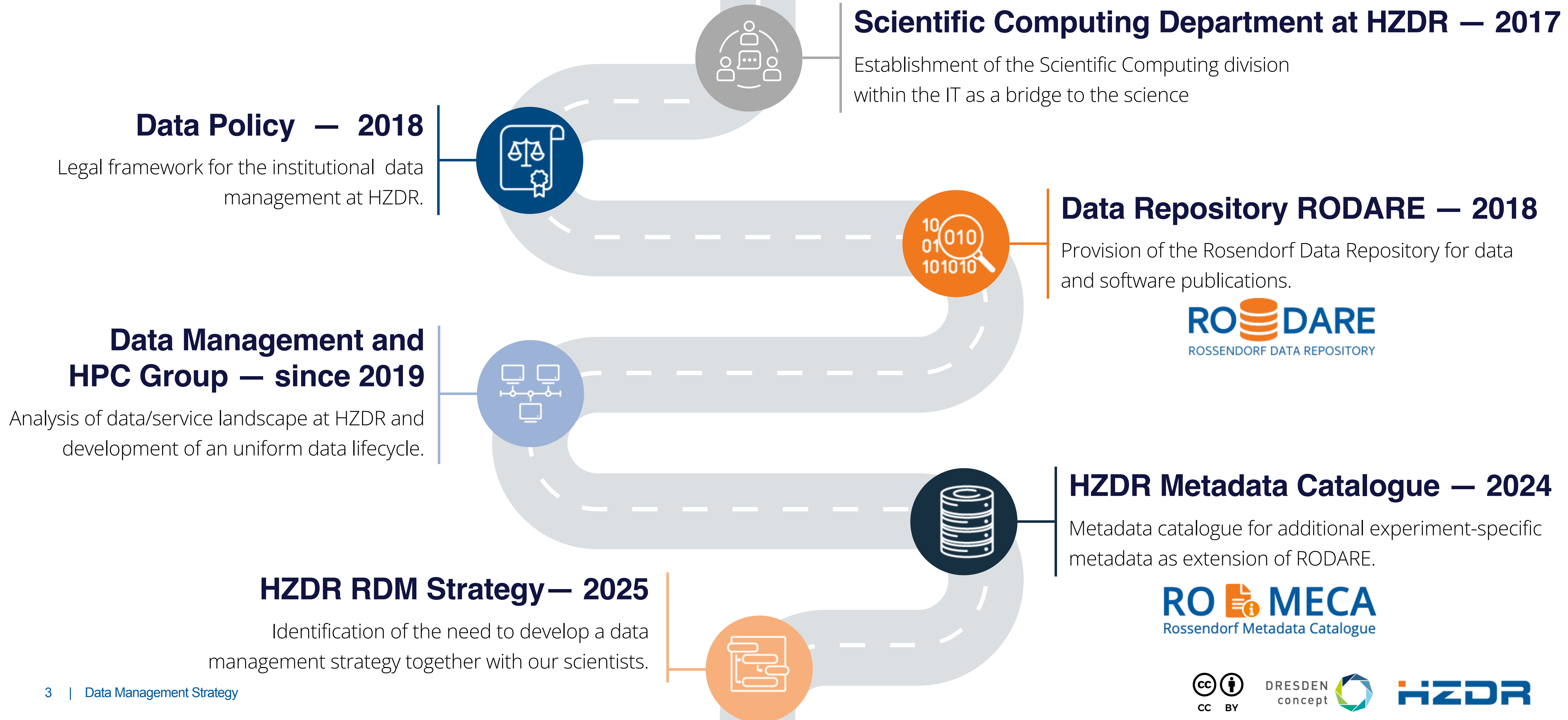
The Data Management Mission of the Computing Department

- Supporting our scientists and research experiment with tools:
 - electronic lab books,
 - interactive analysis,
 - publication repositories for data and software,
 - scientific workflow management,
 - PID (handle) generation and management.
- Providing support in connecting experiments, detectors and diagnostics to our infrastructure.
- Establishment of analysis workflows and HPC applications.



Development of the HZDR

Open Data Ecosystem

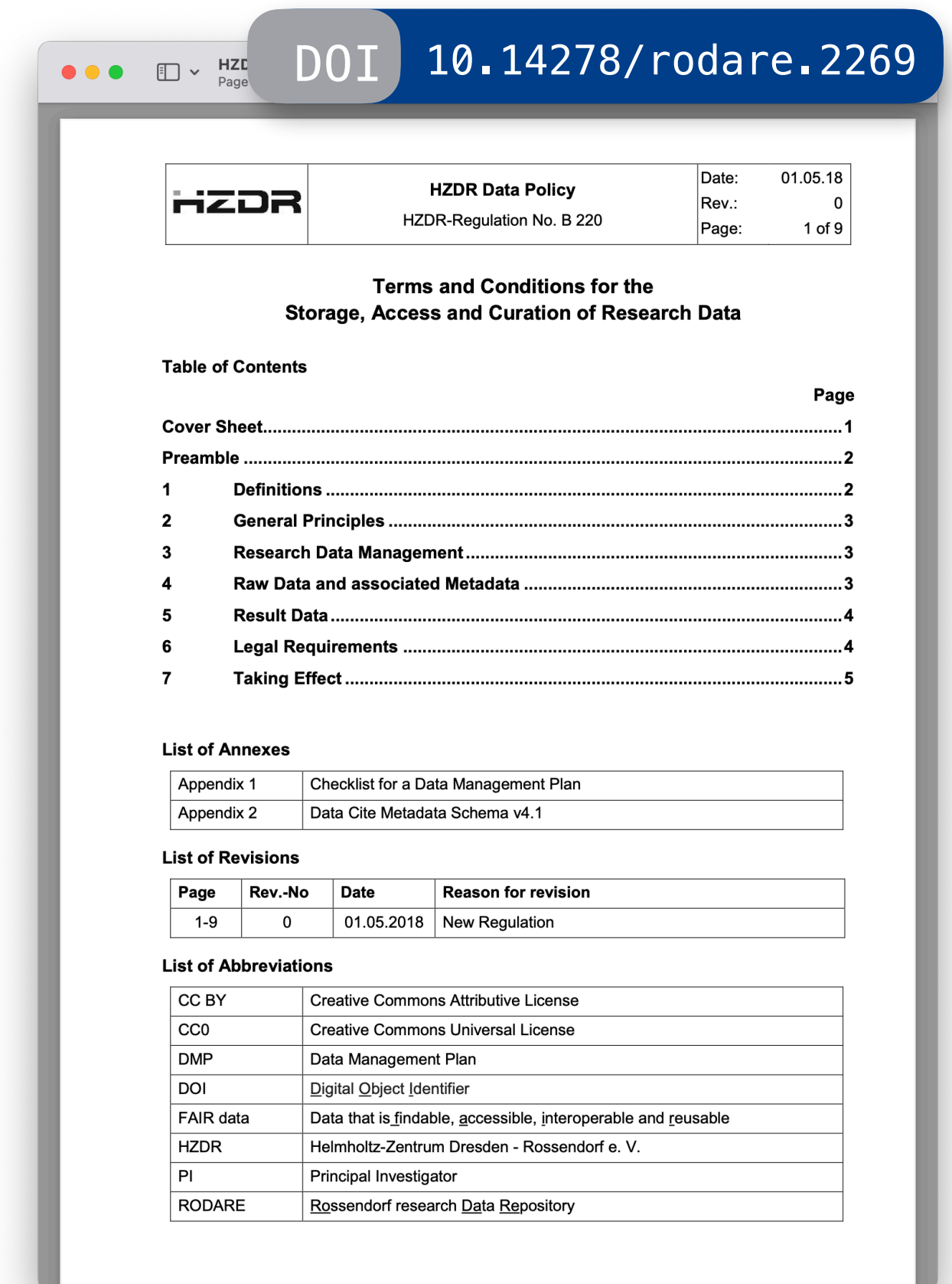
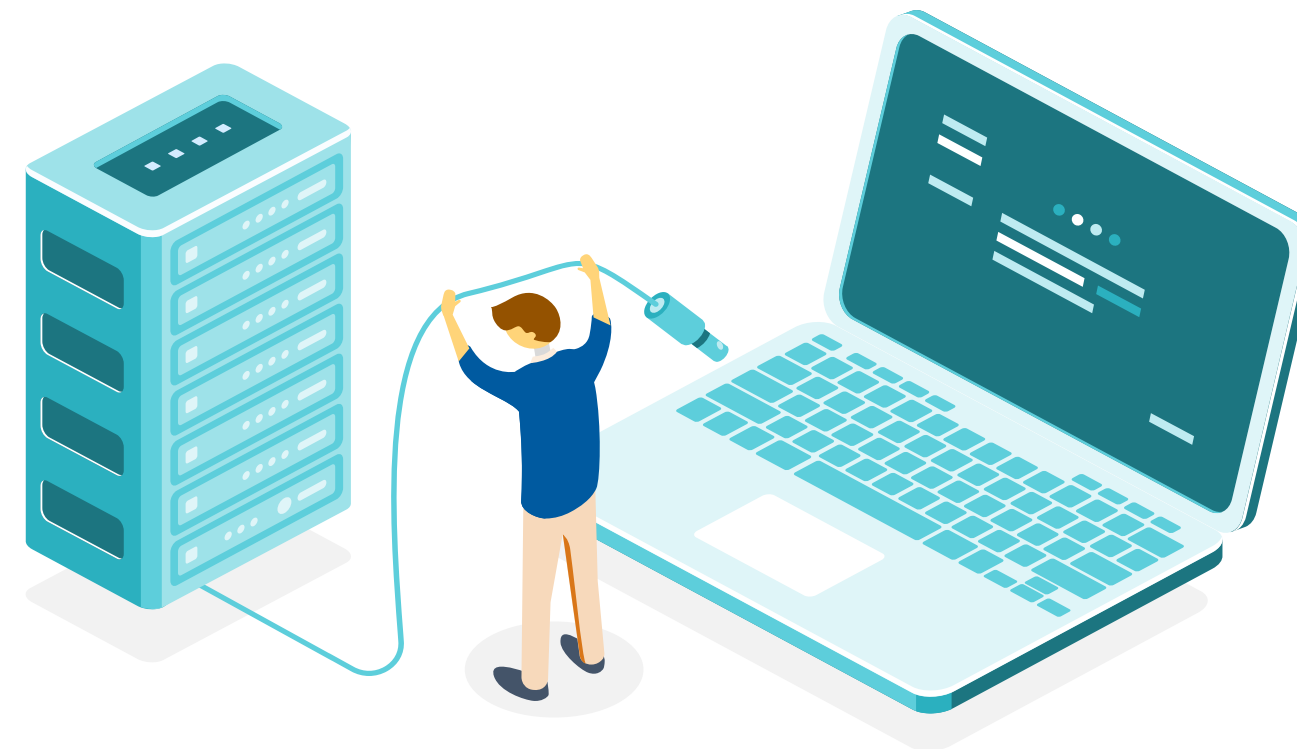


The Consequence of Open Science and FAIR: Institutional Data Policies


- The HZDR has a data policy since May 2018.
- Reasons for the development:
 - Establishment and legitimisation of publication, handling and deletion of data generated or taken at the HZDR,
 - Legal framework for data management and...



... to further develop data management services together with our scientists!



The Data and Software Publication Platform RODARE



[Upload](#)

[Communities](#)

[Log in](#)


Recent uploads

September 24, 2024 (v1)

Dataset

Open Access

Data publication: Cavity-mediated thermal control of metal-to-insulator transition in 1T-TaS2

Jarc, Giacomo; Mathengattil, Shahla Yasmin; Montanaro, Angela; Giusti, Francesca; Rigoni, Enrico Maria; Sergo, Rudi; Fassioli, Francesca;  Winnerl, Stephan; Zilio, Simone Dal; Mihailovic, Dragan; Prelovšek, Peter; Eckstein, Martin; Fausti, Daniele

Original datasets corresponding to the publication.

Uploaded on September 24, 2024



[View](#)

September 19, 2024 (v1)

Dataset

Open Access

Heat flow data from the fungus Schizophyllum commune

 Fahmy, Karim; Günther, Alix; Bertheau, Rahel;  Pape, David

The data set contains three typical heat flow curves recorded from the fungus Schizophyllum commune and exemplifies the evaluation of such data by the software tool metabolator (<https://rodare.hzdr.de/record/3150>).

Uploaded on September 19, 2024







[View](#)

September 19, 2024 (v0.2.0)

Software

Open Access

METABOLATOR: Analysis of Microcalorimetric Metabolic Data Using Monod's Equation

 Pape, David;  Lokamani, Mani; Seal, Ayush;  Kelling, Jeffrey;  Knodel, Oliver;  Fahmy, Karim;  Juckeland, Guido

Curve fitting automation for metabolic load of bacteria in solutions.

Uploaded on September 19, 2024

2 more version(s) exist for this record

[View](#)

September 18, 2024 (v1)


Dataset

Open Access

Data publication: Formation of martensitic microstructure in epitaxial Ni-Mn-Ga films after fast cooling

[View](#)


RODARE Docs



Have a look at the restructured documentation of RODARE. We now can more easily notify about news and features, such as the search options in Rodare.


Visit us <https://rodare.hzdr.de/about>.

Featured HZDR Large-Scale Research Facilities



In order to make our large-scale HZDR facilities more visible, Rodare now offers specific communities and an overview on our front page!

Overview of published data sets of selected large-scale research facilities of the HZDR:

- **ATHENA** — Accelerator Technology Helmholtz iNfrAstructure
- **CARBOSOLA**
- **Dresden High Magnetic Field Laboratory**
- **DRESDYN** — DREsden Sodium facility for DYNamo and thermohydraulic studies
- **ELBE** — Electron Linac for beams with high Brilliance and low Emittance
 - ▶  ELBE Beamlines
- **Felsenkeller** — The underground ion accelerator lab
- **HECToR** — High-power ultrafast computed tomography
- **HIBEF** — Helmholtz International Beamline for Extreme Fields

Powered by:


Harvested via OAI-PMH by:



Registered in:

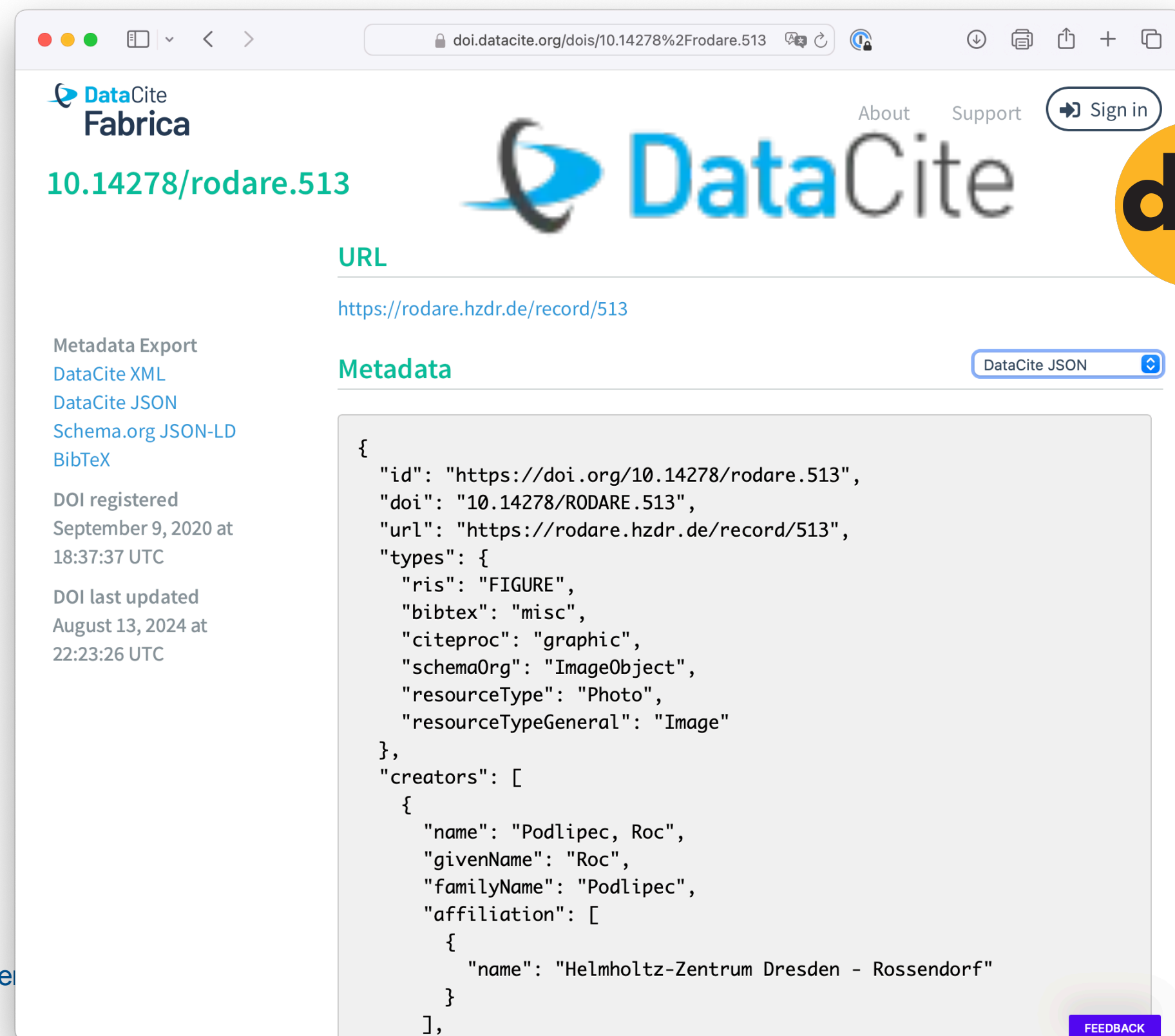
REGISTRY OF RESEARCH DATA REPOSITORIES

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



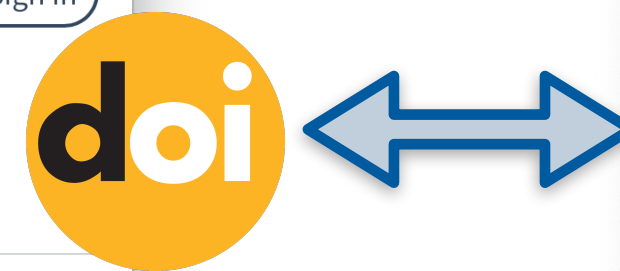
Metadata and Data

- In our data publication system the datasets are described via **DataCite** metadata to be FAIR.
- The DataCite metadata is attached to the DOI and harvested via portals, such as **B2Find**.
- In Theory: max 50 GB per file, max 100 GB per dataset (largest dataset: 7,2 TByte).



The screenshot shows the DataCite Fabrica interface for the DOI 10.14278/rodare.513. The URL is <https://rodare.hzdr.de/record/513>. The metadata is displayed in JSON format:

```
{
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    "schemaOrg": "ImageObject",
    "resourceType": "Photo",
    "resourceTypeGeneral": "Image"
  },
  "creators": [
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      "givenName": "Roc",
      "familyName": "Podlipec",
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        }
      ]
    }
  ]
}
```



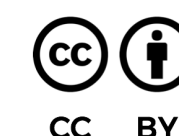
The screenshot shows the RODARE website record for DOI 10.14278/rodare.513. The record includes the title "Chronic Inflammation Prediction for Inhaled Particles, the Impact of Material Cycling and Quarantining in the Lung Epithelium", the author "Podlipec, Roc", and a preview image of a fluorescence micrograph. The record also shows 78 views and 51 downloads, the publication date of September 8, 2020, and the license "Creative Commons Attribution 4.0 International".

↓
File Access:
Rest API

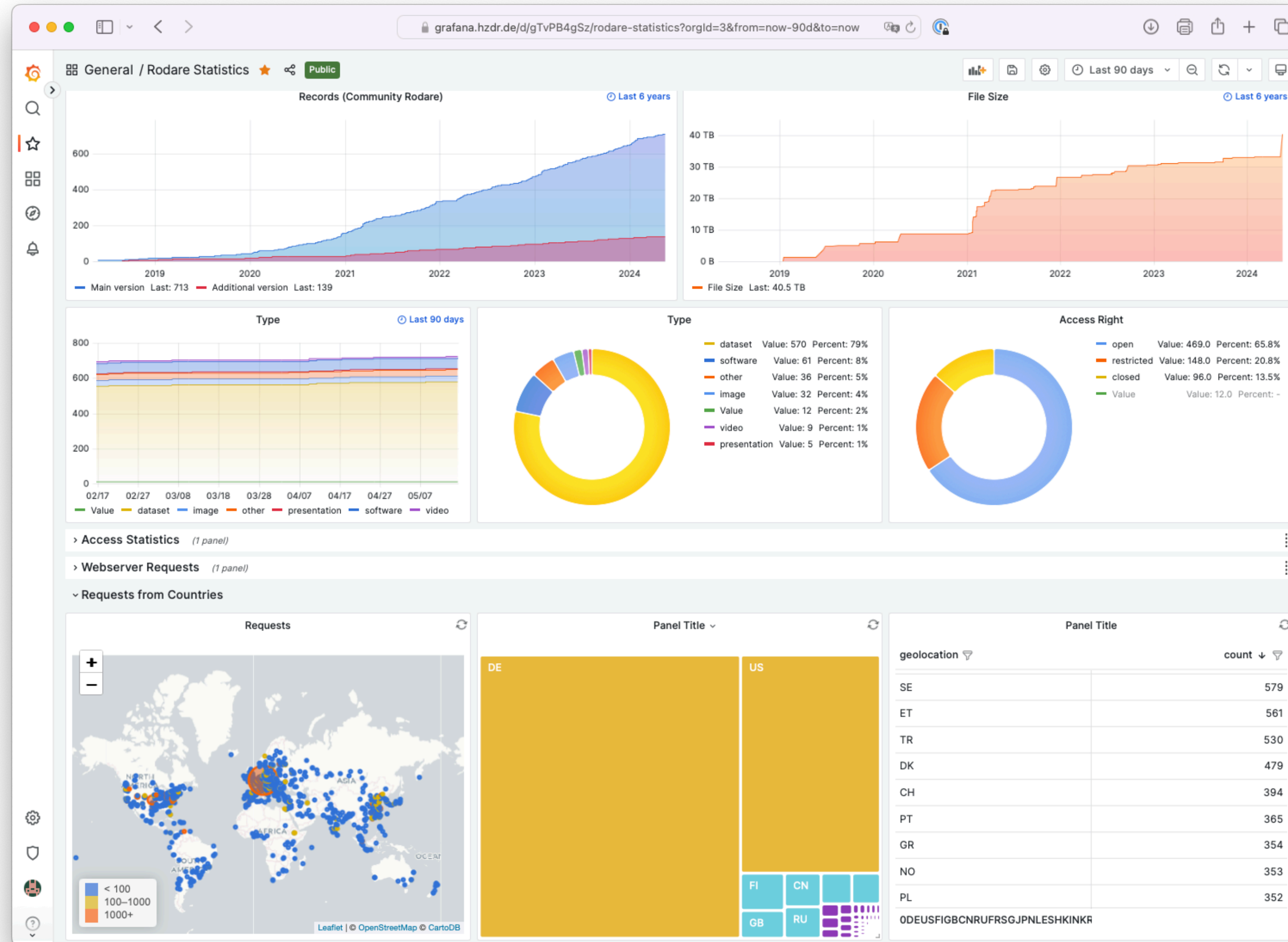


Filesystem

↓
Metadata API:
Rest API, OAI-PMH

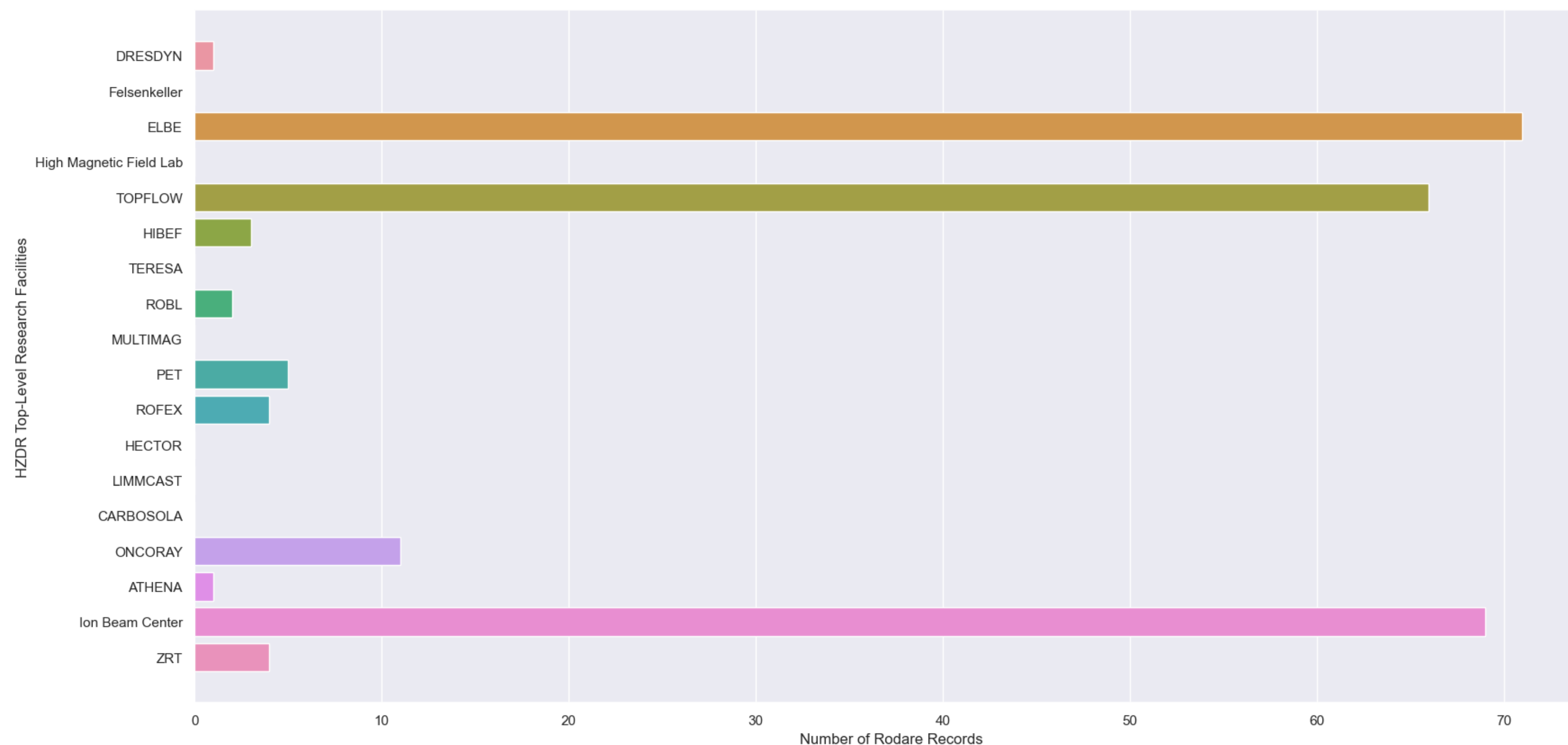


The RODARE Statistics and Worldwide Accesses



Additional Metadata Through Communities

- Experiment-specific metadata is difficult because the RODARE metadata is the same for every entry.
- We integrated the facility information throughout Communities for our large-scale facilities:
 - **18** facilities from different research areas...
 - ...and one facility (ELBE radiation source) with **9** beamlines.



Featured HZDR Large-Scale Research Facilities



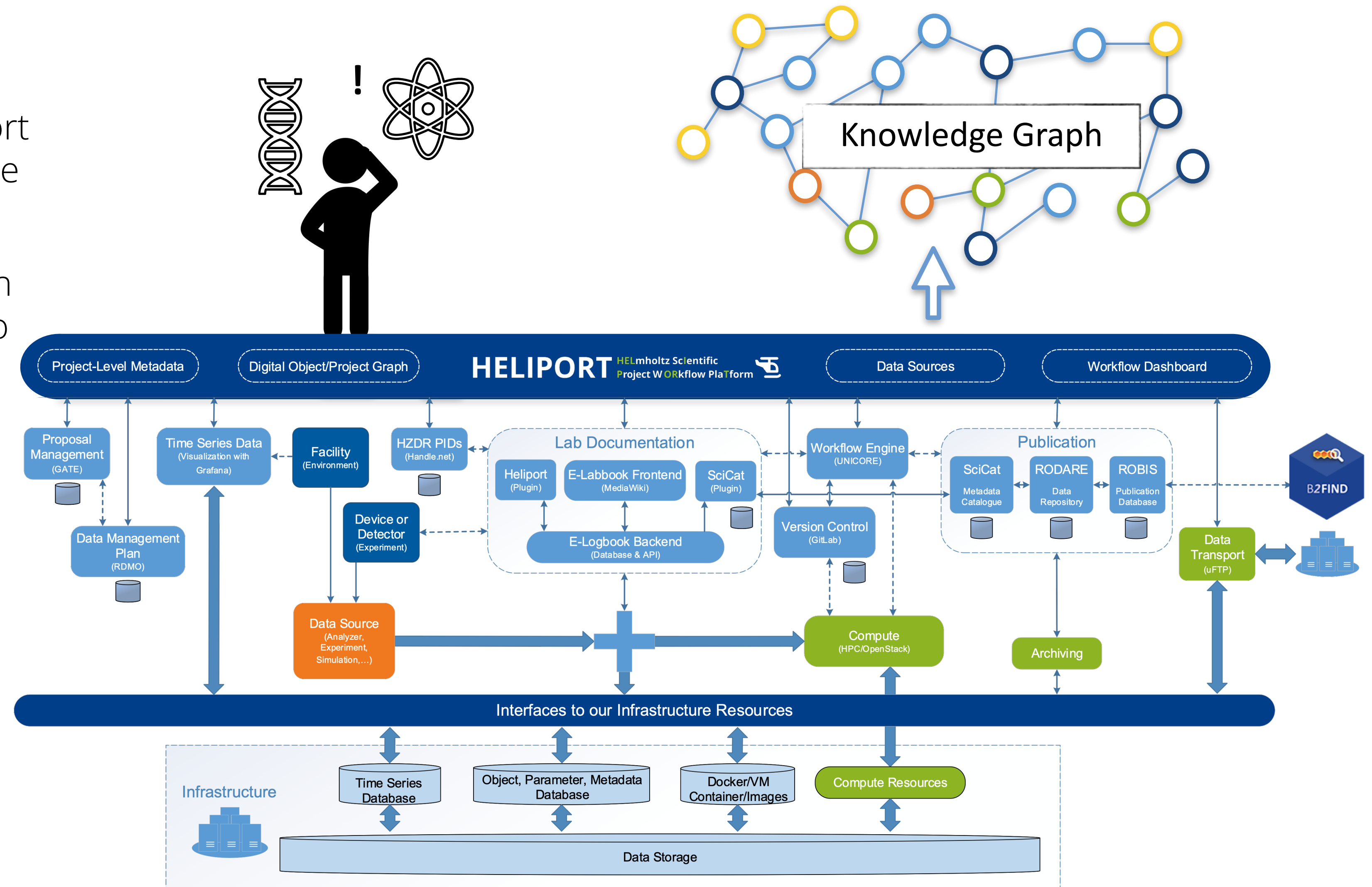
In order to make our large-scale HZDR facilities more visible, Rodare now offers specific communities and an overview on our front page!

Overview of published data sets of selected large-scale research facilities of the HZDR:

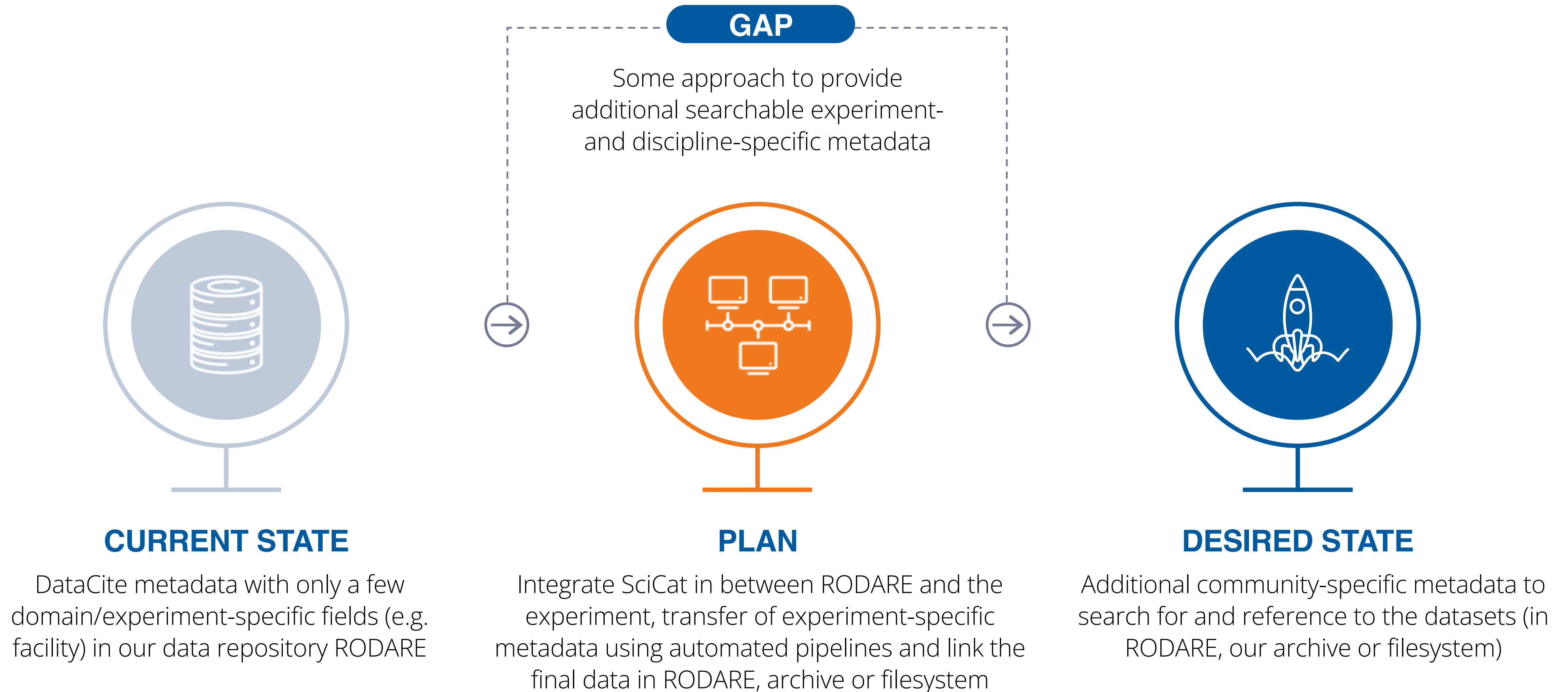
- **ATHENA** — Accelerator Technology
HEImholtz iNfrAstructure
- **CARBOSOLA**
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- **ELBE** — Electron Linac for beams with high Brilliance and low Emittance
 - ▶ **⊕** ELBE Beamlines
- **HECToR** — High-power ultrafast computed tomography
- **HIBEF** — Helmholtz International Beamline for Extreme Fields

The Research Data Management Landscape at HZDR

- Our IT infrastructures can support various experiments, but they are complex...
- Scientists often don't know which services are available and how to use them.
- Offers to our scientists to guide them through the services:
 - IT-Service catalogue: hzdr.de/fdm-services
 - HELIPORT: heliport.hzdr.de



Gap Analysis of our Metadata Ecosystem

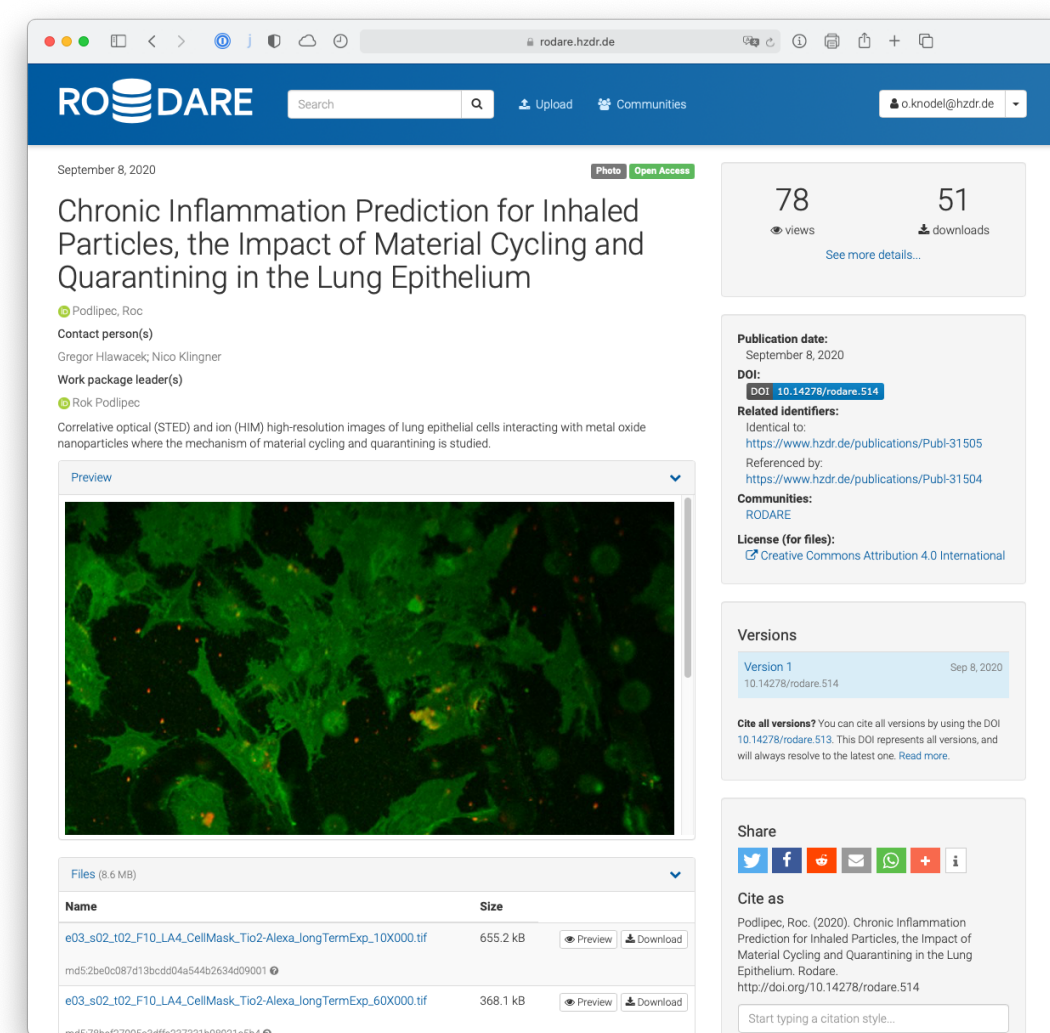
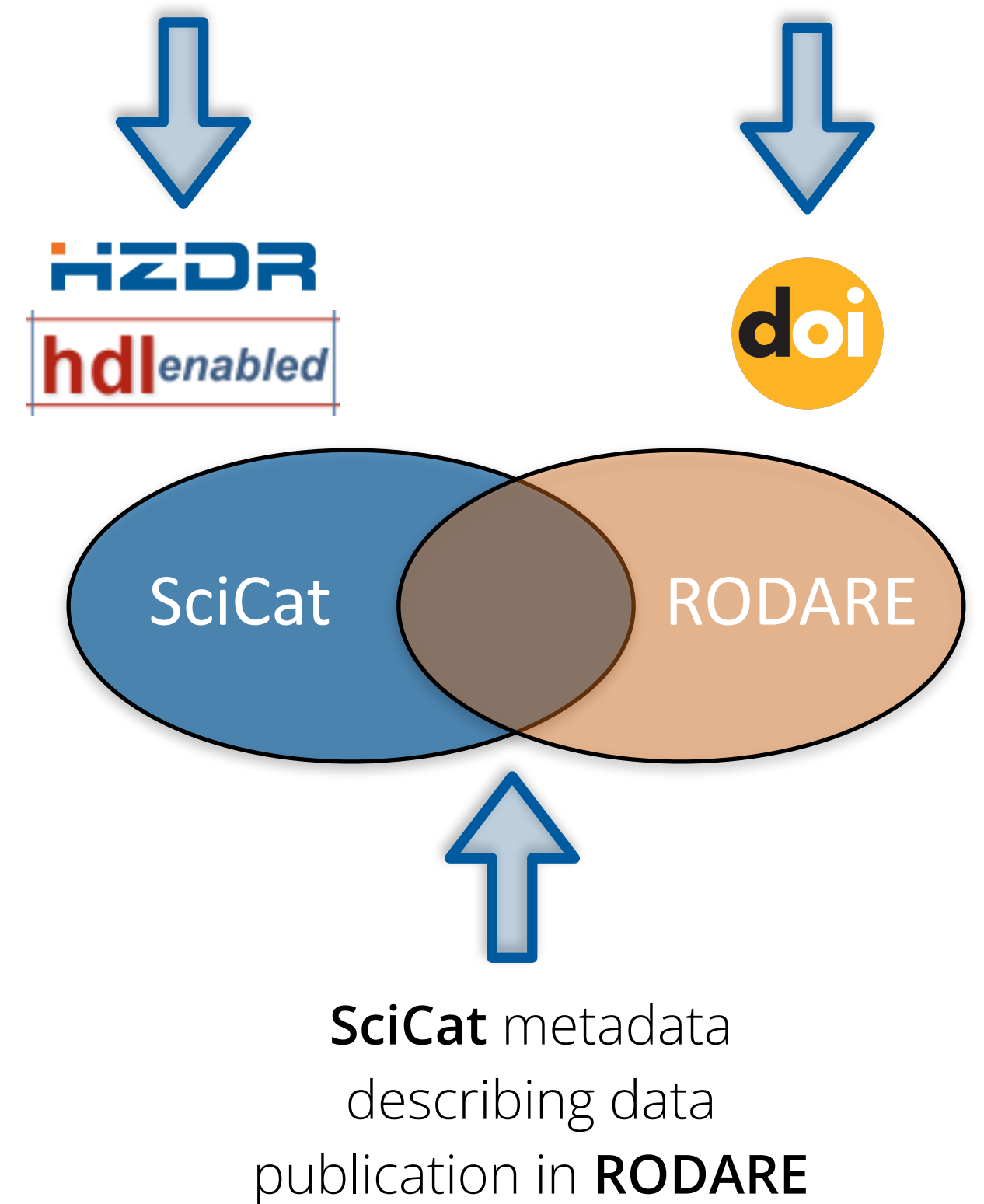


Data, Metadata and Publications at HZDR

- Data Repository RODARE for citable **data/software publications** with **DOIs**
- **SciCat** for public findable metadata describing data and it's different locations with “HZDR Handles” as **PID**:
 - RODARE, if the data is published and used in scientific publications
 - Anywhere on our internal filesystems or cloud storage
 - In our internal archive for long-term storage

SciCat metadata for describing unpublished RAW or derived data located in our filesystems or archives
(external access can be granted)

Data and software publications in **RODARE**
(Open, closed, restricted or embargoed access)



Data publication system RODARE
rodare.hzdr.de

PID	Name	Source Folder	Size	Start Time	Type
20.500.12865/scicat.8edBeda1-eb5b-4268-a05d-9b1b9ff321e	087_Op7THz_LSCO_15K_TPPOP_P1_155_P2_50	...cords/1289	61 GiB	2018-06-13 Wed 23:06	raw
20.500.12865/scicat.351ca141-4e60-45d6-a996-01e097e9c173	087_Op7THz_LSCO_15K_TPPOP_P1_155_P2_50	...cords/1289	66 GiB	2018-06-13 Wed 22:47	raw
20.500.12865/scicat.96a09008-7885-47f6-90d3-c79f1d8dec4	084_Op7THz_LSCO_P0_P0_30K	...cords/1289	19 GiB	2018-06-13 Wed 20:47	raw
20.500.12865/scicat.b90b4efe-40d6-4fc6-a493-abead7c12d1	083_Op7THz_LSCO_P10_P10_30K	...cords/1289	19 GiB	2018-06-13 Wed 20:38	raw
20.500.12865/scicat.aa77629d-97b9-446d-8694-eeeb7844595a	082_Op7THz_LSCO_P16_P16_30K	...cords/1289	19 GiB	2018-06-13 Wed 20:30	raw
20.500.12865/scicat.faf05c6a-a69b-4031-9be8-405ba38a5937	081_Op7THz_LSCO_P22p5_P22p5_30K	...cords/1289	19 GiB	2018-06-13 Wed	raw

SciCat metadata catalogue
scicat.hzdr.de

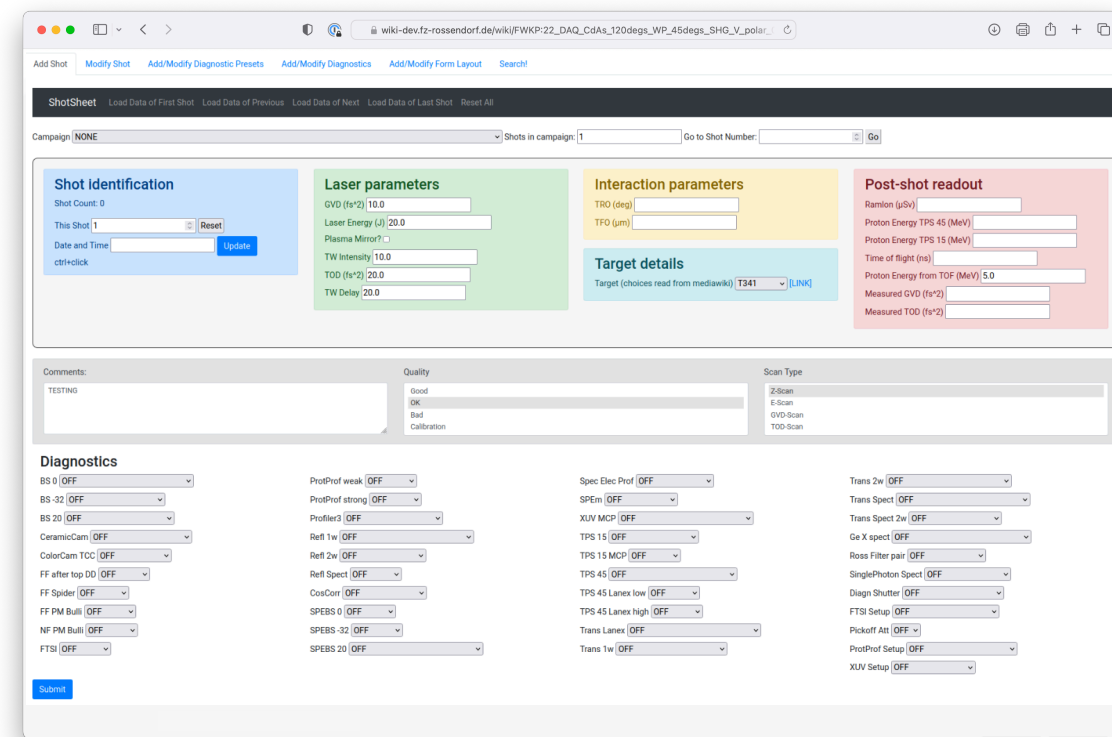
From the Experiment over the Metadata to the Publication of Data

Curated Metadata Sources

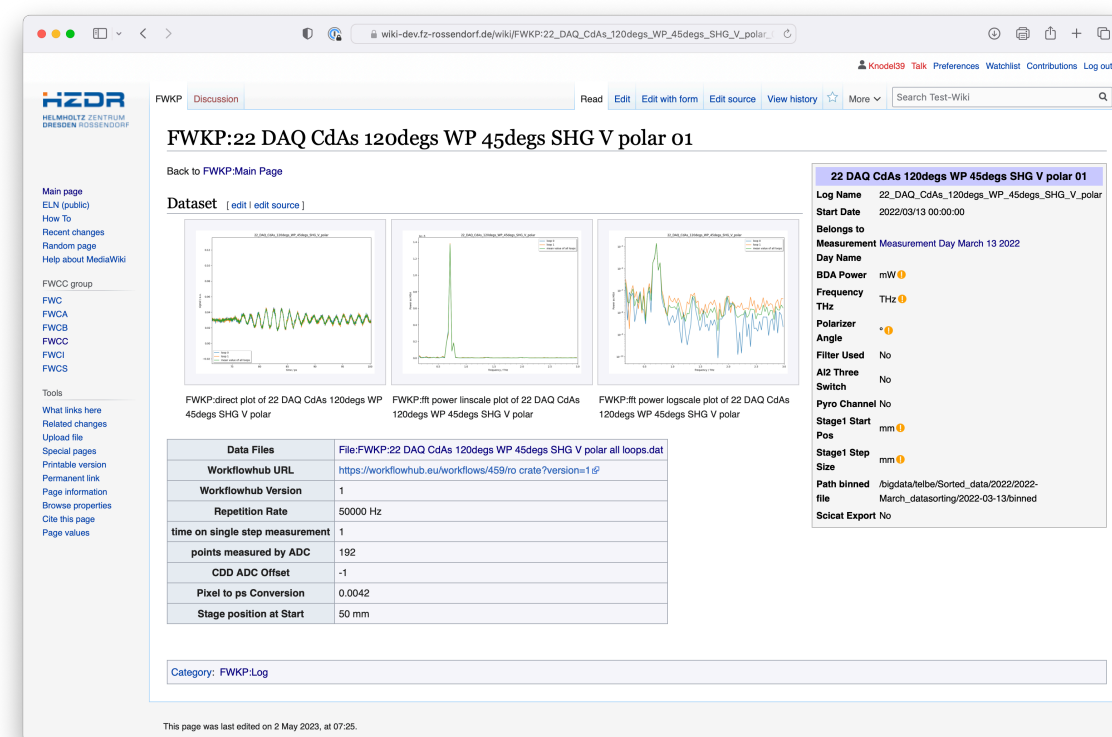
Public Metadata Catalogue

Subsequent Access to Data

ExperimentLogging app (ExL)



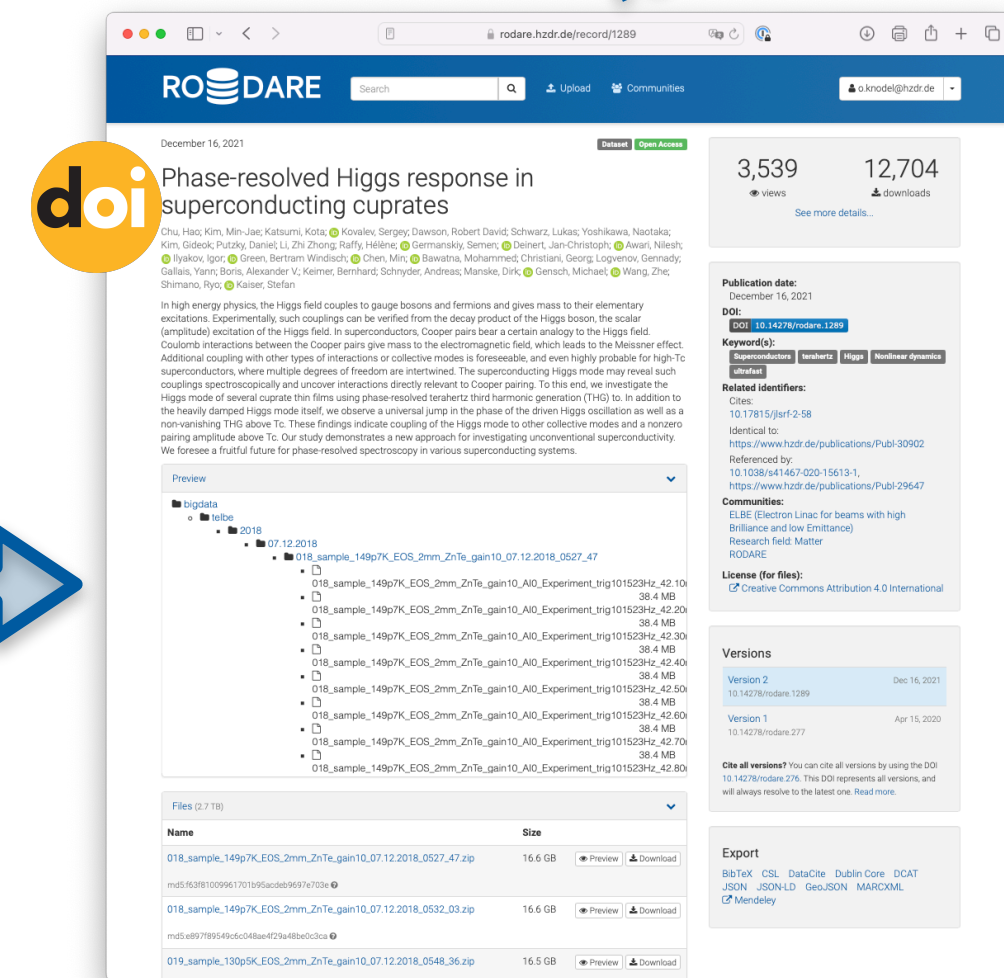
E-Logbook



SciCat



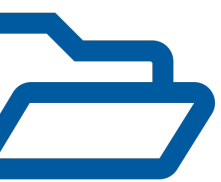
RODARE (Invenio)



Dataset



Filesystem



Tape Archive

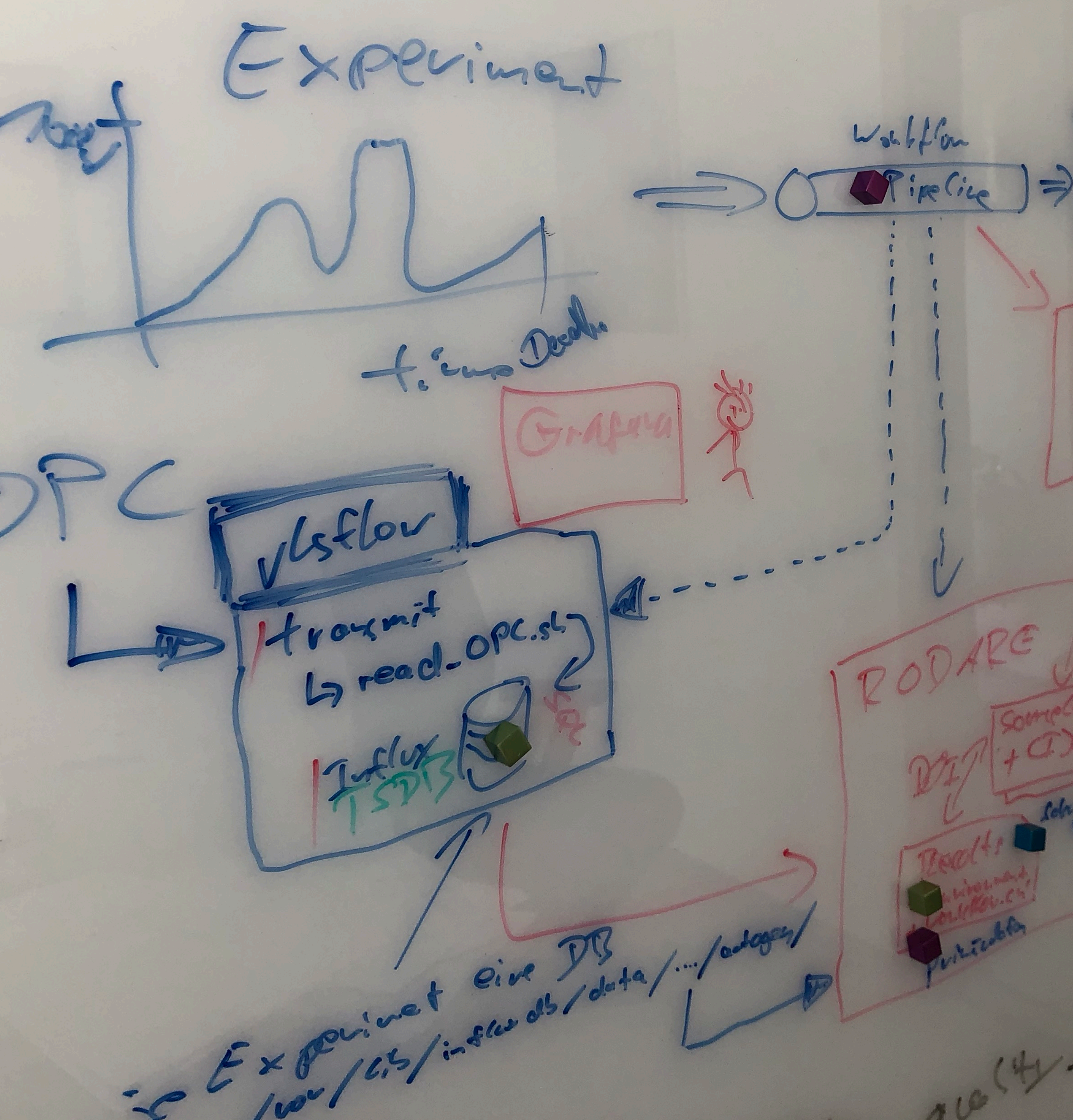


Fully Automated Process for DRACO

Access: Private/Internal

Access: Public



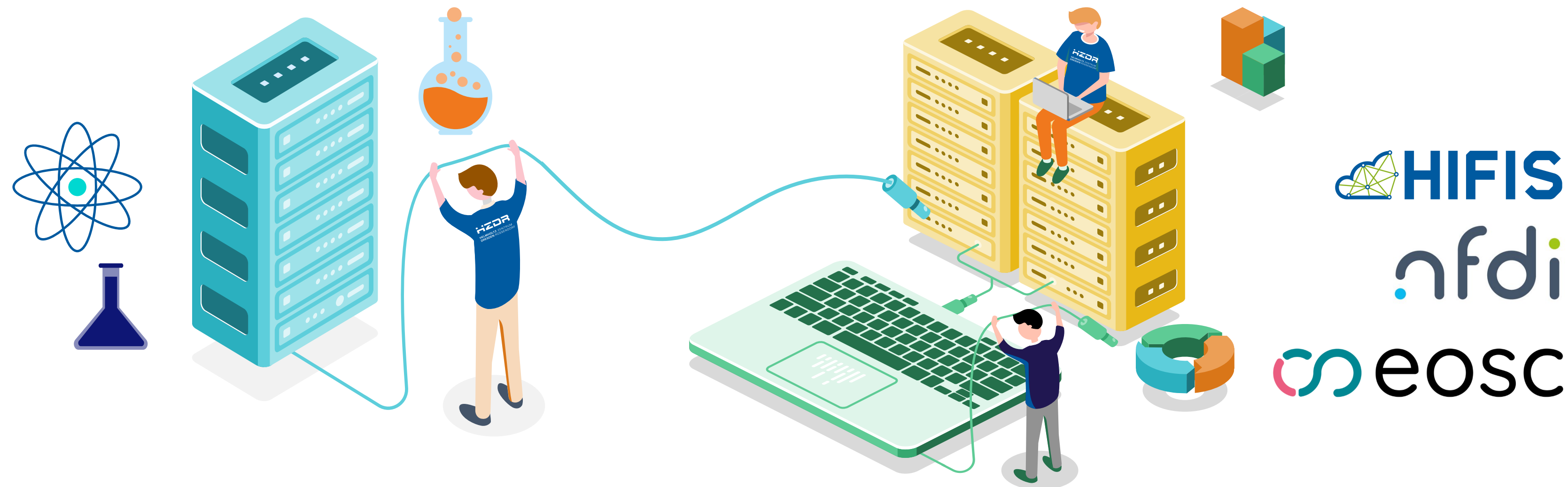


Why a
**HZDR Data
Management
Strategy**
is necessary



Motivation for the Development of a HZDR Data Management Strategy

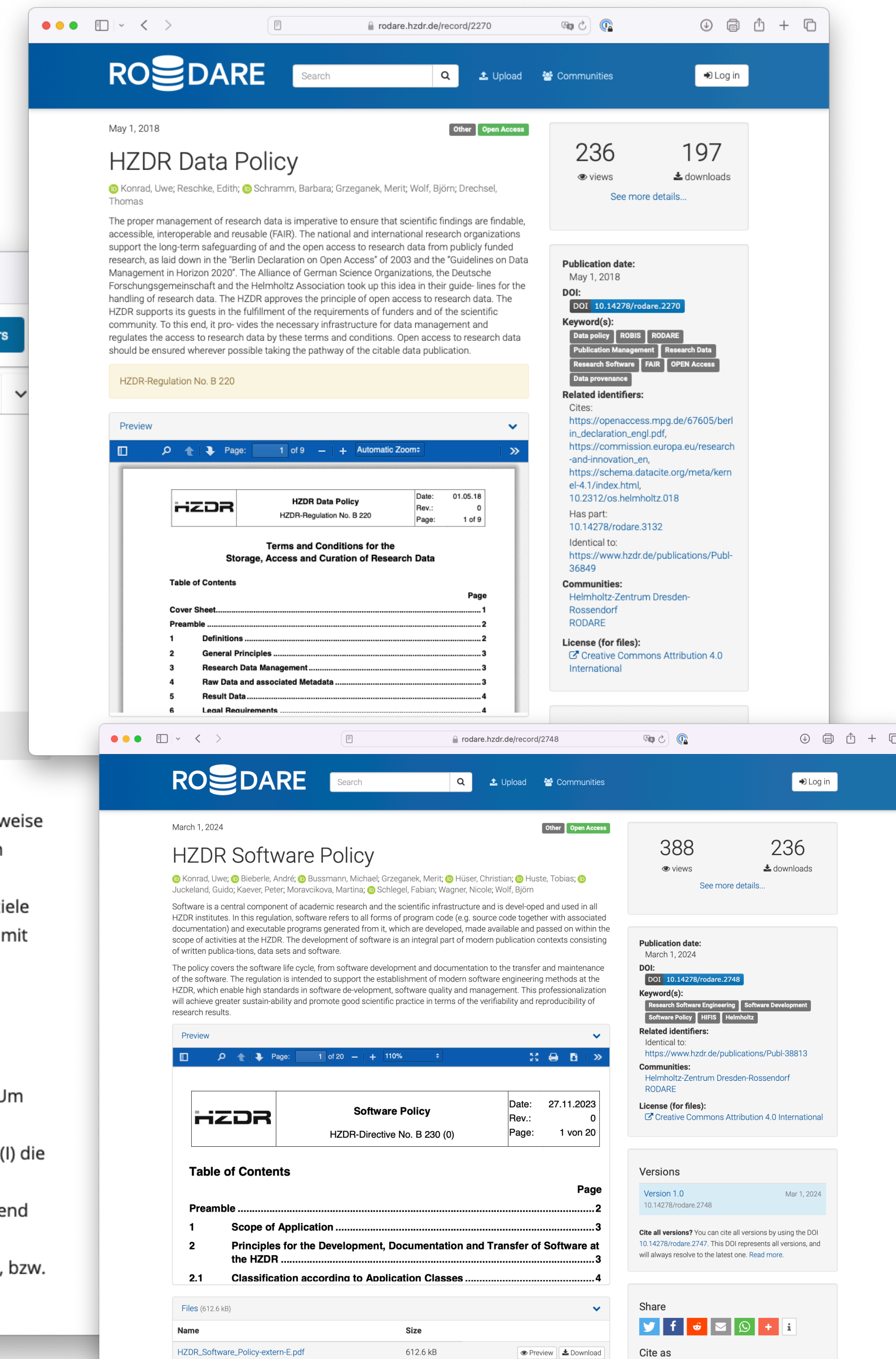
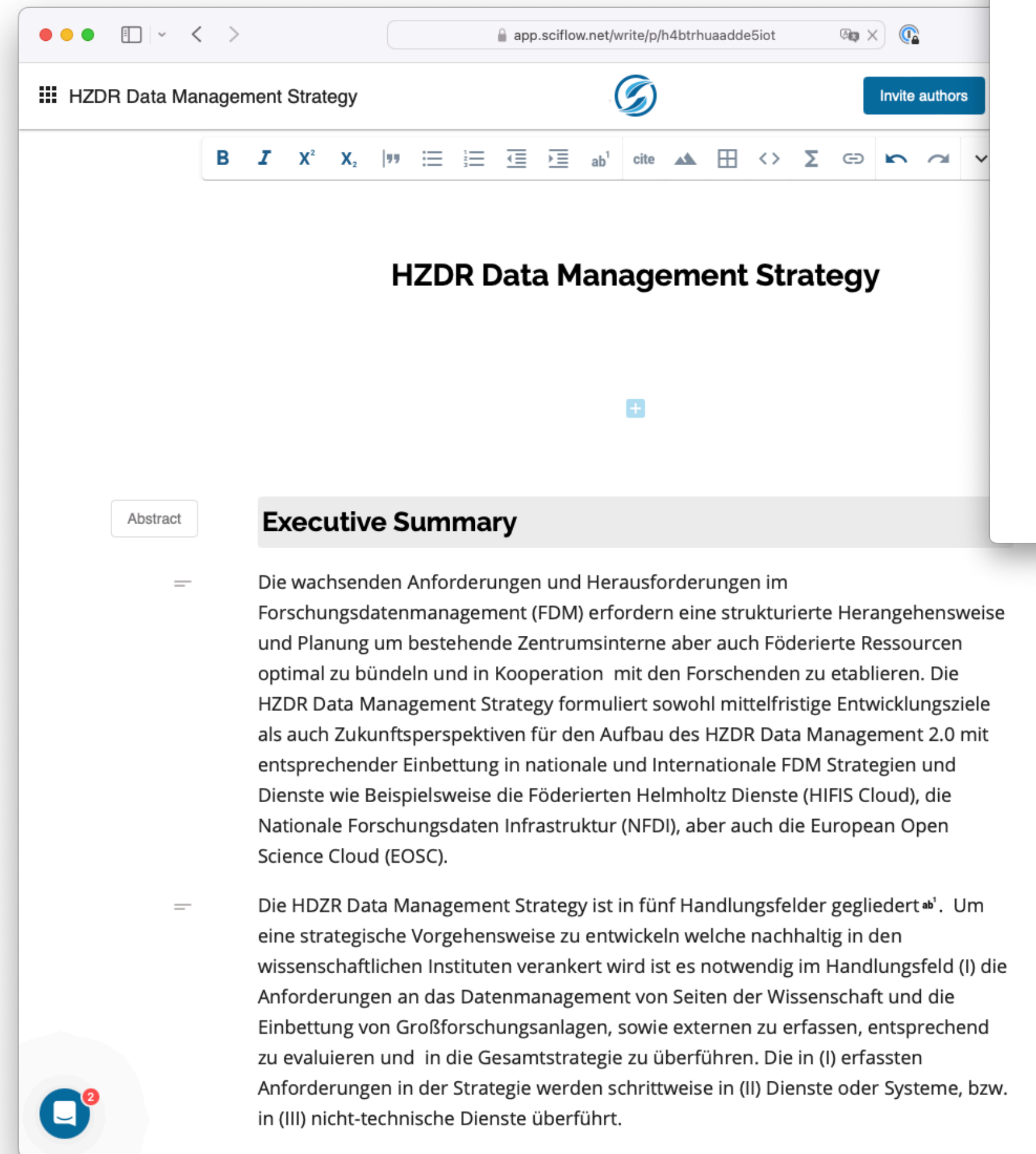
- We have a complex ecosystem of tools and services at the HZDR, within HiFiS and beyond: NFDI and EOSC.
- A clear and transparent roadmap for our developments in coordination with our internal and external stakeholders is necessary.
- The HZDR scientists, large-scale instruments and experiments must always be at the top of the agenda.



→ We want to work with you to develop a clear and transparent roadmap to define priorities, allocate resources and obtain appropriate funding.

Data Management Strategy

- A document that describes the HZDR data management,
- integrated into our guidelines and policies,
- including future developments based on
- a clear roadmap and subproject,
- with appropriate prioritisation and
- embedded in a larger context beyond the HZDR.



Conclusions

- With the workshops today and tomorrow we want to initially discuss the requirements of our scientists and experiments.
- We want to finalise a first draft by the end of the year.
- Together with our scientists and stakeholders, we will iteratively transform the draft into a comprehensive document.

