ETH zürich

IT Services

Supporting the reproducible research value chain in bioinformatics: from raw data to final publication

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SIB Days, 24.06.2024

Open Science and Open Research Data

Open Research Data

Requirement from funding agencies, journals, academic institutions

FAIR data

Persistent Identifier; metadata

Open protocol

Data format

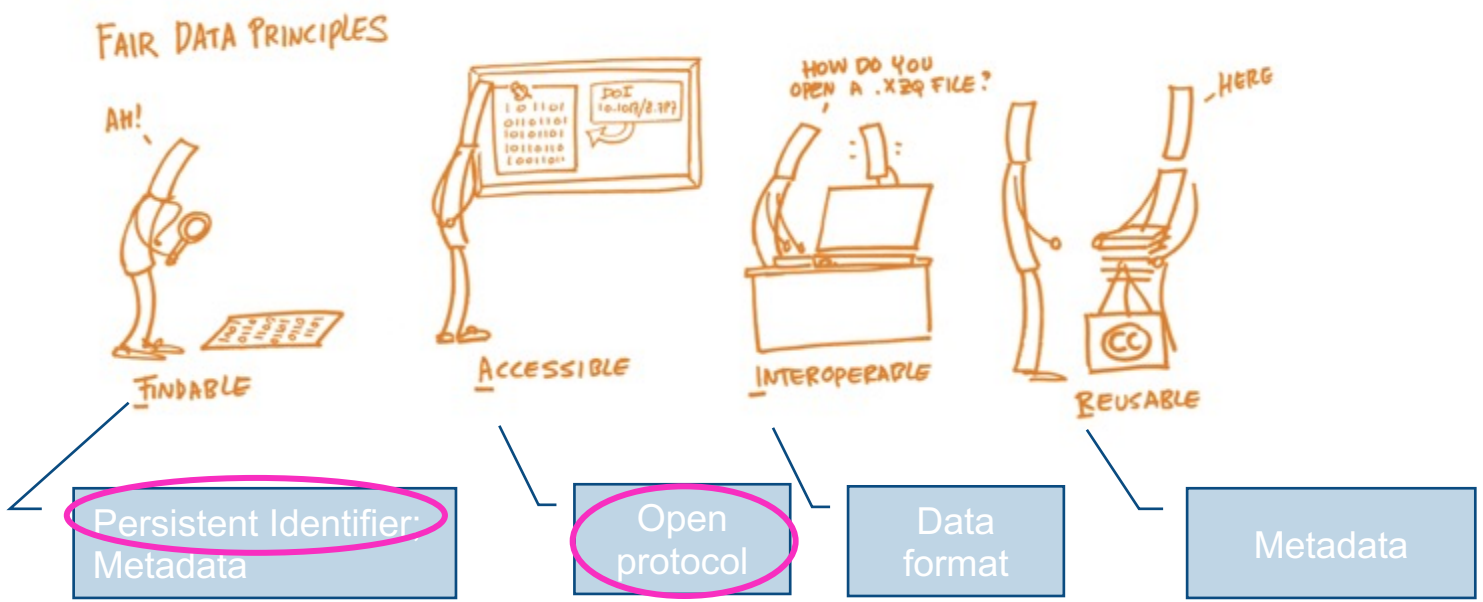
Metadata

The FAIR Data Principles

F	F1. (Meta)data are assigned a **globally unique** and **persistent identifie**r. F2. Data are described with **rich metadata** (defined by R1 below). F3. Metadata clearly and explicitly include the identifier of the data they describe. F4. (Meta)data are registered or indexed in a searchable resource.
A	A1. (Meta)data are retrievable by their identifier using a **standardised communications protocol**. A1.1 The **protocol is open, free, and universally implementable**. A1.2 The protocol allows for an authentication and authorisation procedure, where necessary. A2. **Metadata are accessible**, even when the data are no longer available
I	I1. (Meta)data use a **formal, accessible, shared, and broadly applicable language for knowledge representation**. I2. (Meta)data use **vocabularies** that follow FAIR principles. I3. (Meta)data include qualified references to other (meta)data
R	R1. (Meta)data are richly described with a plurality of **accurate** and **relevant attributes**. R1.1. (Meta)data are released with a clear and accessible data usage license. R1.2. (Meta)data are associated with detailed provenance. R1.3. (Meta)data meet domain-relevant community standards

https://www.go-fair.org/fair-principles/

Prepare to meet the FAIR requirements when data are generated



When data are **published**

How can we share data in a FAIR way?

A few generic [data repositories recommended by SNSF]

ETH zürich Research Collection

OIOS

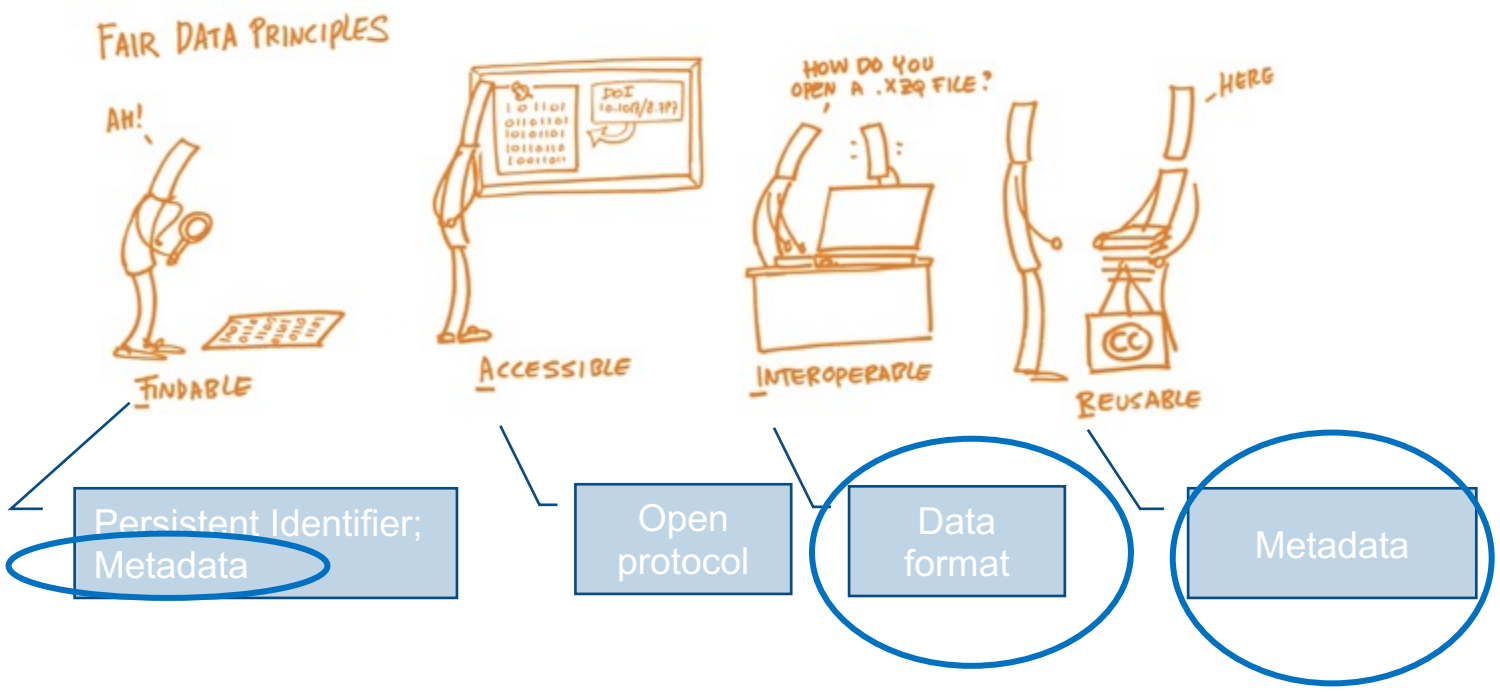
OSF

zenodo

DRYAD

re3data.org
REGISTRY OF RESEARCH DATA REPOSITORIES

Prepare to meet the FAIR requirements when data are generated



When data are **generated**

Data and information generation during a research project

Sample preparation

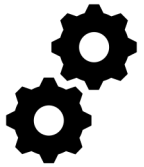
- Sample info
- Sample preparation info (protocol)

Measurement

- Machine info
- Machine settings

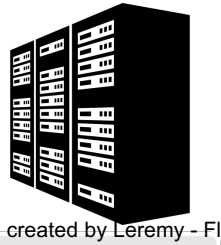
Data collection

- Data collection info



Processing

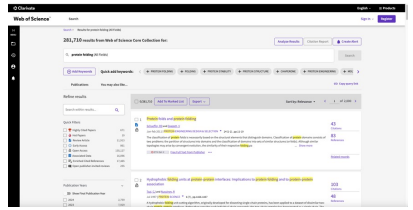
- Code/programs
- Settings/Procedures



Icon created by Leremy - Flaticon

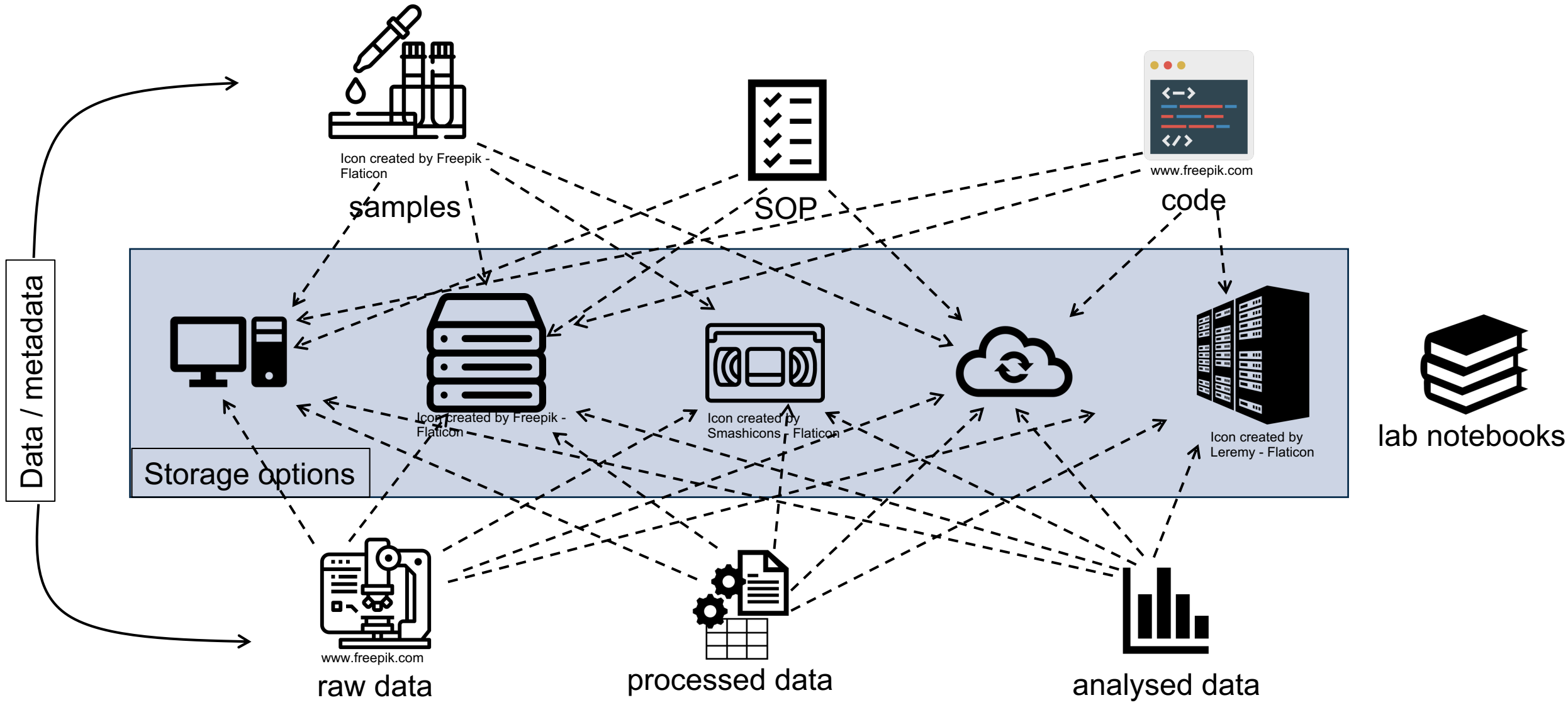
Analysis

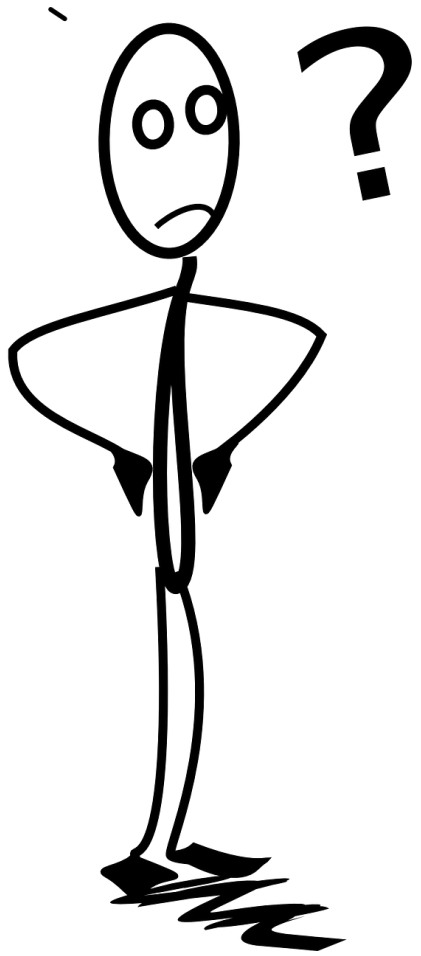
- Code/programs
- Settings/Procedures



Publication

The “Data Spread”: a Common Scenario in Academic Research

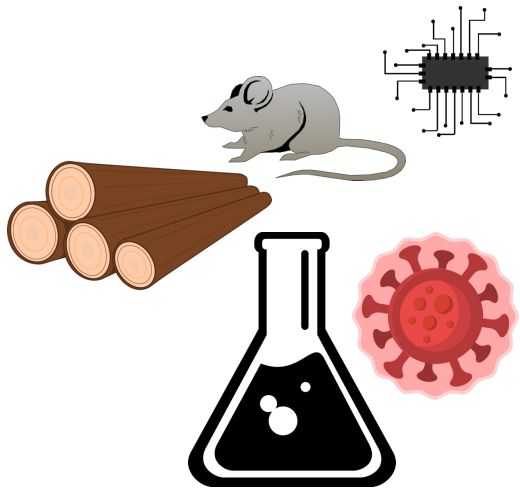


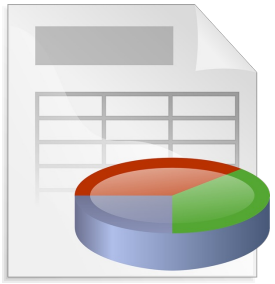


Which tools can we use to manage all these data and information?

RDM
Research Data Management

Management of materials and samples





Not scalable

No sharing

No efficient search

Easy to use

Spreadsheets / tabular files

+Scalable

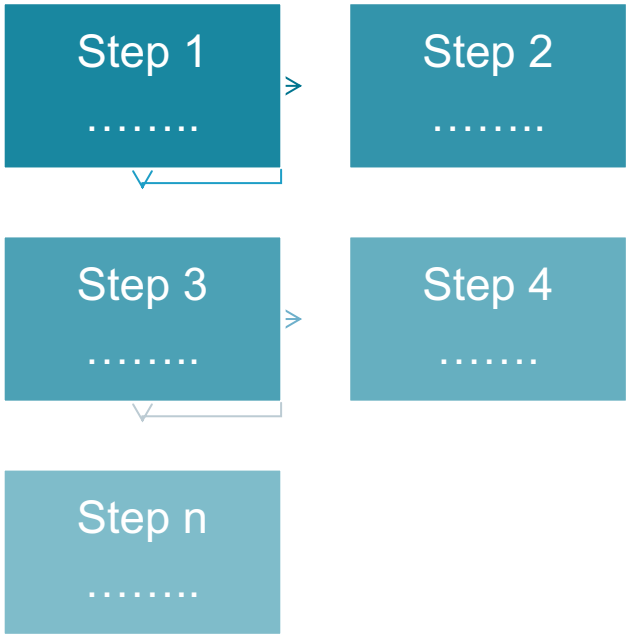
+ Sharing

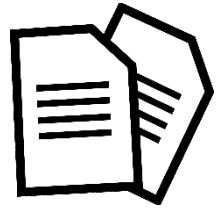
+ Search functionality

- Require time for set up and maintenance

Database/ LIMS

Management of protocols





Text files

Not scalable
No sharing
No efficient search
Easy to use

WIKI

Scalable
Sharing
Search functionality
Versioning

Database/ LIMS

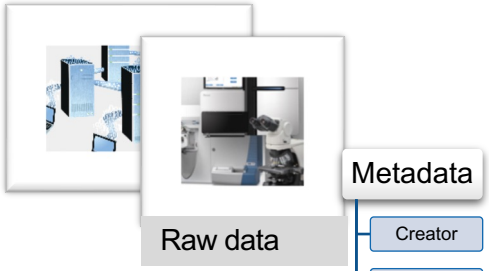
Scalable
Sharing
Search functionality
Require time for set up and maintenance

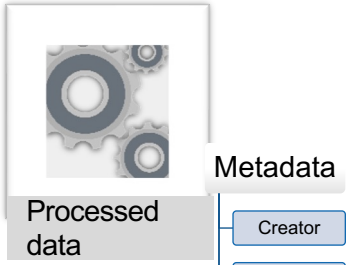
Laboratory Information Management System (LIMS)

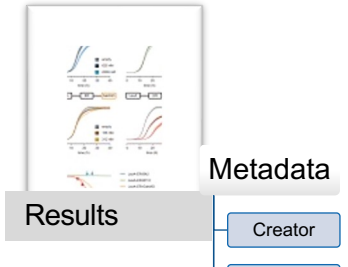
- LIMS are software for managing laboratory operations:
  - **sample tracking**
  - **sample data tracking**
  - **protocol management**

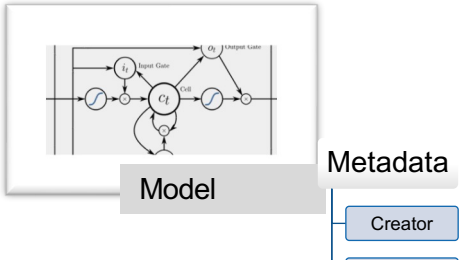
- Nowadays **LIMS are often combined with ELNs** in one platform.

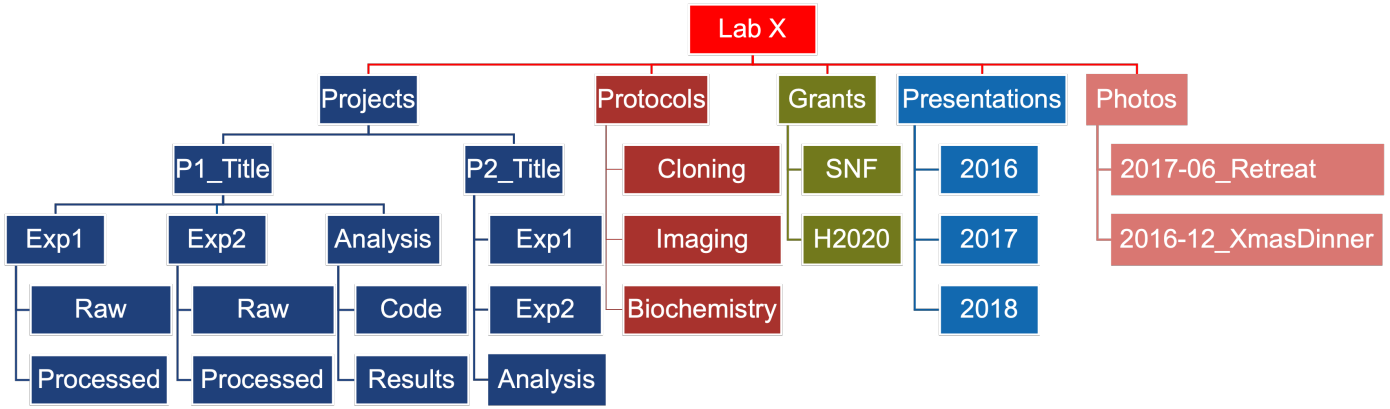
Management of research data files



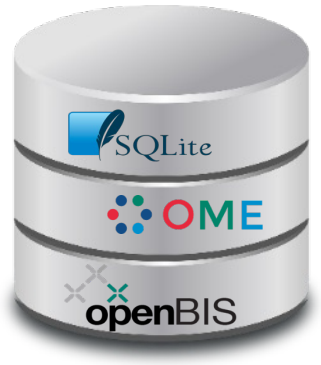








Files / folders hierarchy



Data management platform

Data management platforms

Generic

PostgreSQL

FileMaker
An Apple Subsidiary

SQLite

Microsoft Access

Scientific

PostGIS
Spatial PostgreSQL

openBIS

SLIMS
Agilent Technologies

rasdaman
raster data manager

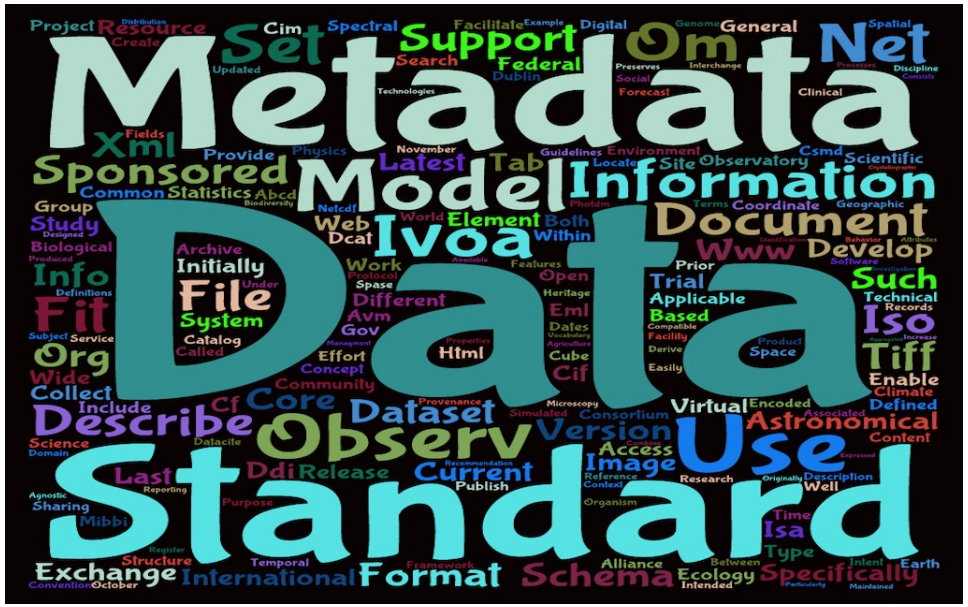
OME

RSpace

- System that allows **structured organization** of data
- Data are described by **metadata**
- Usually more FAIR-compliant than Files / Folders
- Searchable, scalable, flexible
- Allows user rights management

Metadata

- **Metadata** is the *data about your data*
- (Machine-readable) **Metadata** is a key element of the **FAIR data** principles
- Use of structured metadata **facilitates data organization** and searches
- Existing **metadata schemas** are preferred (can be extended, if necessary)



https://rdamsc.bath.ac.uk/

Metadata schema

- ❑ Defines the structure for the metadata.
- ❑ Schema defined by a scientific community to enable the best description of a resource type for their needs.
- ❑ **Generic metadata** schema examples:

DublinCore

DataCite

Table 1: DataCite Mandatory Properties

ID	Property	Obligation
1	Identifier (with mandatory type sub-property)	M
2	Creator (with optional given name, family name, name identifier and affiliation sub-properties)	M
3	Title (with optional type sub-properties)	M
4	Publisher	M
5	PublicationYear	M
10	ResourceType (with mandatory general type description sub-property)	M

https://schema.datacite.org/

Table 2: DataCite Recommended and Optional Properties

ID	Property	Obligation
6	Subject (with scheme sub-property)	R
7	Contributor (with optional given name, family name, name identifier and affiliation sub-properties)	R
8	Date (with type sub-property)	R
9	Language	O
11	AlternateIdentifier (with type sub-property)	O
12	RelatedIdentifier (with type and relation type sub-properties)	R
13	Size	O
14	Format	O
15	Version	O
16	Rights	O
17	Description (with type sub-property)	R
18	GeoLocation (with point, box and polygon sub-properties)	R
19	FundingReference (with name, identifier, and award related sub-properties)	O

Metadata schema

- ❑ Defines the structure for the metadata.
- ❑ Schema defined by a scientific community to enable the best description of a resource type for their needs.
- ❑ **Discipline-specific** metadata schema examples:

OME

Microscopy images

DDI

Social Sciences

EML

Ecology

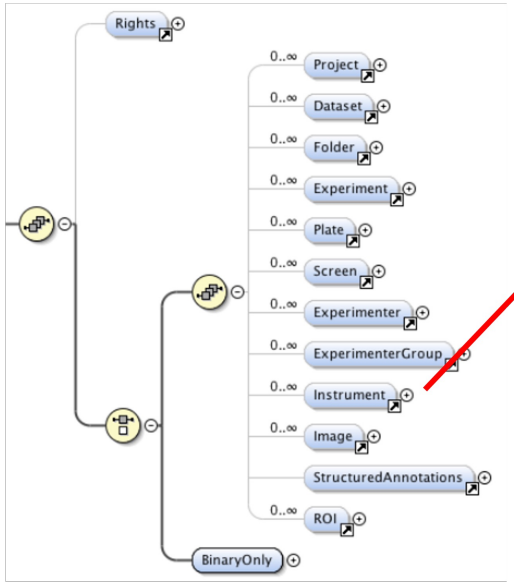
Biodiversity Information Standards TDWG

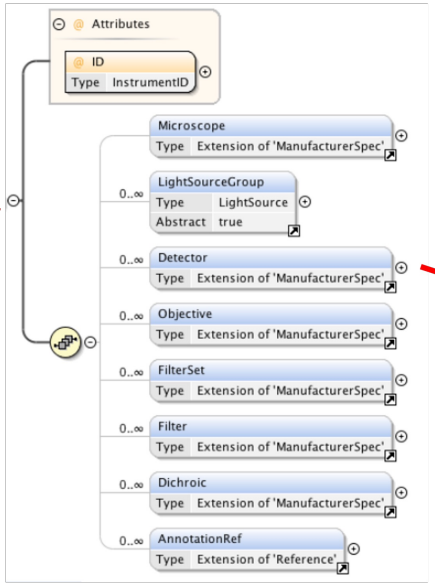
Biology

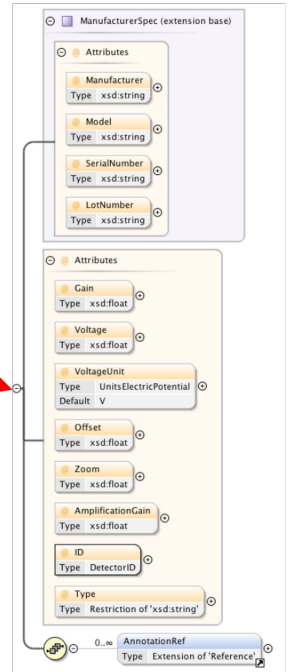
SPHN Swiss Personalized Health Network

SPHN Meta-Data Catalogue

Health data



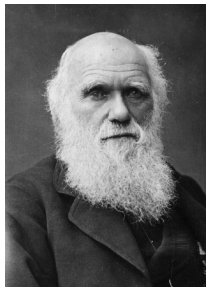




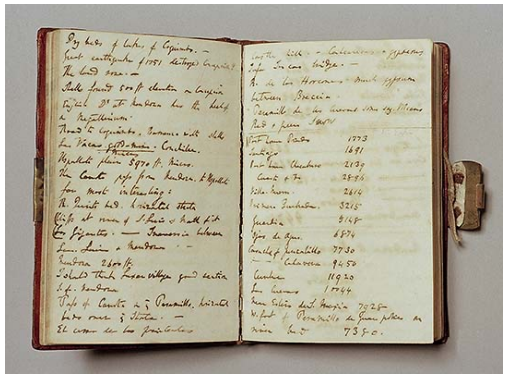
https://www.openmicroscopy.org/Schemas/

Electronic Laboratory Notebooks

- Scientists have always documented their findings in paper notebooks.

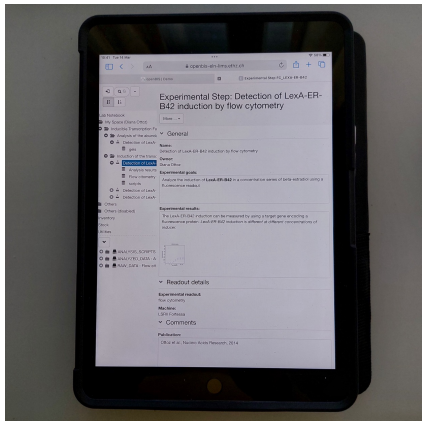


C. Darwin



Beagle voyage notebooks

1831-1836



ELN example

2023

- An **electronic laboratory notebook** (also known as **electronic lab notebook** or **ELN**) is a software program or package designed to replace more traditional paper laboratory notebook (*https://www.limswiki.org/index.php/Electronic_laboratory_notebook*).

ELNs vs. paper notebooks

- Sharing
- Rights management
- Search functionality
- Easier to link digital data
- Can be backed up
- No issues with handwriting
- Track changes

- Learning curve
- Change in working mode required
- Time needed for introduction in lab

Wiki and note-keeping applications

Confluence

- Wikis and note-keeping applications often considered ELN solutions.
- Popular in academia for ease of use.
- These are a straight replacement of paper notebooks, with some added functionalities, but do not provide a solution for data management.

Structured ELNs

openBIS

labfolder

SCINOTE

eLabFTW

Chemotion

RSpace

LabArchives

NOMAD

BIOVIA

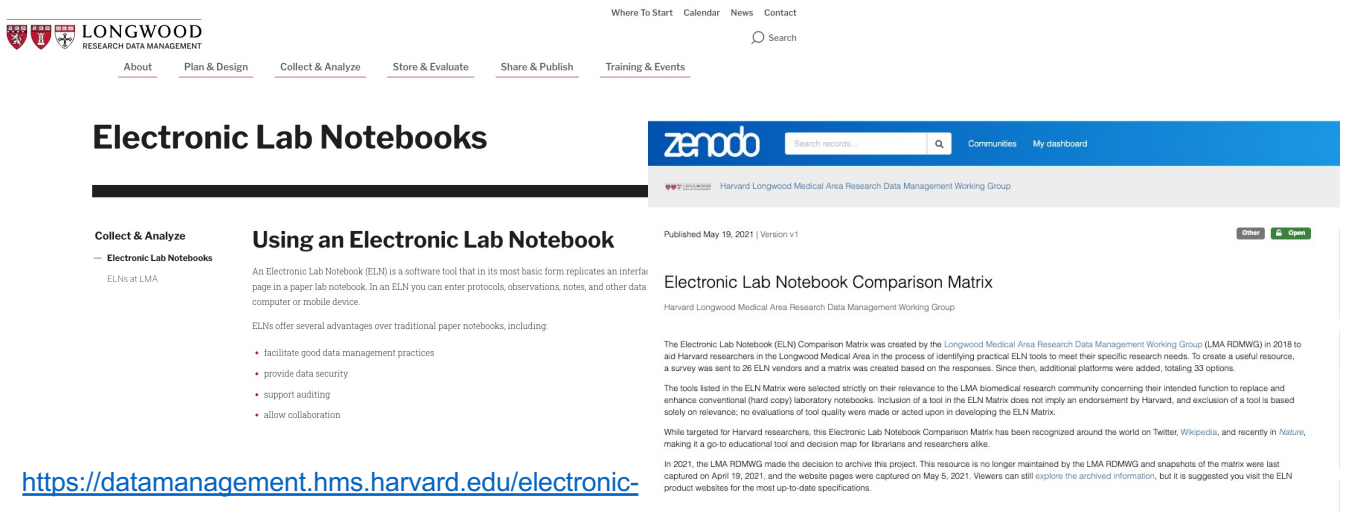
- Additional functionalities compared to note-keeping applications (e.g. workflow management, chemical structures drawing, etc).
- Can be **discipline-specific** or **cross-disciplines**.
- Can have **LIMS** functionalities.
- Some systems offer an all-in-one solution for **RDM**.
- Can be integrated with third party applications.

Where to start when choosing which ELN to use?

- ❑ Is it for personal use or group use?
- ❑ Can I/we use a cloud-based solution?
- ❑ Do I/we need specific features?
- ❑ What do I/we want to do with the ELN? (e.g. only write experimental descriptions, manage samples, manage data – how big?, etc.)
- ❑ Commercial v. open-source.
- ❑ Budget?
- ❑ Can I export my data?

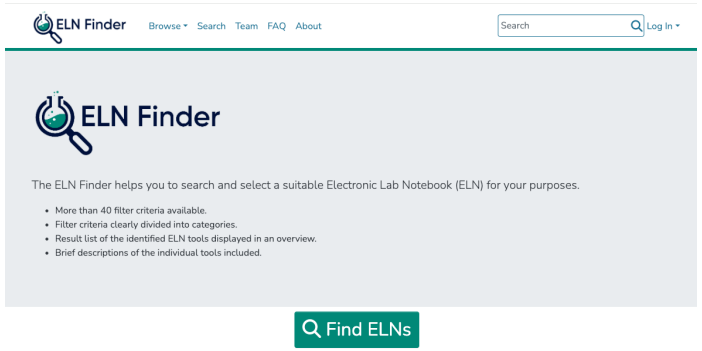
Some useful references on how to choose an ELN

https://www.nature.com/articles/d41586-018-05895-3



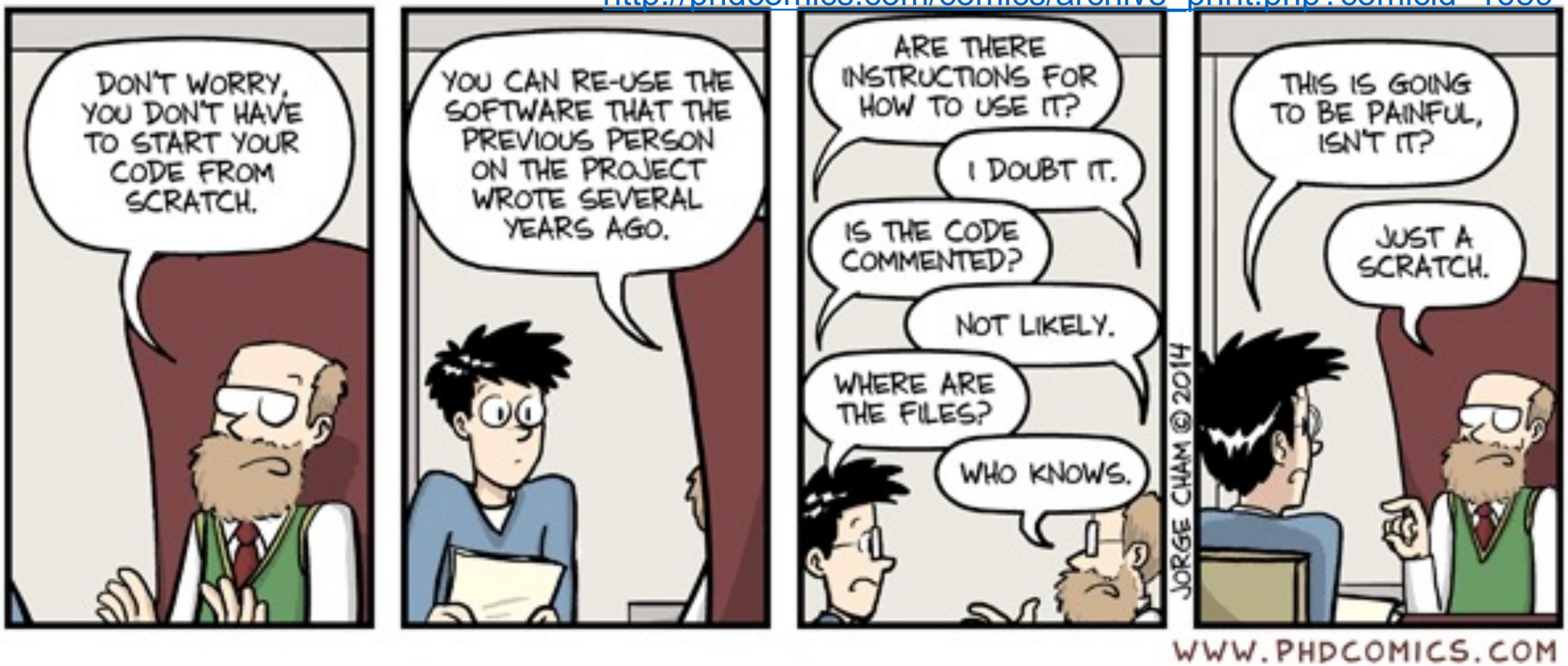
https://datamanagement.hms.harvard.edu/electronic-lab-notebooks

https://zenodo.org/records/4723753



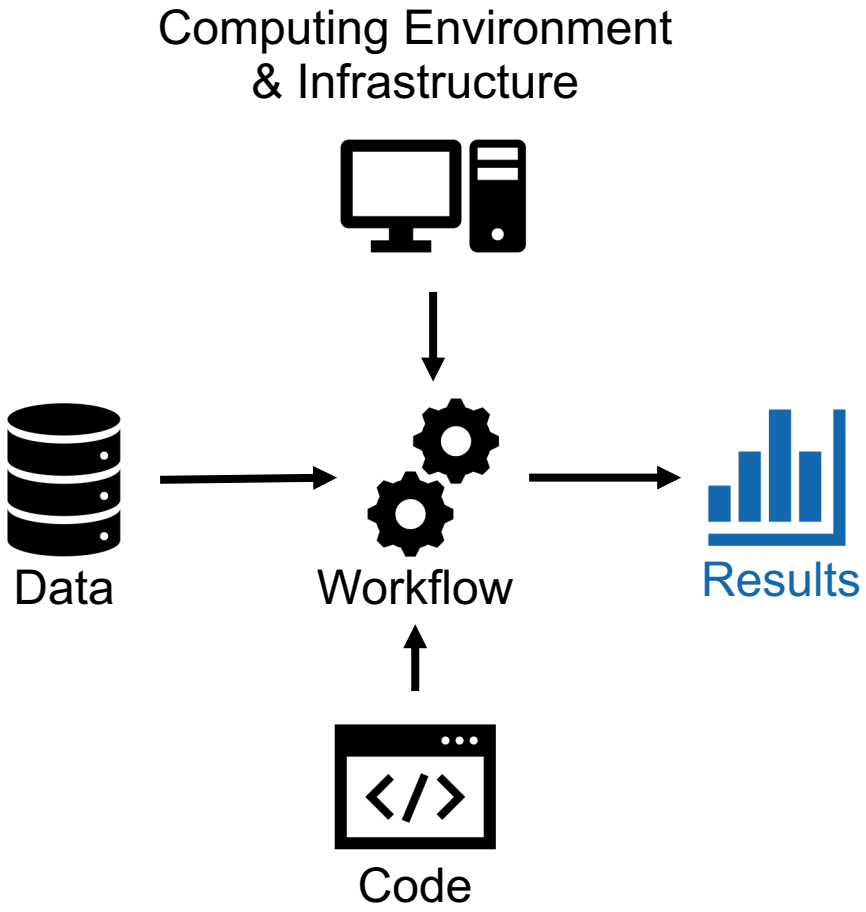
https://eln-finder.ulb.tu-darmstadt.de/home

http://phdcomics.com/comics/archive_print.php?comicid=1689



Reproducible Data Analysis

What do we mean by *Reproducibility*?

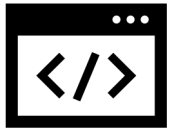


« ***Reproducibility*** is **obtaining consistent results** using the same input data; computational steps, methods, and code; and conditions of analysis. This definition is synonymous with "computational reproducibility"… »

- All components need to be reproducible!

National Academies of Sciences, Engineering, and Medicine. 2019. Reproducibility and Replicability in Science. https://doi.org/10.17226/25303.

Code management



Version control systems

> Software tools specialized on managing and documenting changes to source code over time

> Necessary for managing large code bases

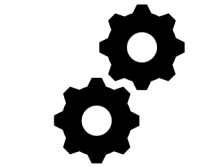
> Standard in professional software development

Interactive notebooks

> Applications that combine documentation, code, input and output generated by the code, e.g. graphs, plots (*Nature 515, 151–152*)

> Useful for exploratory data analysis and reproducibility

Workflow Management



An incomplete list of **286** Computational Data Analysis Workflow Systems

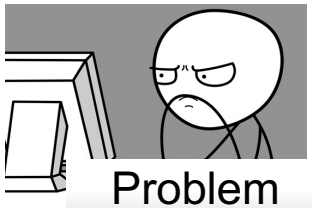
https://github.com/common-workflow-language/common-workflow-language/wiki/Existing-Workflow-systems

A curated list of **109** Awesome Pipeline frameworks & libraries + **30** Workflow platforms

https://github.com/pditommaso/awesome-pipeline

Reproducible Environment

Computing Environment and Infrastructure



Problem

Solution

Full reproducibility requires the possibility to recreate the system that was originally used to generate the results.

Bundle your application and all dependencies = Environment Isolation + Dependency Management

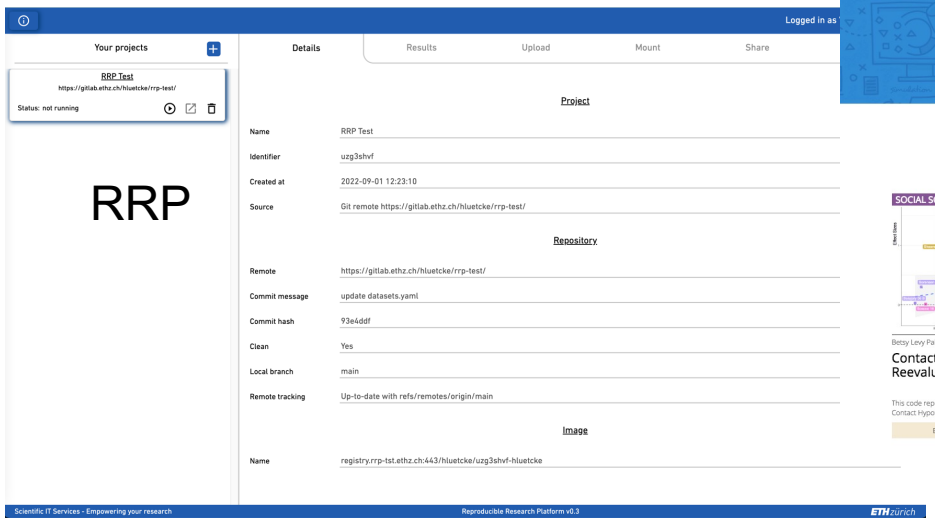
Environment and Package Management

Containers

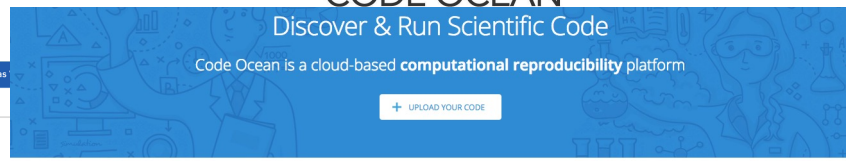
Virtual Machines

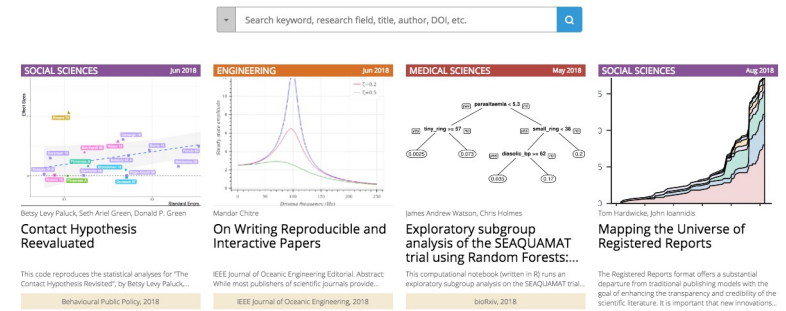
Environment & package management

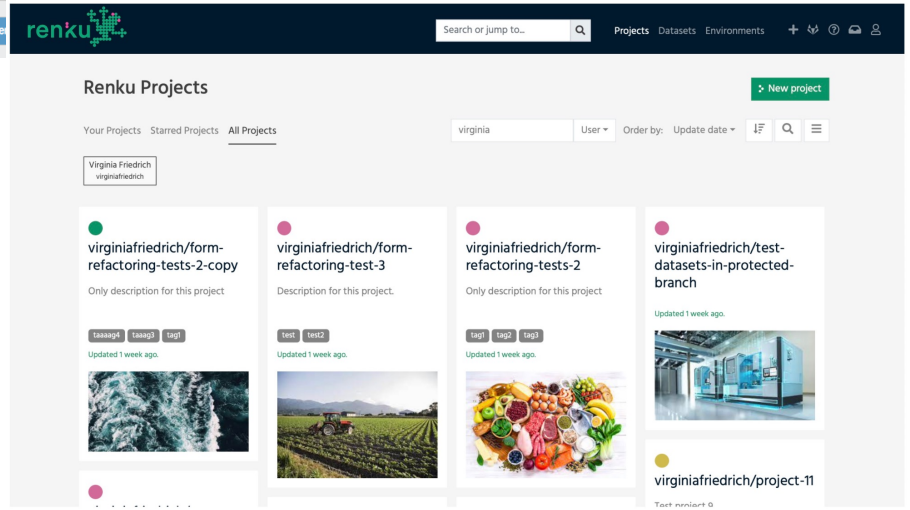
Platforms for running code reproducibly

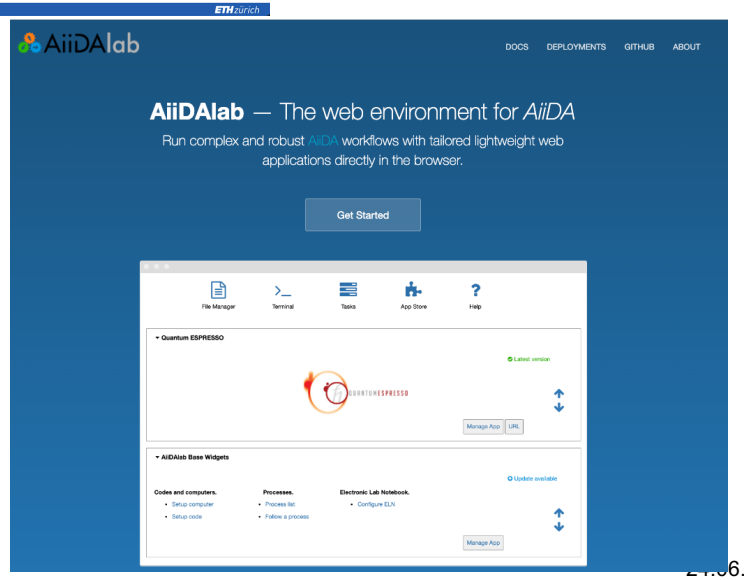


RRP





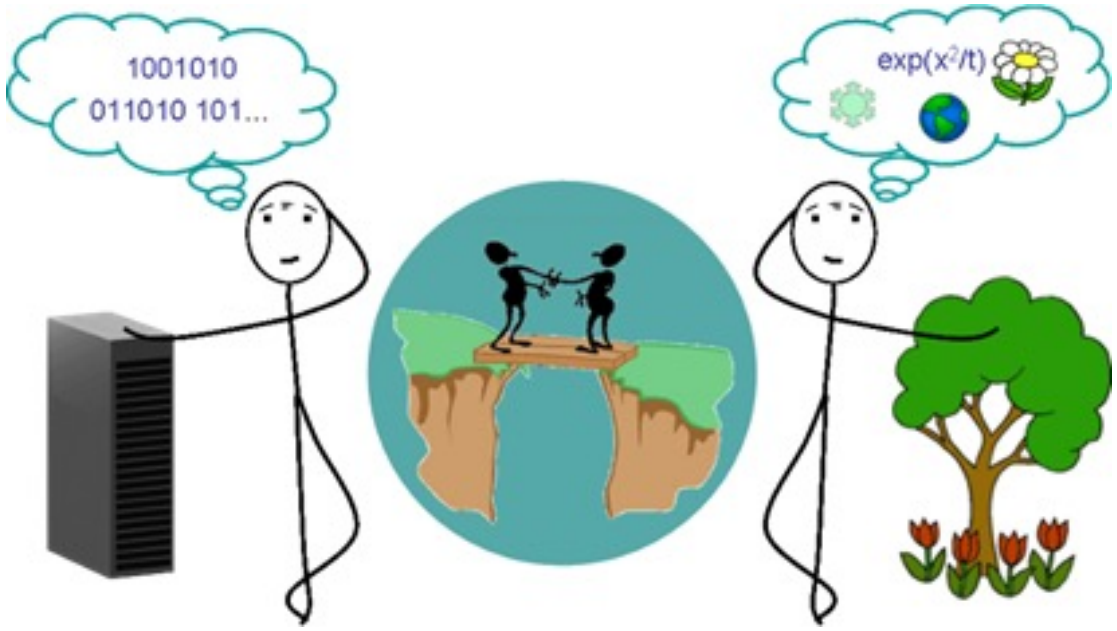




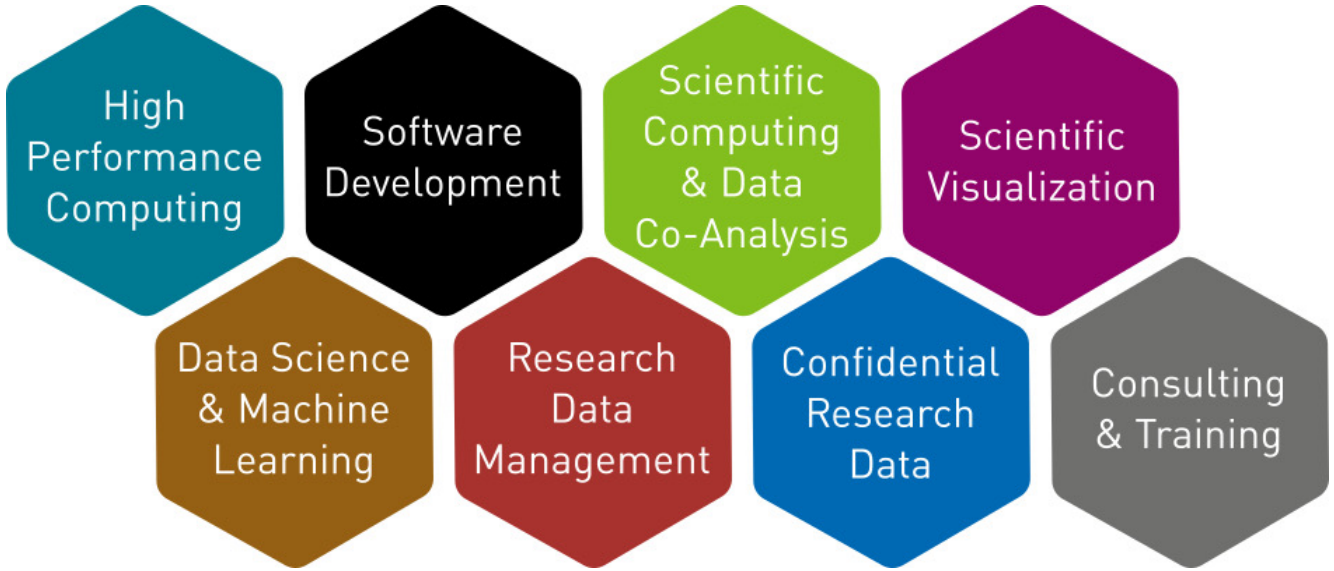
Take home messages

- Efficient RDM during the lifetime of a project is necessary to meet FAIR data requirements.
- RDM should be an integral part of every researcher's daily work.
- Several tools are available for RDM. There is no „*one-fits-all*" solution, but every use-case should find the most appropriate solution(s) for them.
- Talk to the RDM experts in your institution!

Scientific IT Services: bridging the gap between research and IT

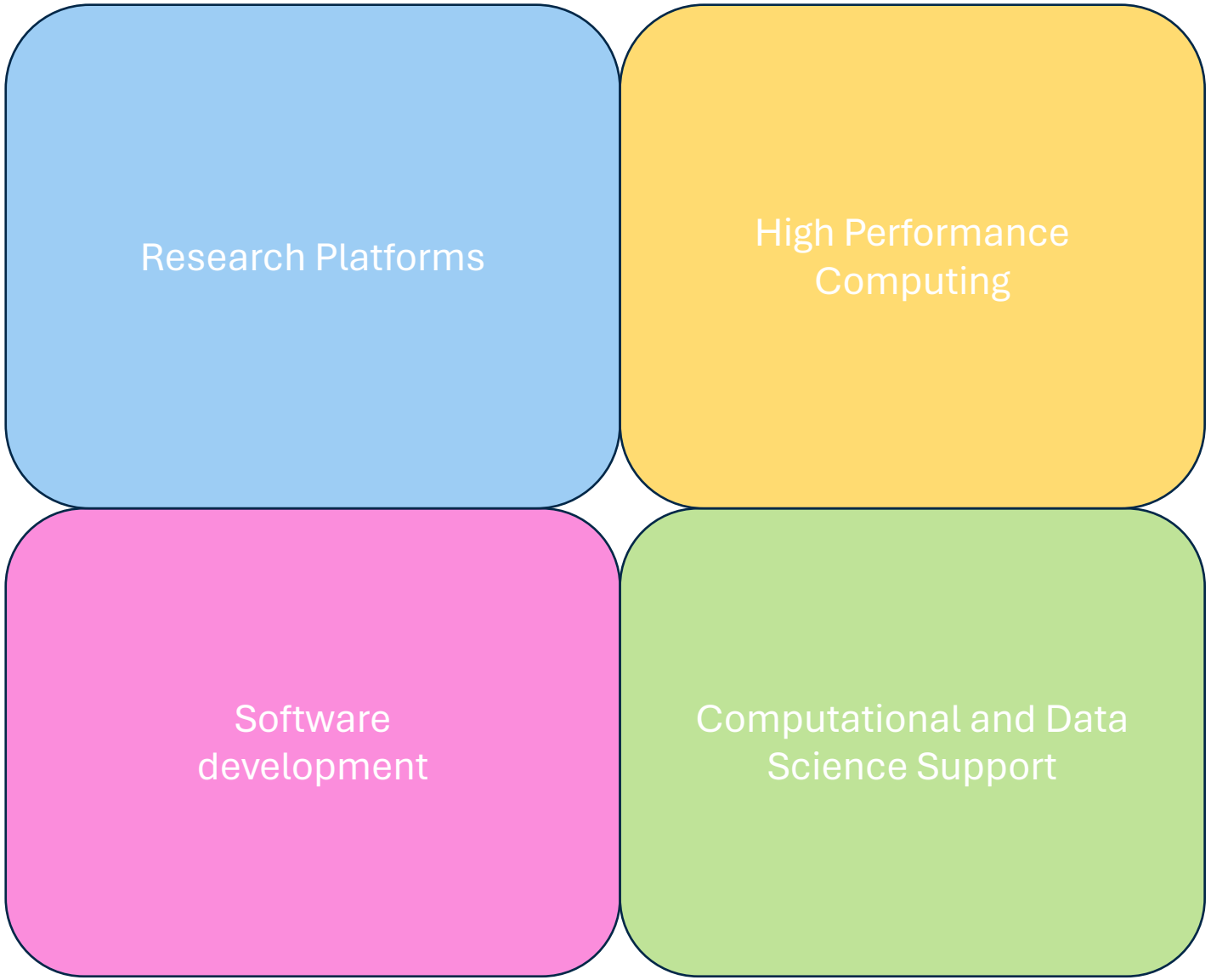


Who is Scientific IT Services of ETH Zurich?



- ❑ A section of ETHZ IT Services
- ❑ Around 50 experts in various areas of scientific computing
- ❑ With a background in different areas of science

Scientific IT Services: 4 groups

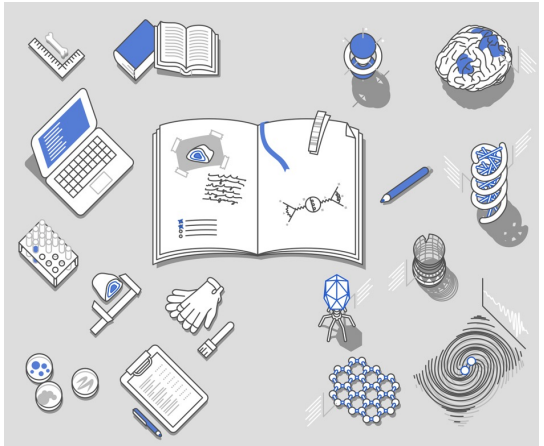


Scientific IT Services

Research Platforms

- Research data management services (openBIS)
- Confidential research data
- LeonhardMed
- GFB sequencing core facility data support

openBIS

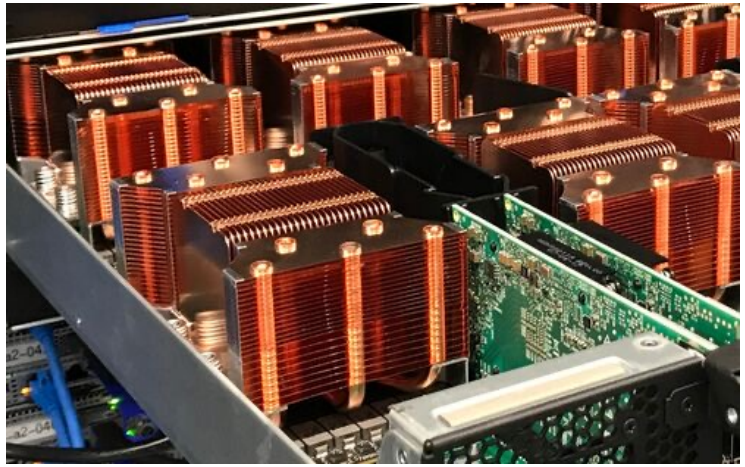


NGSvivo

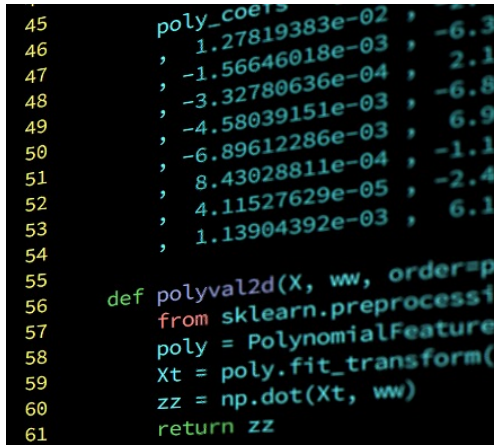
Scientific IT Services

- Scientific computing
- EULER cluster

High Performance Computing



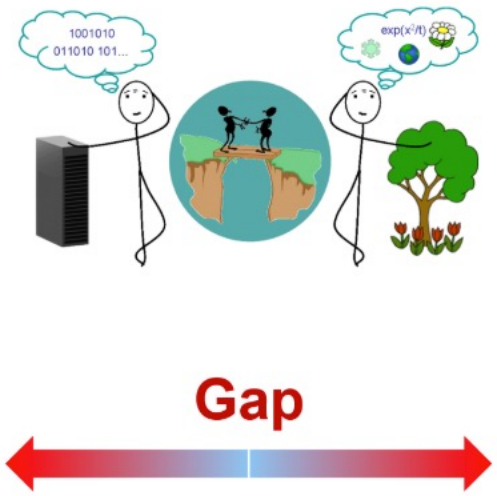
Scientific IT Services

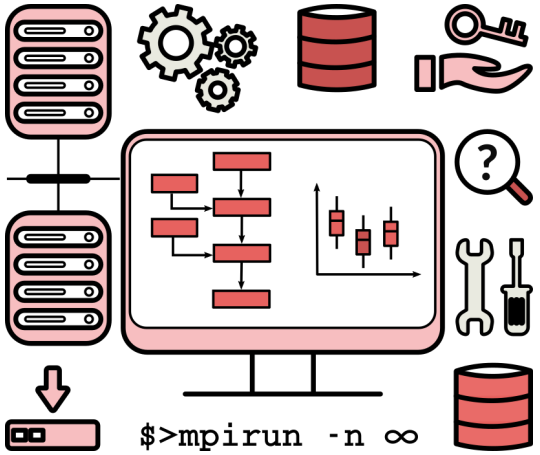


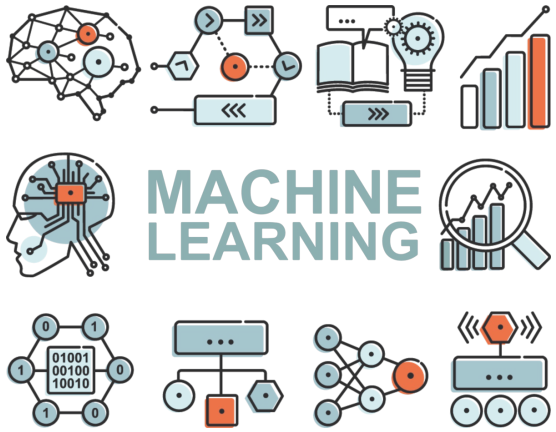
Software development

- ❑ openBIS development
- ❑ Custom software development
- ❑ Scientific visualizations
- ❑ Scientific code support

Scientific IT Services



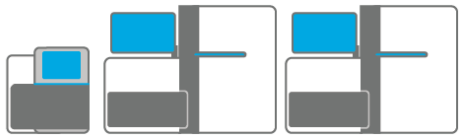




- ❑ Scientific IT consulting
- ❑ “Glue” between the SIS units
- ❑ Data science
- ❑ Data co-analysis
- ❑ Machine Learning/ AI

Computational and Data Science Support

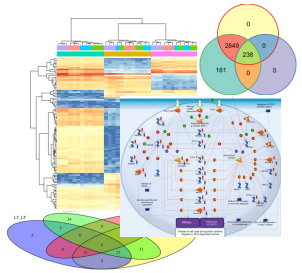
Bionformatics consulting



sequencing facilities

sequencing data

researcher



results

publications

Research

data analysis

co-analysis

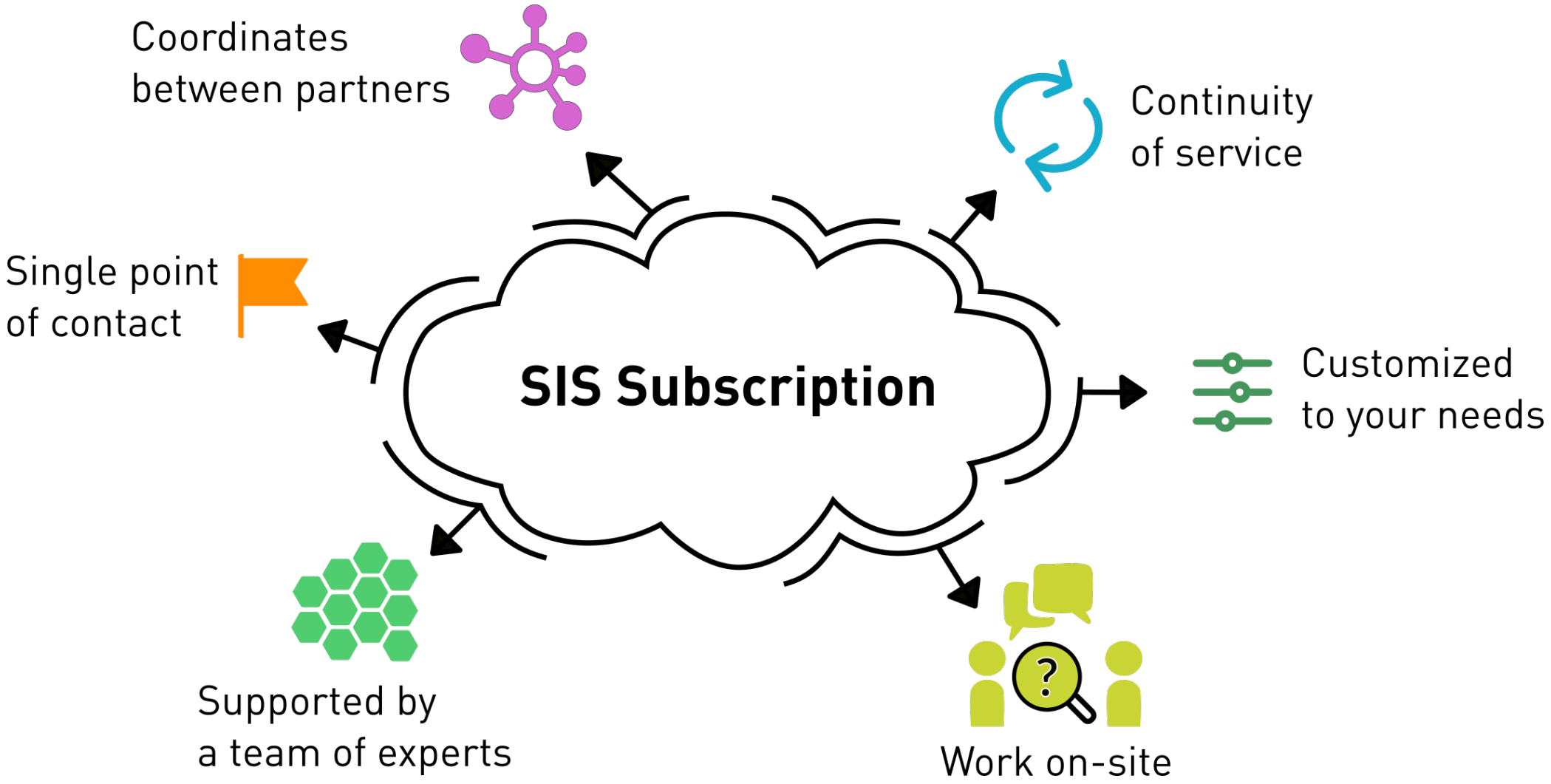
SIS bioinformatics consultant

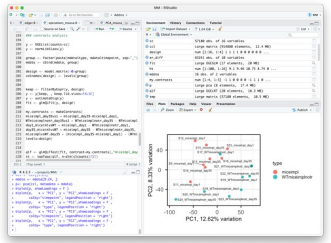
High performance computing clusters

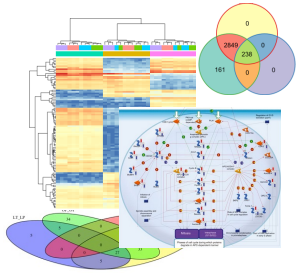
genomes and databases

bioinformatic software

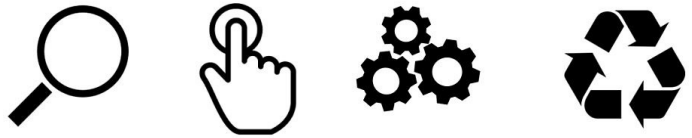
Scientific IT Services

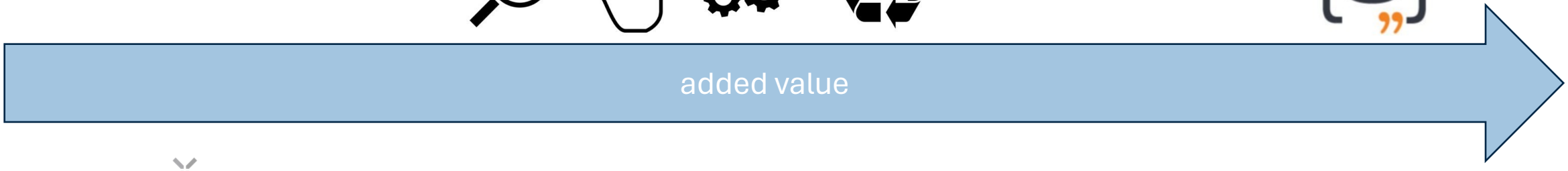






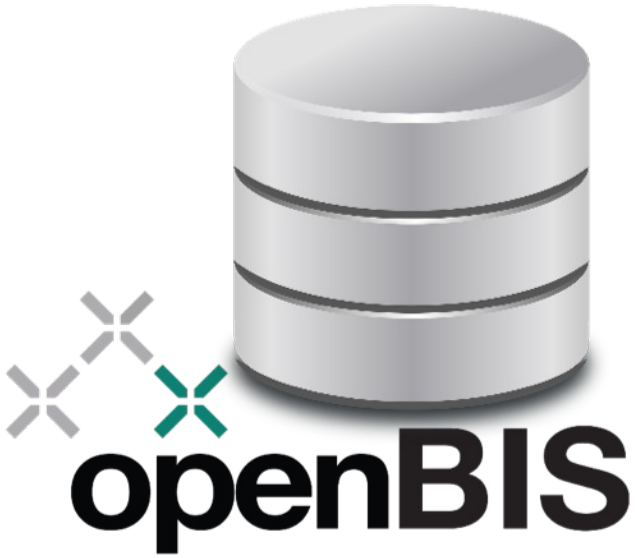
Findable Accessible Interoperable Reusable





openBIS

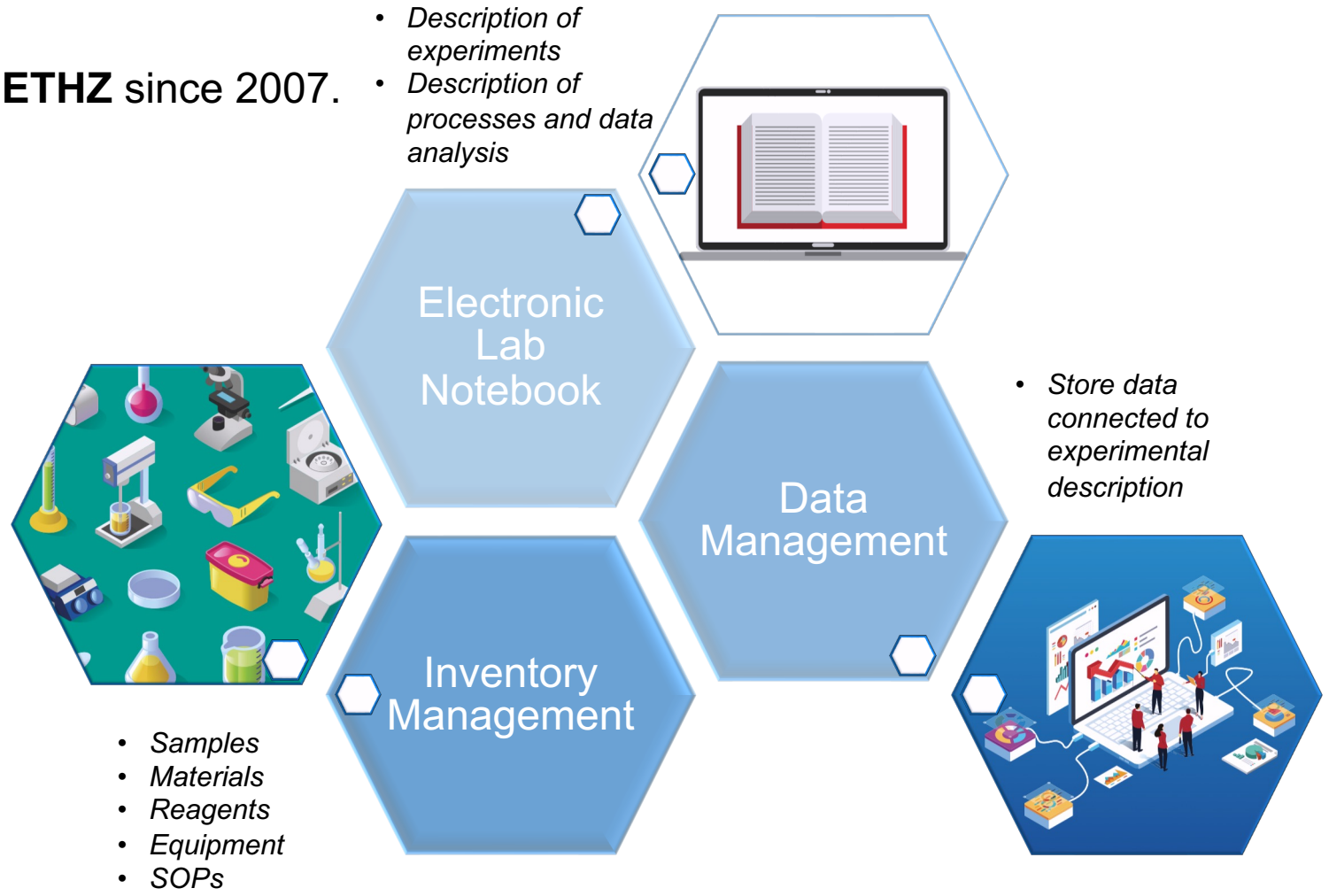
NGSvivo



The ETHZ Scientific IT Services data management solution for research groups

openBIS: a complete solution towards FAIR data management

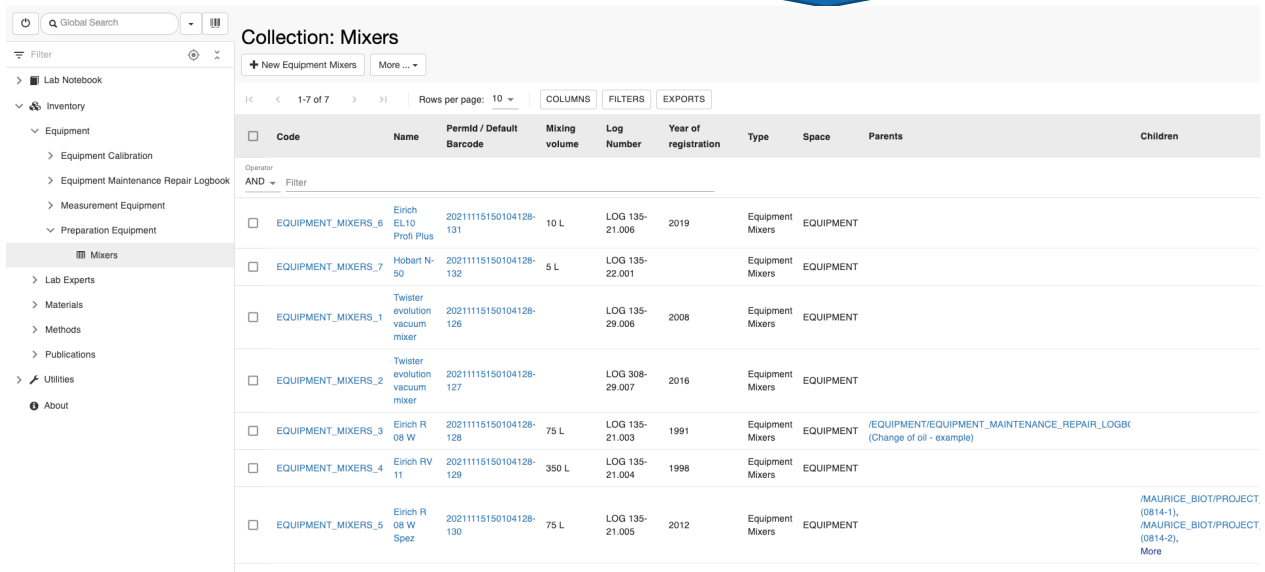
- Developed at **ETHZ** since 2007.



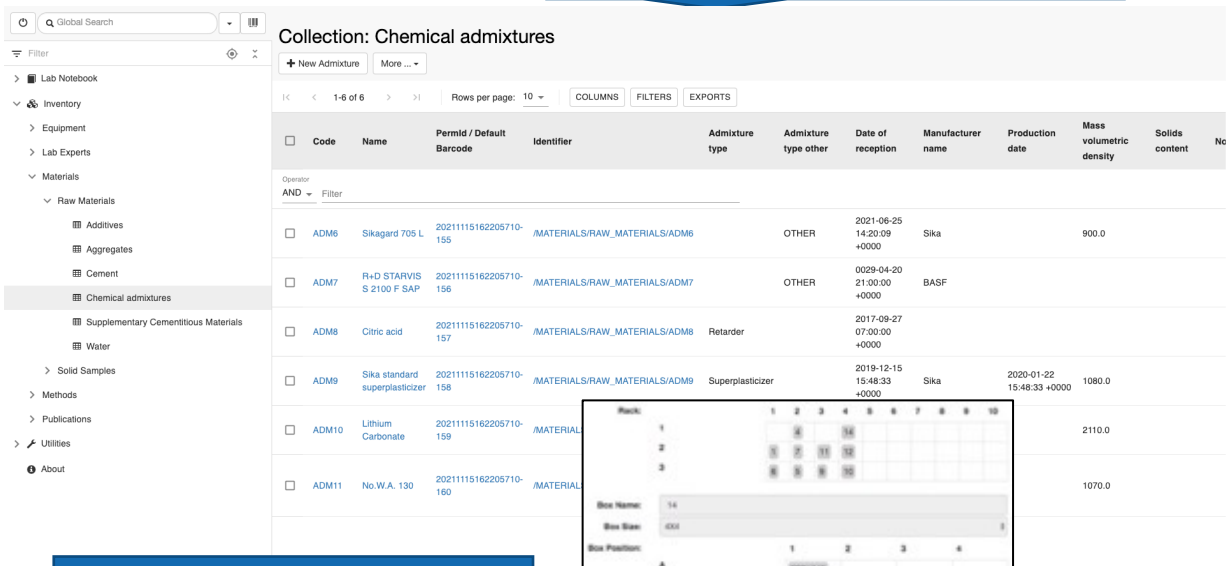
Inventory management

openBIS

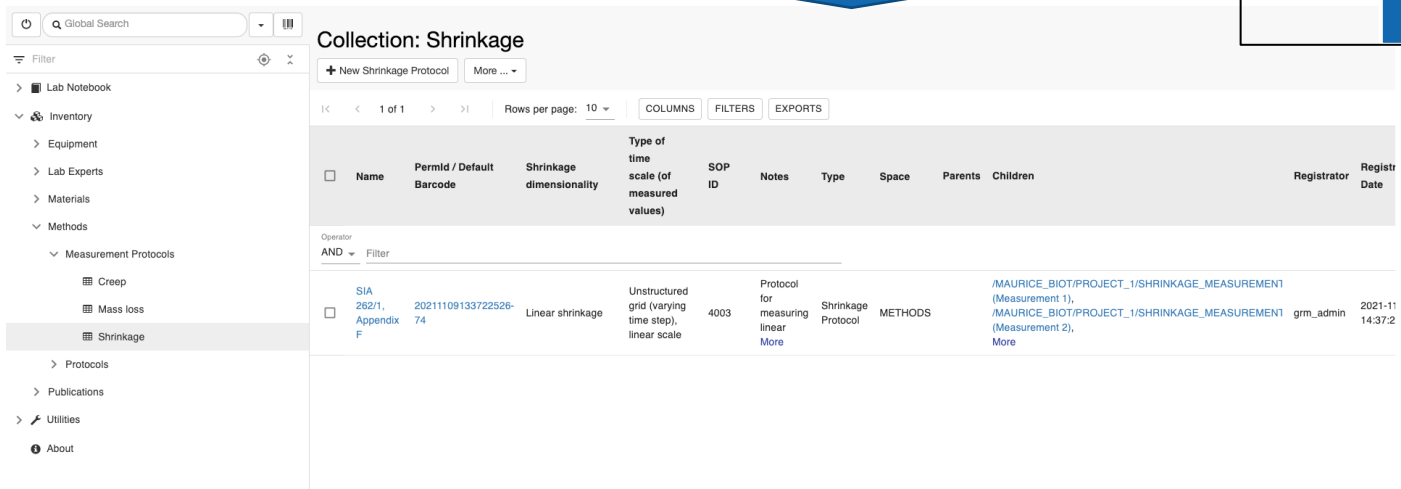
Lab equipment

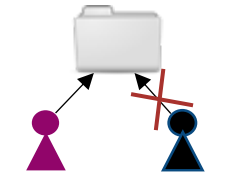


Lab samples & materials



Lab procedures



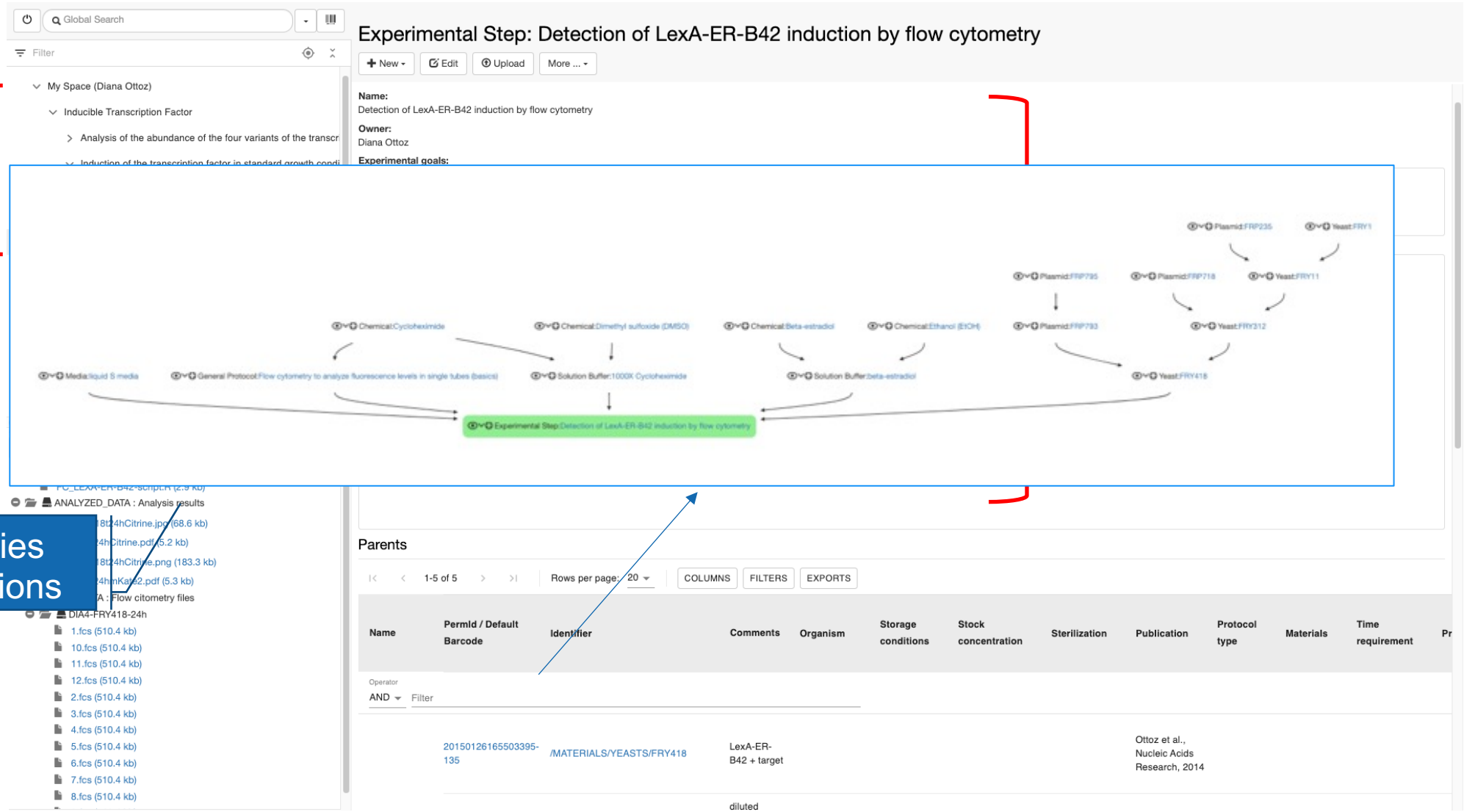


User rights management

Samples' storage manager

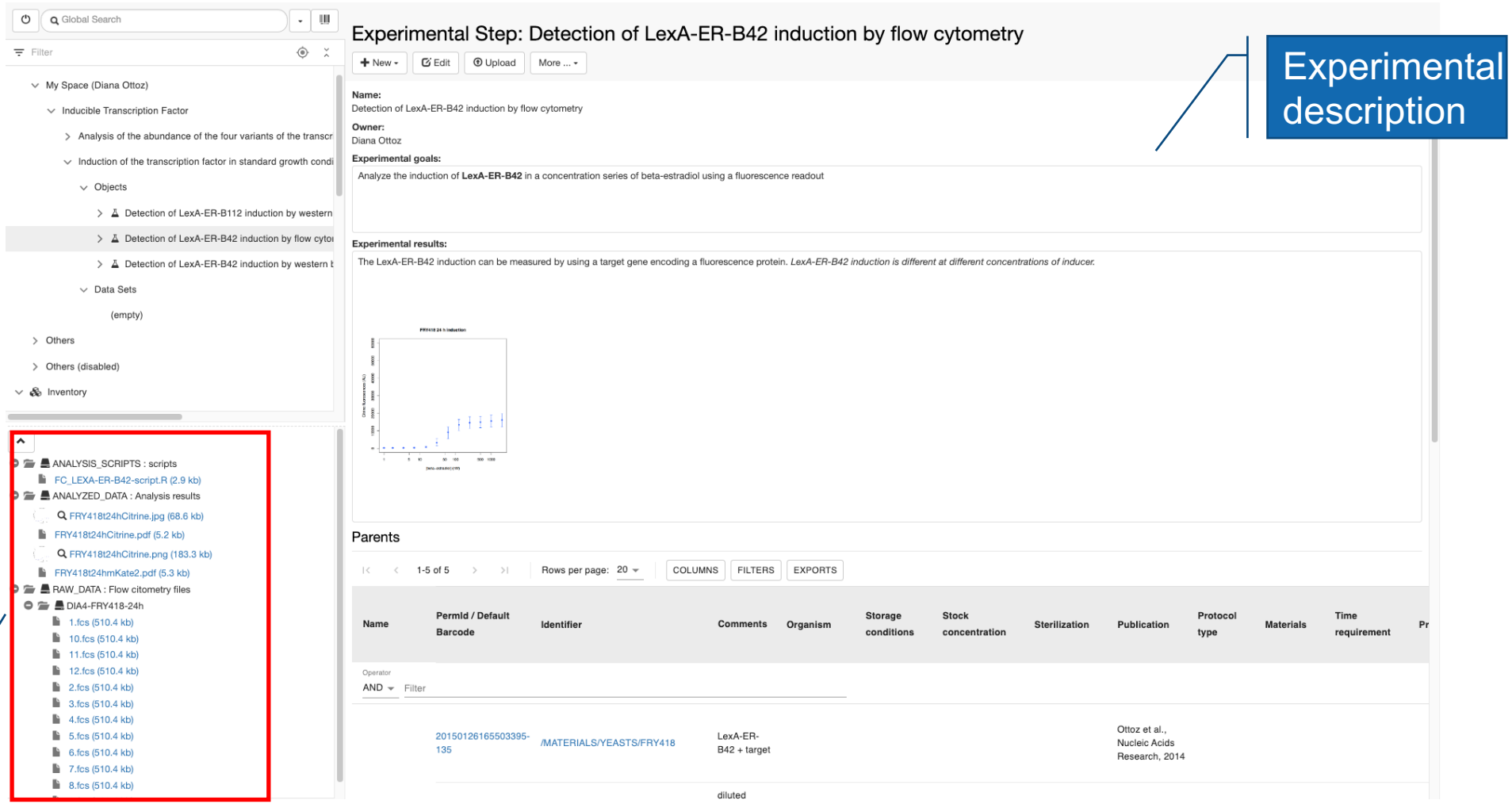
Barcode reader

Electronic Lab Notebook

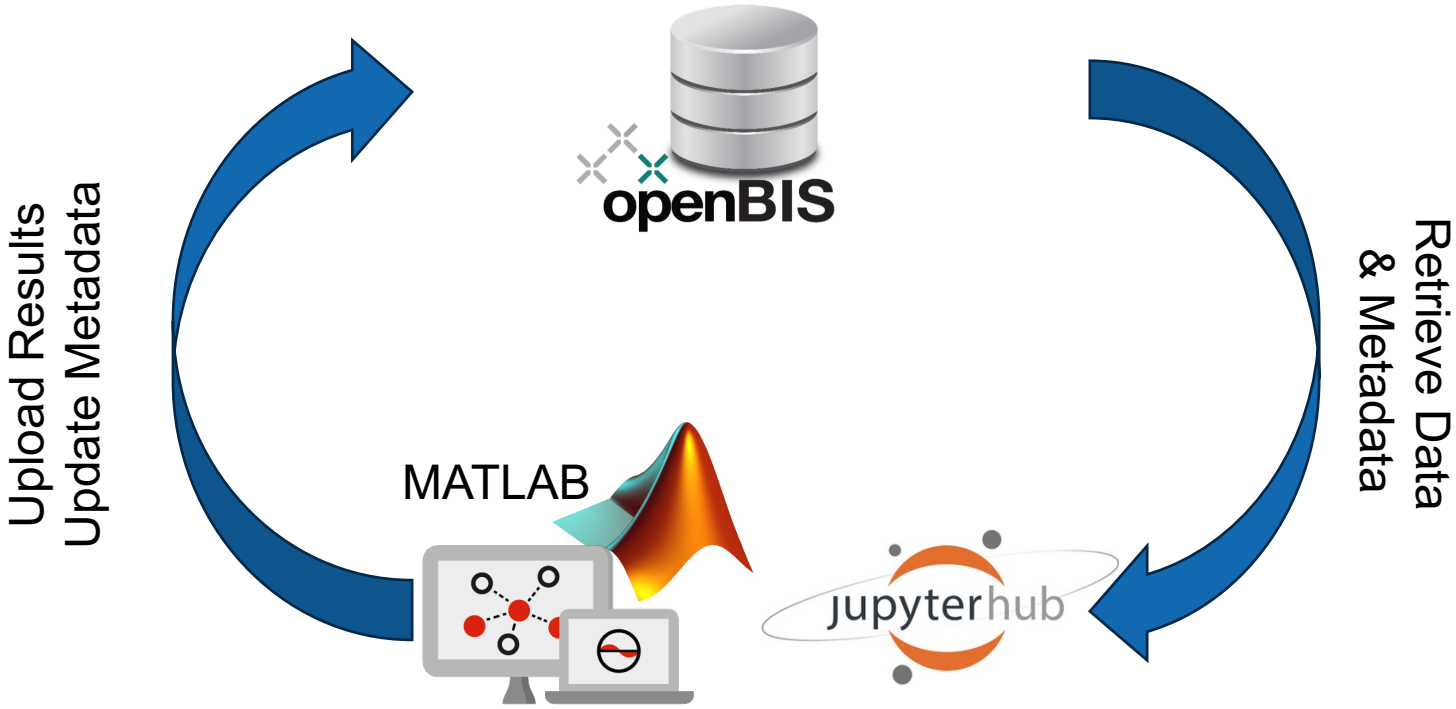


Data management

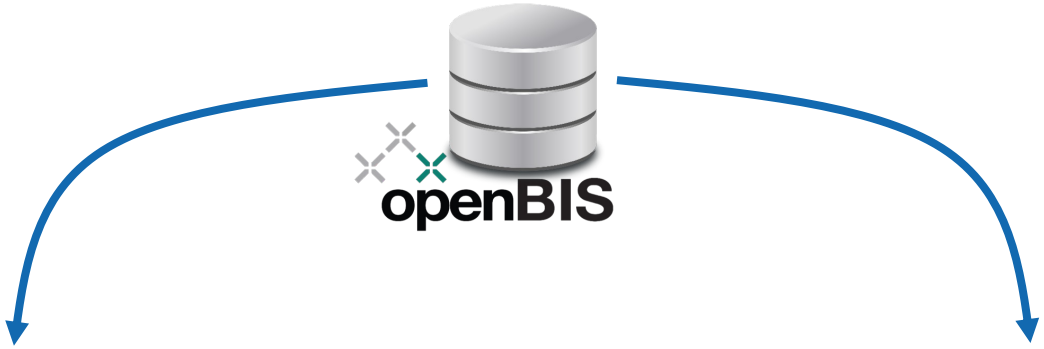
- Data are always connected to experimental descriptions

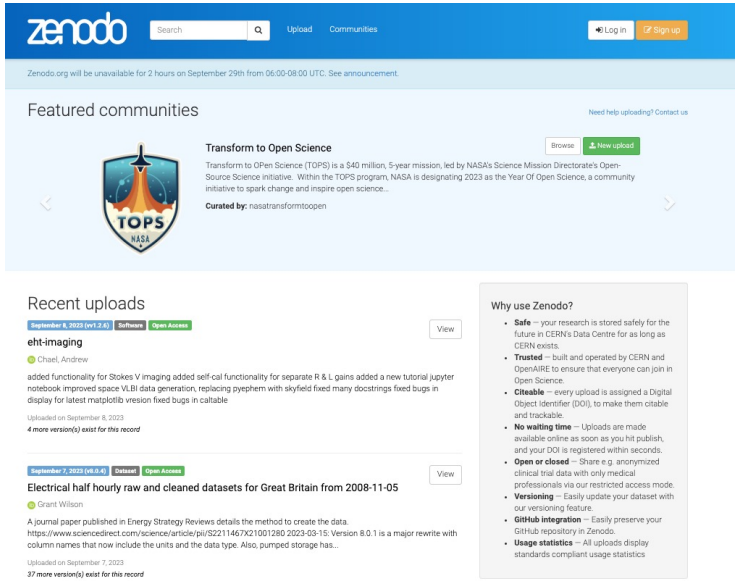


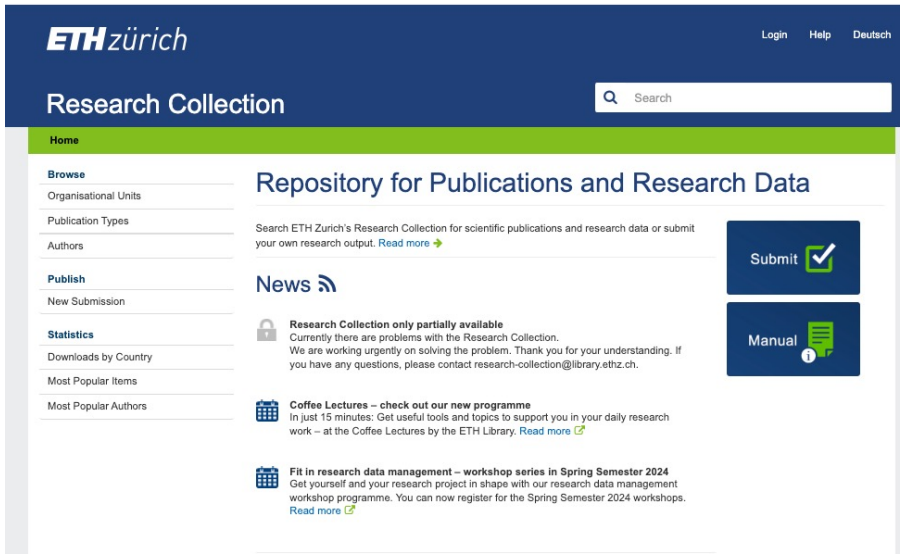
Data analysis: JupyterHub & MATLAB



Data publication: export to ETH Research Collection & Zenodo

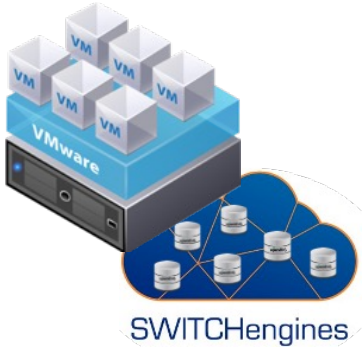






RDM services offered BY ETHZ SIS

- Services for ETHZ researchers
- Services for Swiss academic scientists (openrdm.swiss)



openBIS installation on ETHZ infrastructure (ETH customers) /cloud (Swiss academic customers).

openBIS + OS maintenance & upgrades

Consulting

Tailored data modelling

Training

User support