Research Data Management at HZDR

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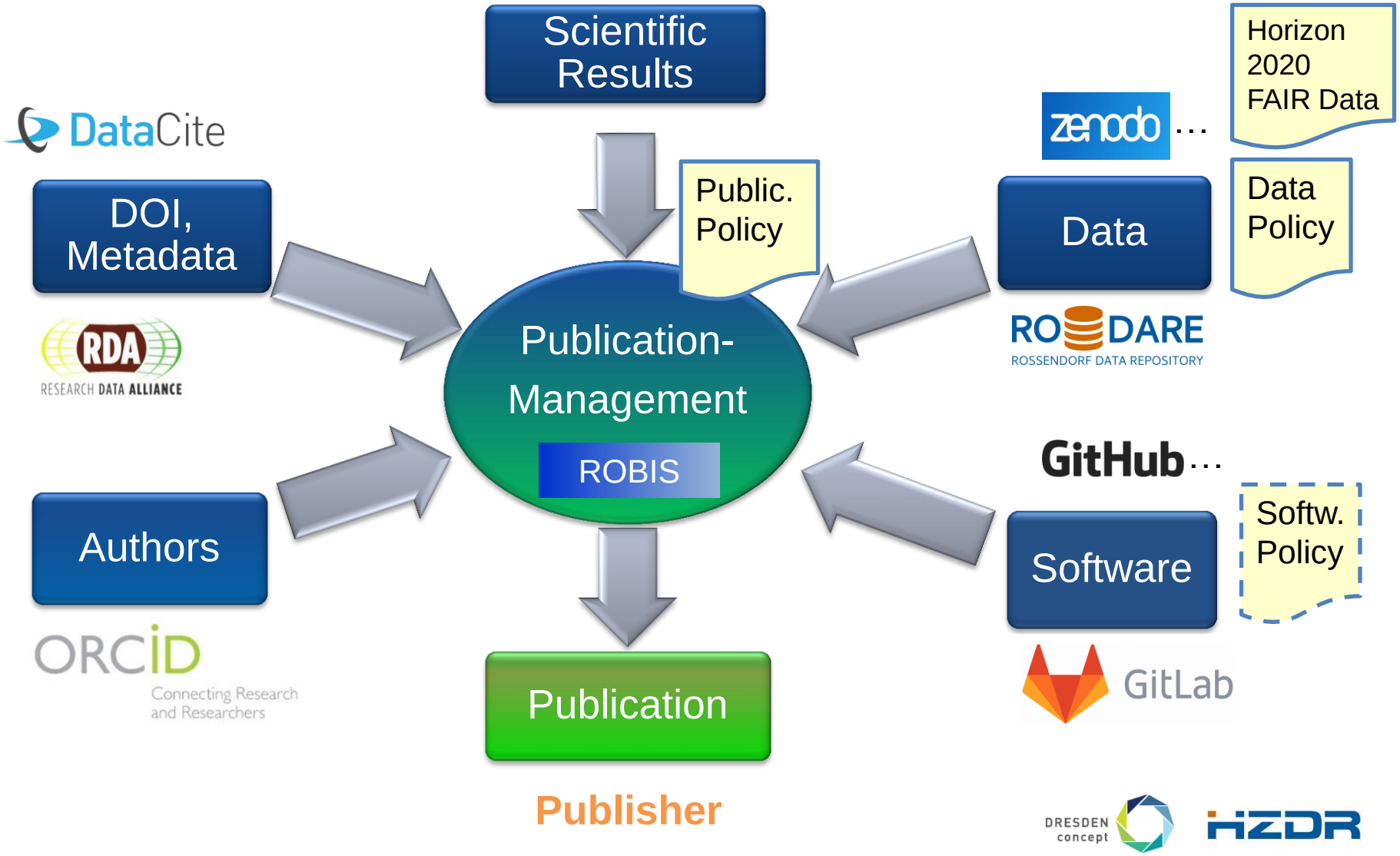
HZDR

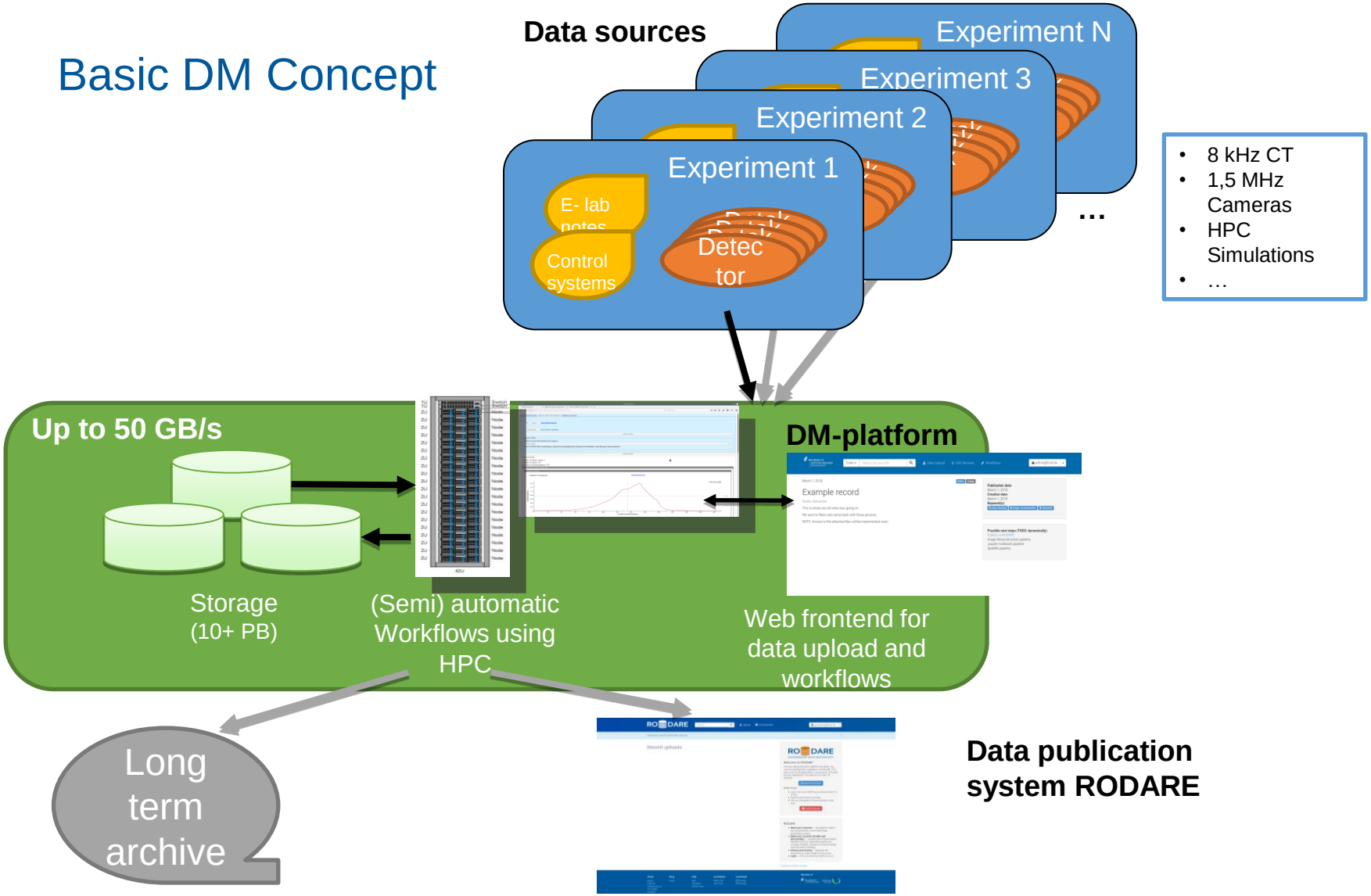
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Publication Components



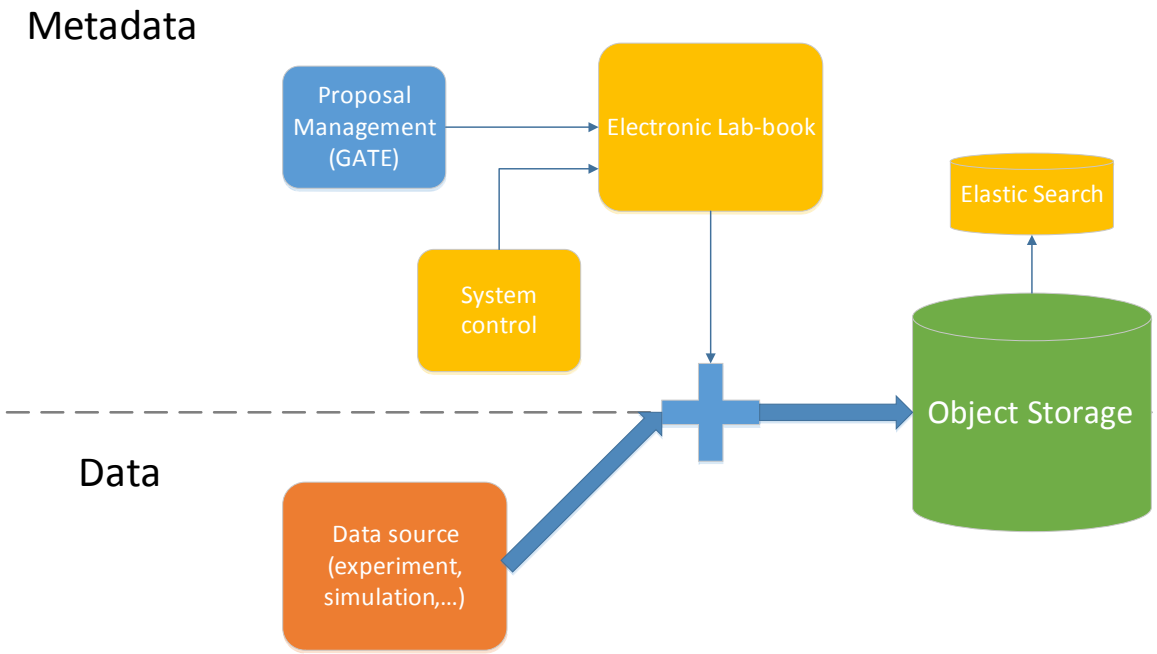
The Concept

Basic DM Concept



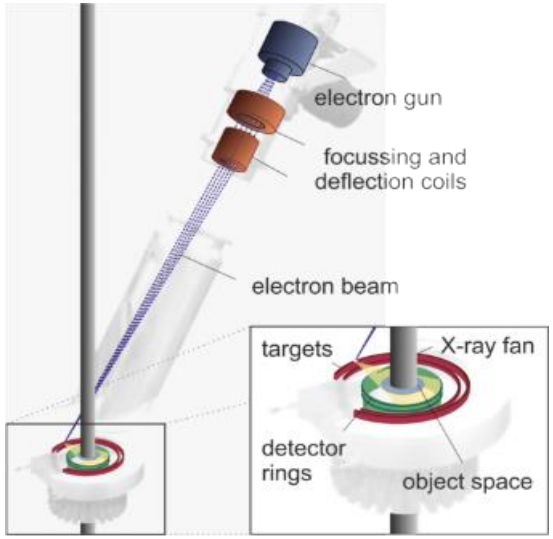
Data Ingest

- Goal: publication-ready records already on ingest by collecting necessary metadata from available sources (e.g. GATE system, eLab-Books)
- Stepwise inclusion of facilities(T-ELBE, ROFEX)

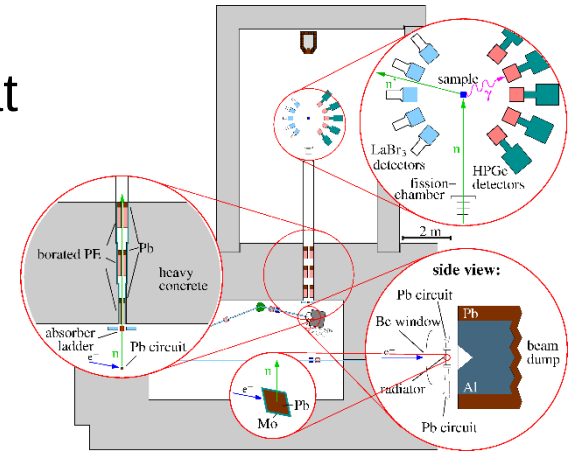


How to deal with heterogeneous metadata schemes?

- Invenio uses jsonschemas to describe what each record has to look like
- Allows instant validation
- Plan:
  - Extract metadata schema for each resource type together with scientists
  - Characterize facilities in data-base
  - Write tools to extract metadata from existing gadgets if possible
  - convert data into a self explanatory format together with its metadata (e.g. HDF5, ADIOS or Nexus)

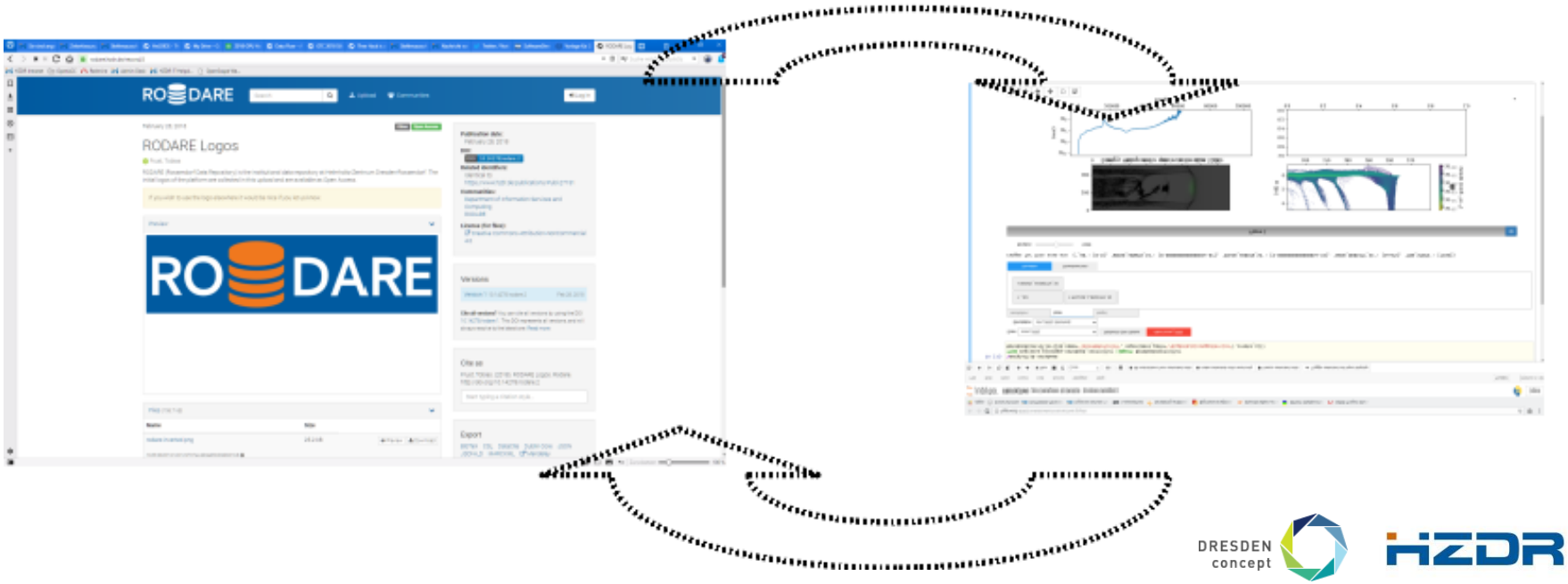


(Fischer et al., 2008)



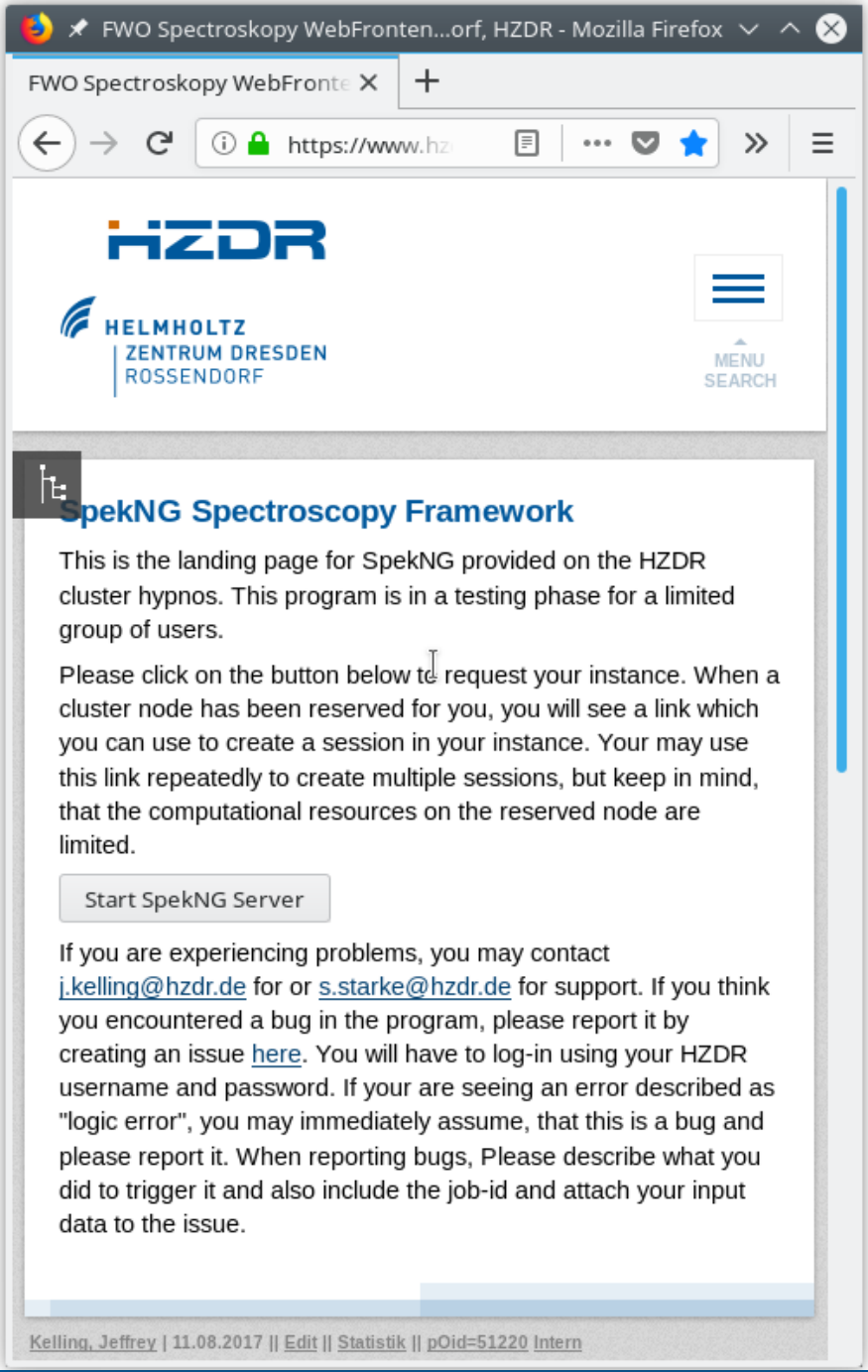
HZDR Data Management

- Built using Invenio (like Zenodo) → Elastic Search for large data repositories
- Start predefined compute workflows base on selected input data
- Ingest workflow output again into repo and link to input data set



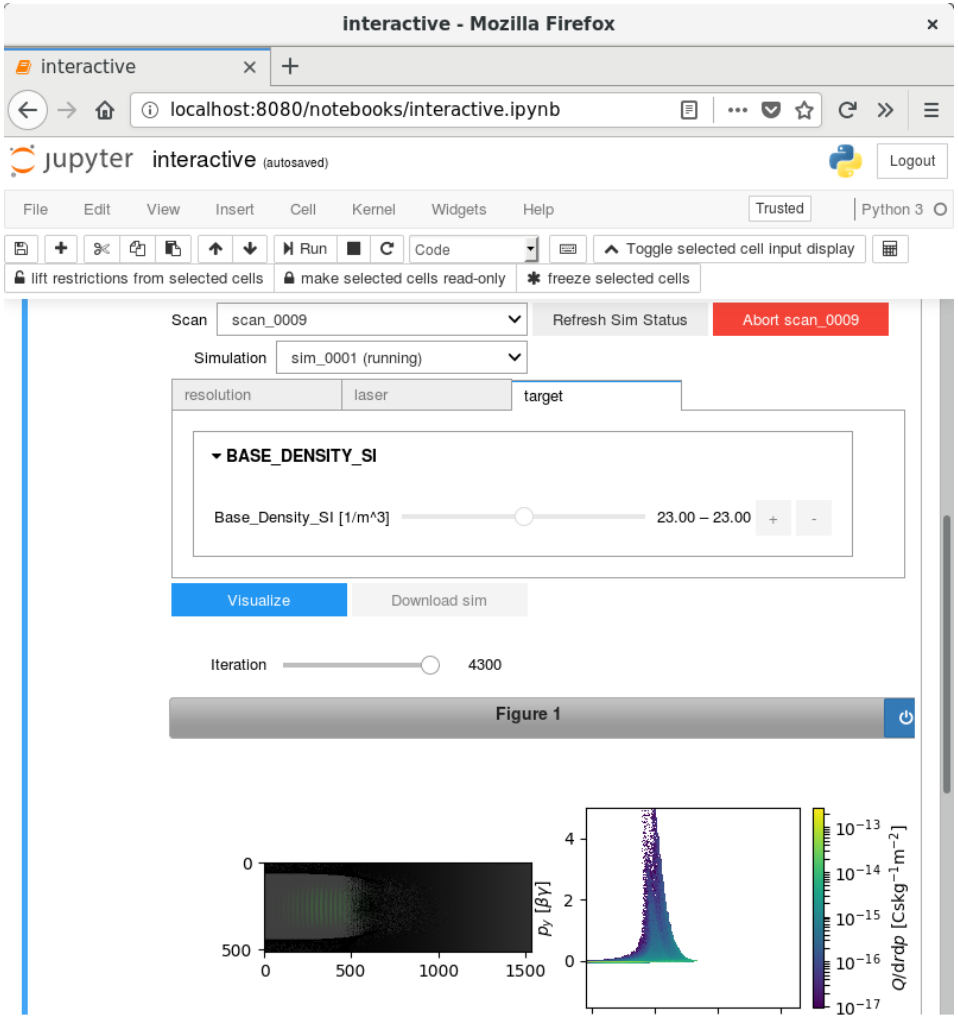
Tightly coupled, even isolated

- Typical cloud (micro-)service
  - fixed workflows / machine
  - service is feature complete
- “Web“: HTTP & WebSocket
  - persistent, sharable sessions
  - browser, app, CLI
- Existing infrastructure
  - Got intranet? CMS Spawner
  - Qt expert? Try Wt



Loosely coupled, fully enabled

- Prepared Jupyter notebook
  - same user, same rights
  - transparently load: modules/containers/environments
- Lend out (G)UI design principles
  - data ↔ representation
  - client request ↔ HPC scheduling
- Transparent (“Hackable“) by design
  - share full workflow as a file: migrate, re-connect
  - add cells, code, extensions, ...
  - !spack install … (pip, docker, ...)



HZDR data publication system: RODARE

- Decision for Invenio web framework
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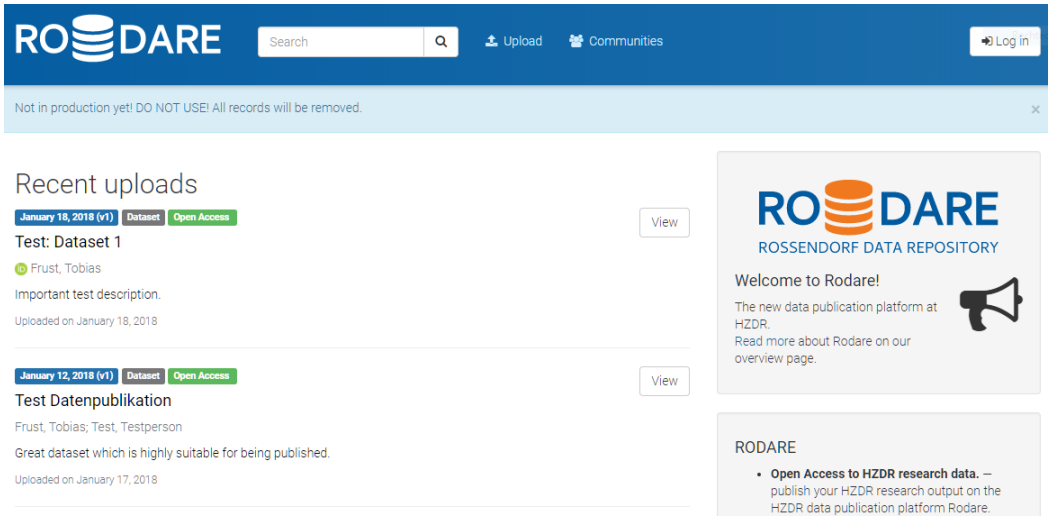
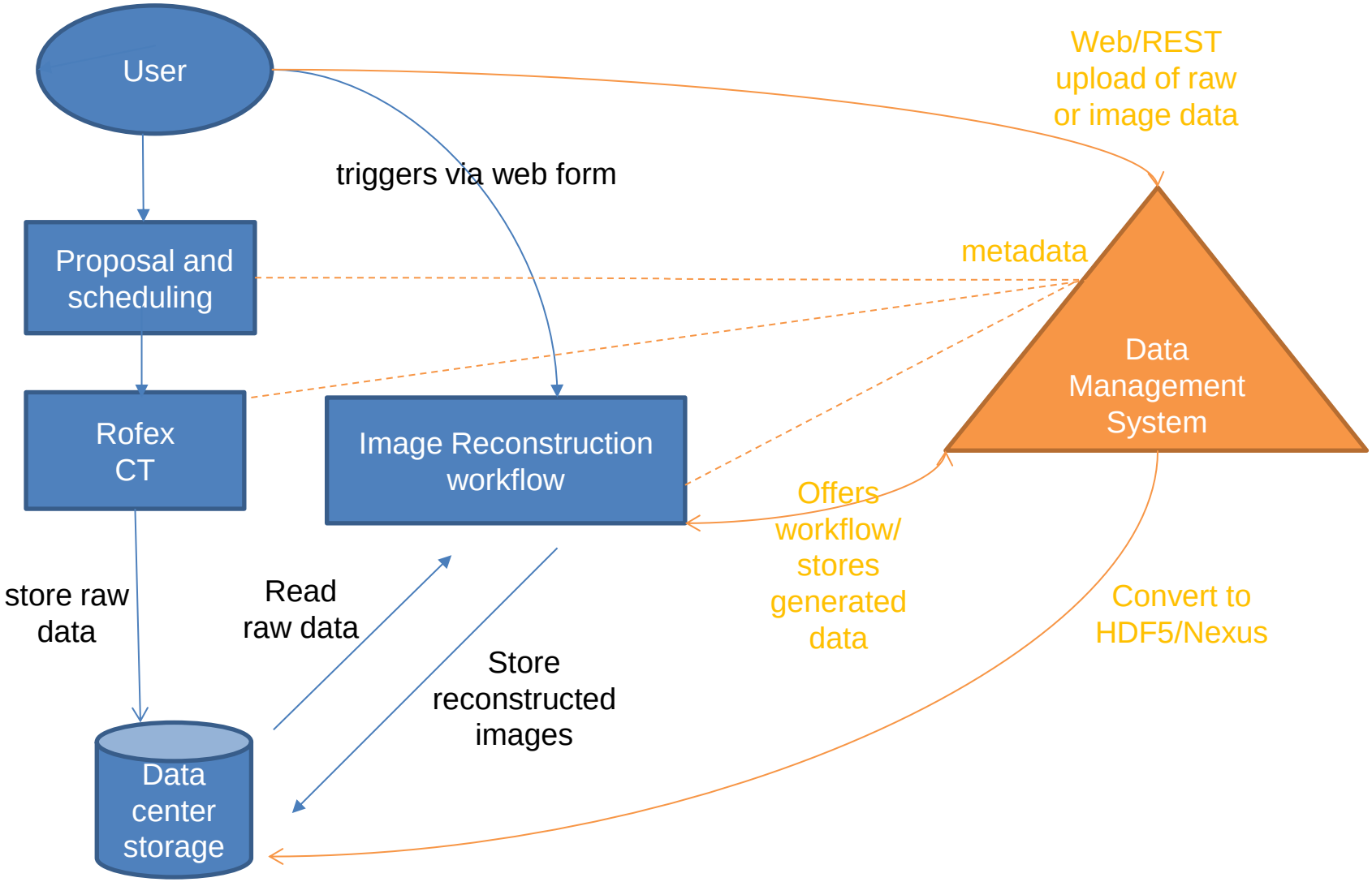
- Advantages:
  - Actively developed at CERN, also used at e.g. DESY
  - Provides the codebase for Zenodo as well
  - supports deployment via Docker → scalability



Looking at an Example: ROFEX CT

Data flow for ROFEX: Now and future

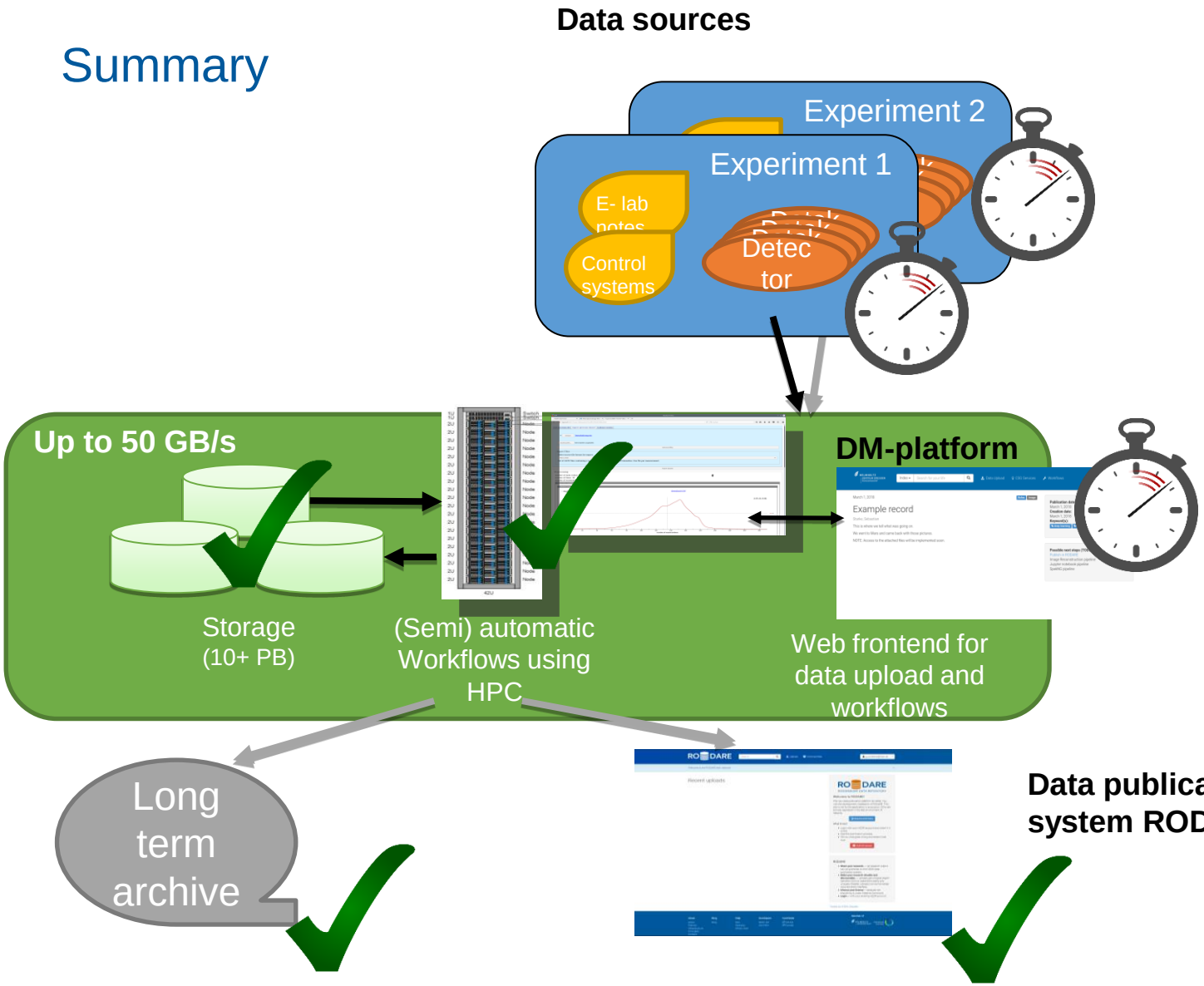


Data management and analytics platform: vision

- Under current development
- Also based on Invenio modules

- Long term goals:
  - Authentication via Umbrella ID for broader audience
  - Tightly linked to web workflows using HPC resources
  - Allow tracking of processing steps for each record along its lifecycle
  - **“No metadata has to be typed more than once!”**
  - Extract as much metadata as possible from other available sources (e.g. GATE system, eLab-Books, …)
  - Connect this tool with all relevant HZDR facilities
  - Try to interfere with scientists workflow as little as possible

Summary


Data sources
Experiment 2
Experiment 1
E- lab notes
Control systems
Detec tor
Up to 50 GB/s
DM-platform
Example record
Storage
(10+ PB)
(Semi) automatic Workflows using HPC
Web frontend for data upload and workflows
Long term archive
Data publication system RODARE

Backup

HZDR Data Policy: Management of Research Data

- The policy is based on the data guidelines of other data initiatives (e.g. PaN-Data, ESRF, BESSY) and the Horizon 2020 “FAIR Data” principles.
- The draft is currently being discussed in a HGF committee as a template for Helmholtz.
- General Principles:
  - A Data Management Plan (DMP) documents the responsibilities and processes
  - Raw data and results are stored in a trusted research data infrastructure (RODARE) and kept for at least 10 years. Metadata is defined according to the Data Cite Scheme.
  - Access to the data is initially limited to the respective user group for 5 years after completion of the experiment (embargo period). The HZDR acts as curator of the data.
  - Thereafter, the data of publicly funded research are freely published (Open Access). The access and licensing is defined in the DMP. Data publications as well as software publications are to be registered in the publication database (ROBIS).
  - The policy has been discussed with user groups of Elbe and HLD and within the HGF and EU projects (CALIPSO+, PanData).