

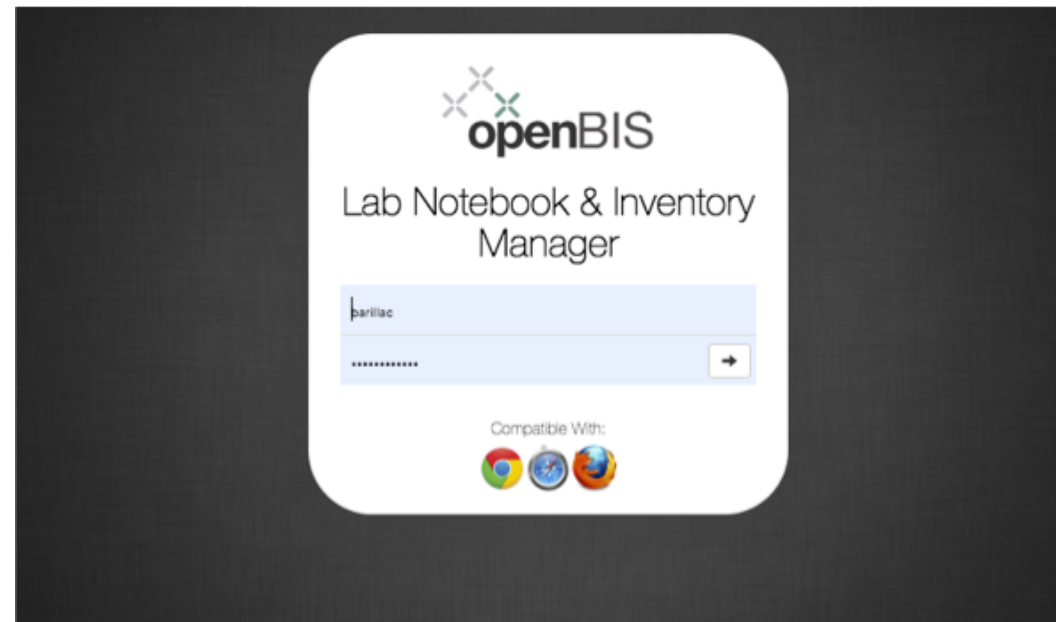


openBIS Training

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Scientific IT Services, ETH Zurich

Zurich, 09.10.2019

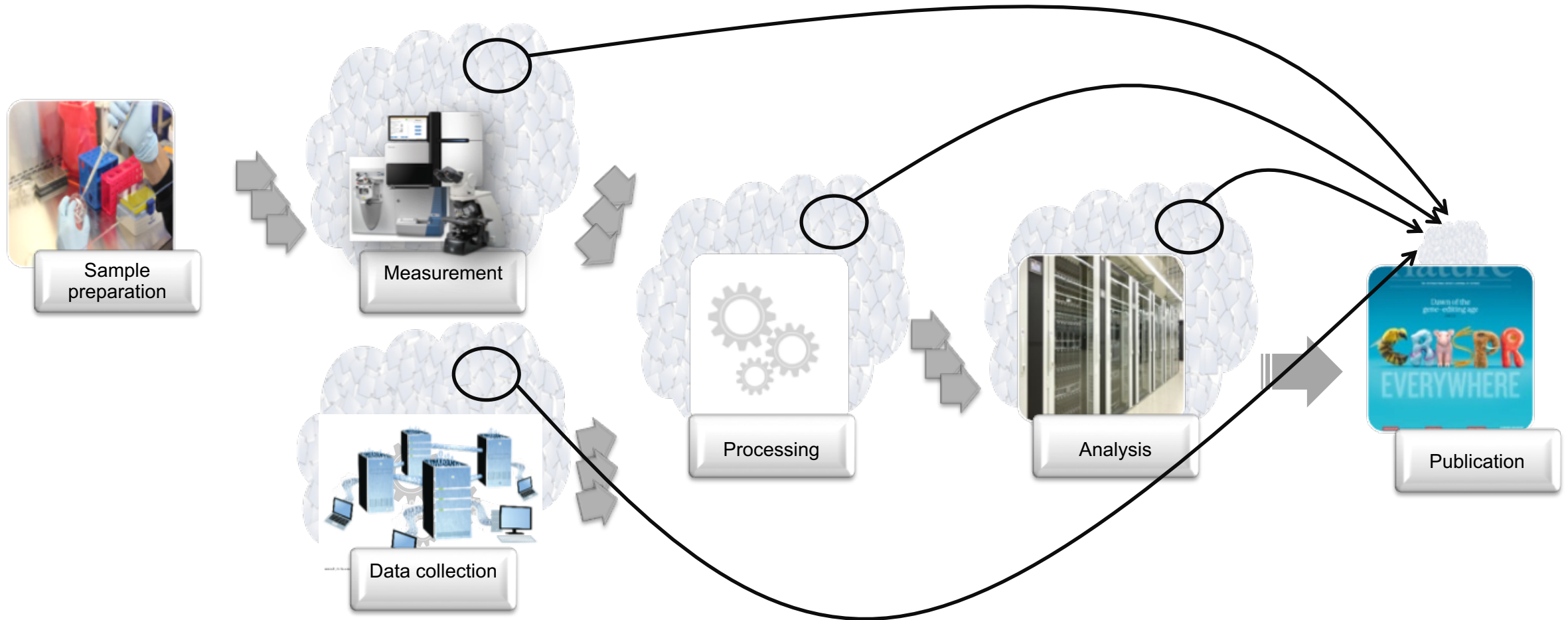
<https://openbis-tst.ethz.ch/openbis/webapp/elN-lims/>



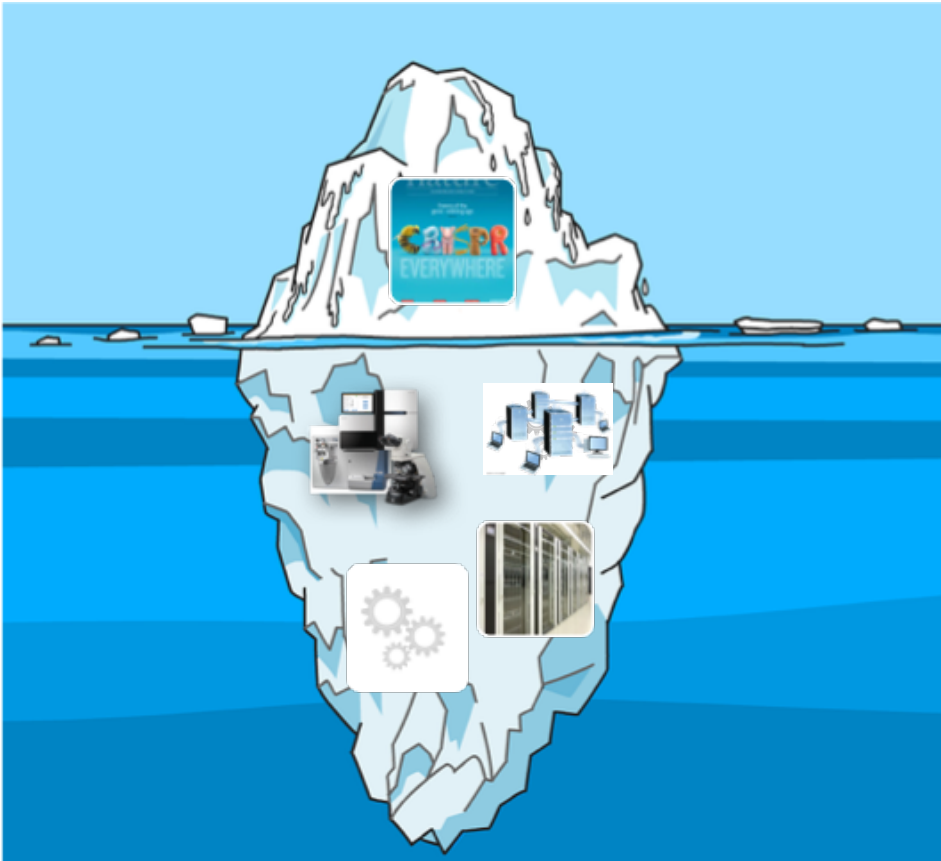
Overview

1. Overview of research data management with openBIS
2. Introduction to basic openBIS concepts
3. Hands-on tutorial:
 1. Registration of samples
 2. Registration of protocols
 3. Recording experiments and uploading data
 4. Data analysis with Jupyter notebooks
 5. Data analysis with MATLAB

Research workflow in experimental & computational labs



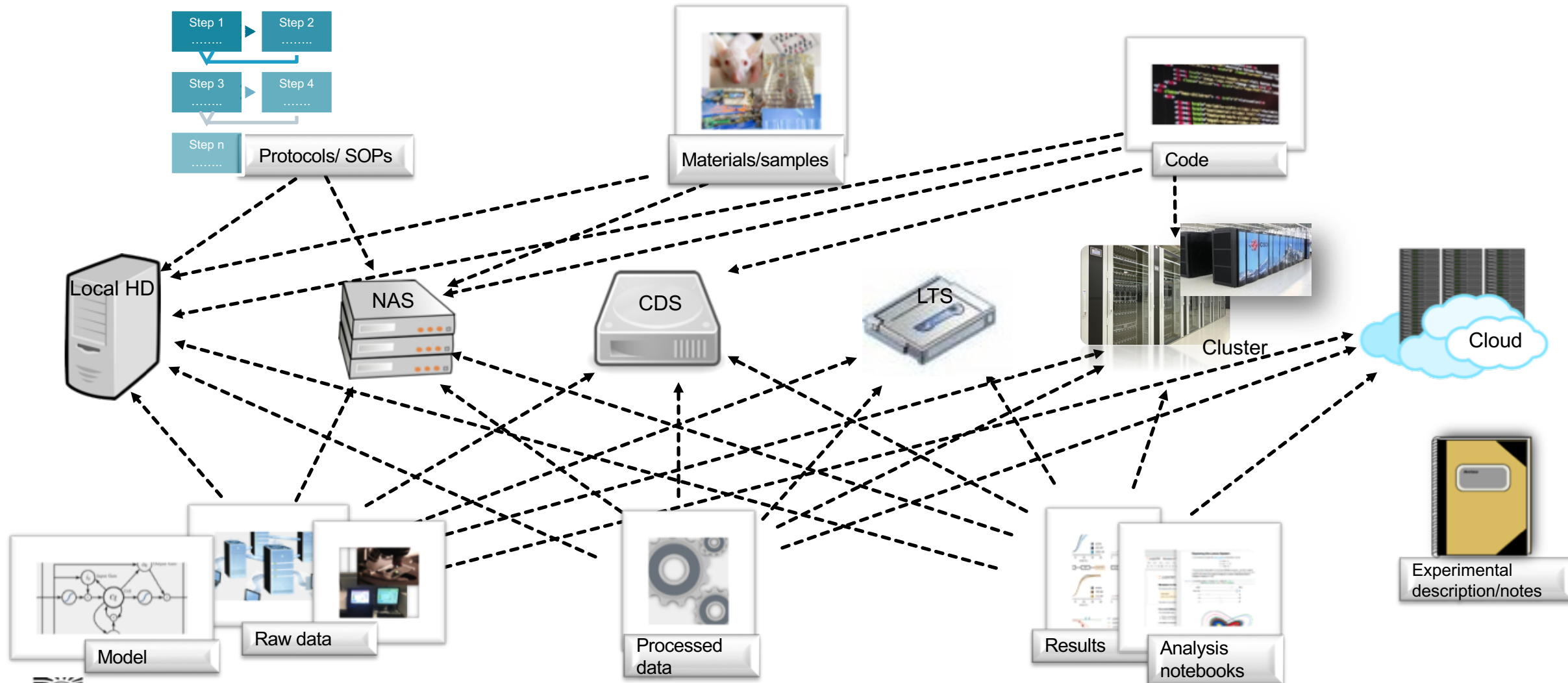
The “Data Iceberg”



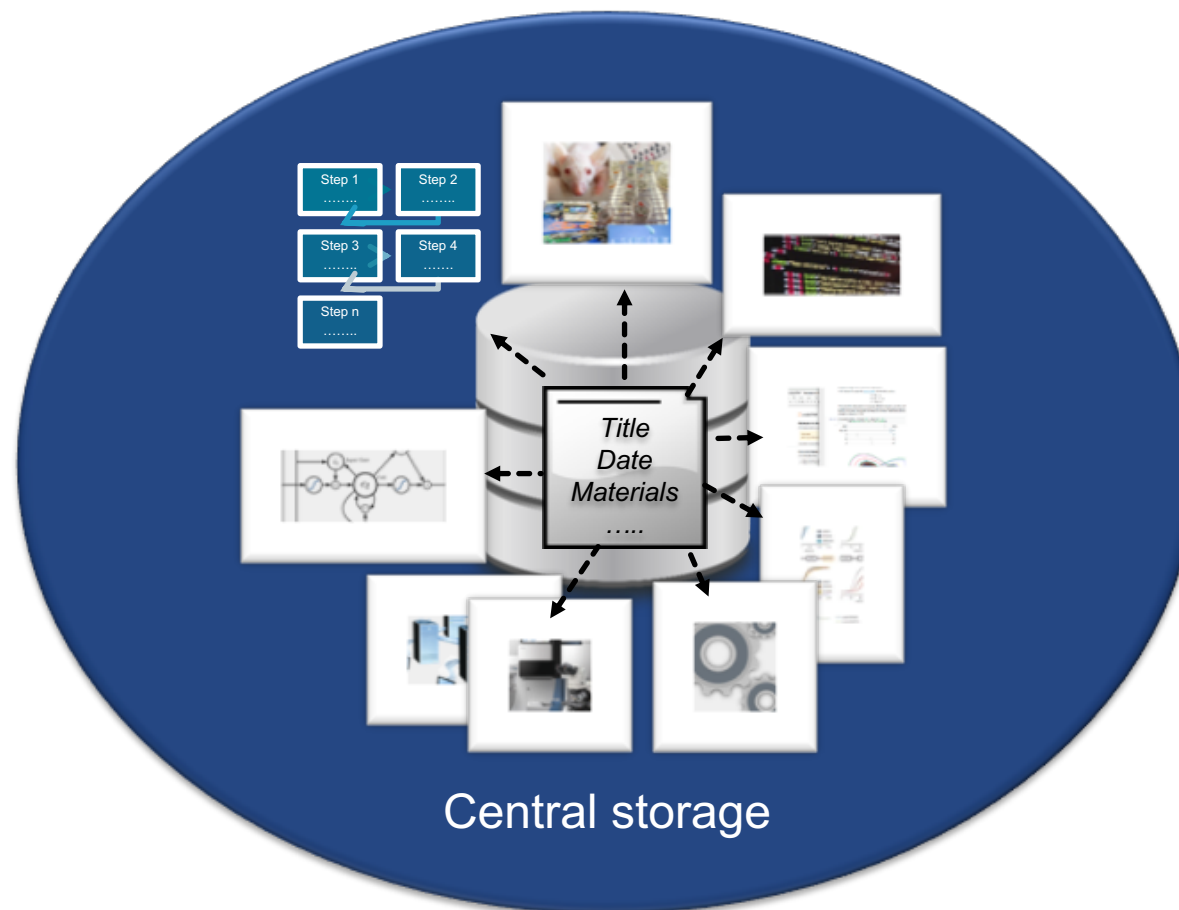
- Funding agencies and journals increasingly demand that data is published according to the **FAIR**¹ data principles (**F**indable, **A**ccessible, **I**nteroperable, **R**eusable).
- Published data is only the “tip of the iceberg”.
- Published data can be FAIR only if **all collected data** that led to the publication is **FAIRly managed from the start**.

1. The FAIR Guiding Principles for scientific data management and stewardship, *Scientific Data*, Issue 3, 2016. 10.1038/sdata.2016.18.

A common scenario @ ETHZ

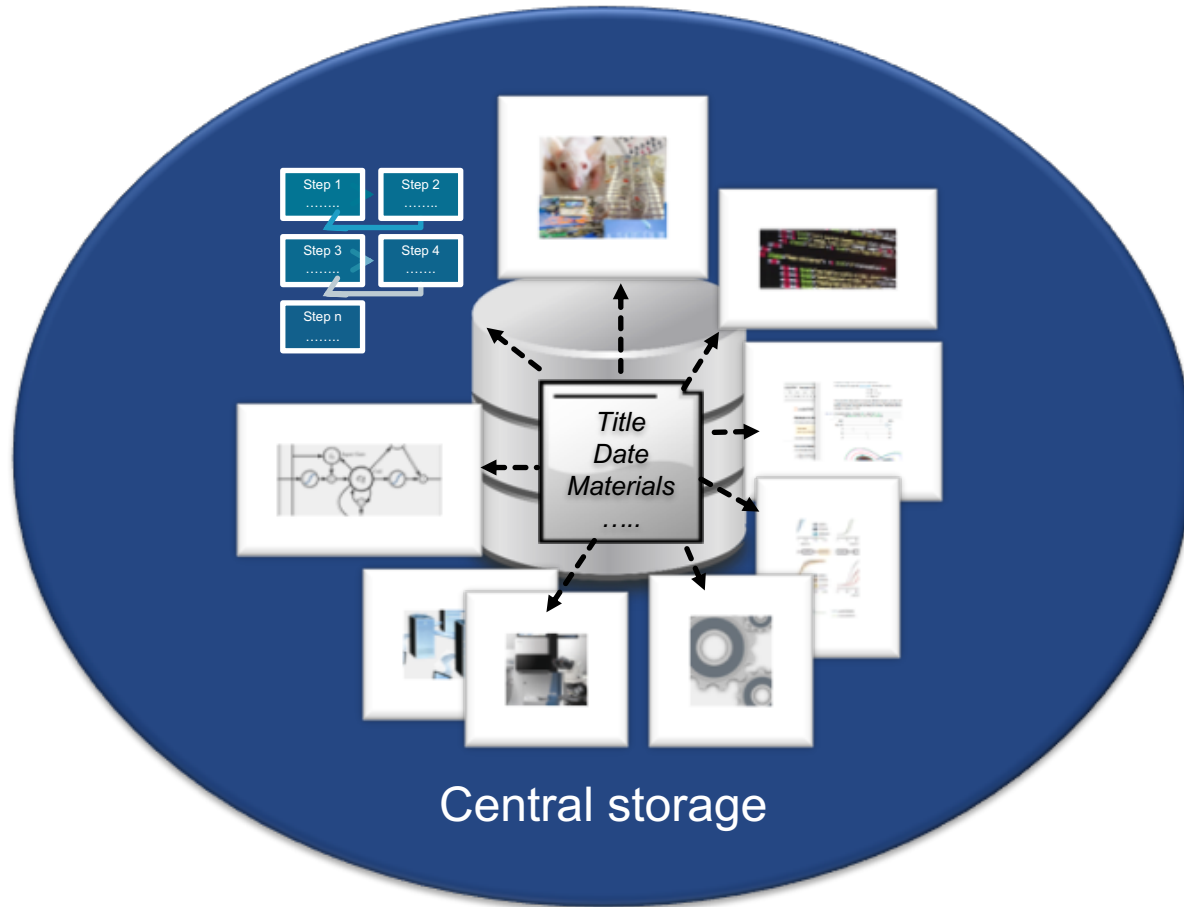


The ideal scenario



A combined ELN/LIMS can provide such solution

The ideal scenario



A combined ELN/LIMS can provide such solution

openBIS-based services at ETHZ

Research Data Hub

openBIS available to any ETH group

- Centrally managed
- Shared resource
- Limited Customization

Departmental Data Hubs

openBIS available to any ETH group of a certain department

- Centrally managed
- Shared resource
- Department customization

Research Data Nodes

openBIS available to single ETH research groups

- Individually managed
- Dedicated resource
- Individual customization

openBIS-based services in Switzerland



University of
Zurich^{UZH}



SWITCHengines

National service for RDM based on openBIS: Cloud-hosted openBIS

- Virtual servers per research group, institute or institution
- Optionally with JupyterHub server for analytics

Self-hosted openBIS

- Support for set up on local IT infrastructure

Training & 'best effort' user support

- Optional: support contract with ETH SIS

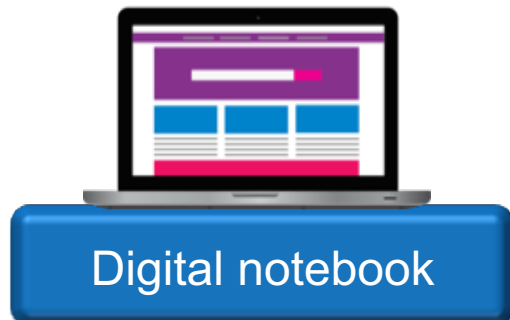
What is openBIS used for?

- openBIS is a software for:
 - ✓ Keeping track of lab materials



- ✓ Keeping track of lab methods

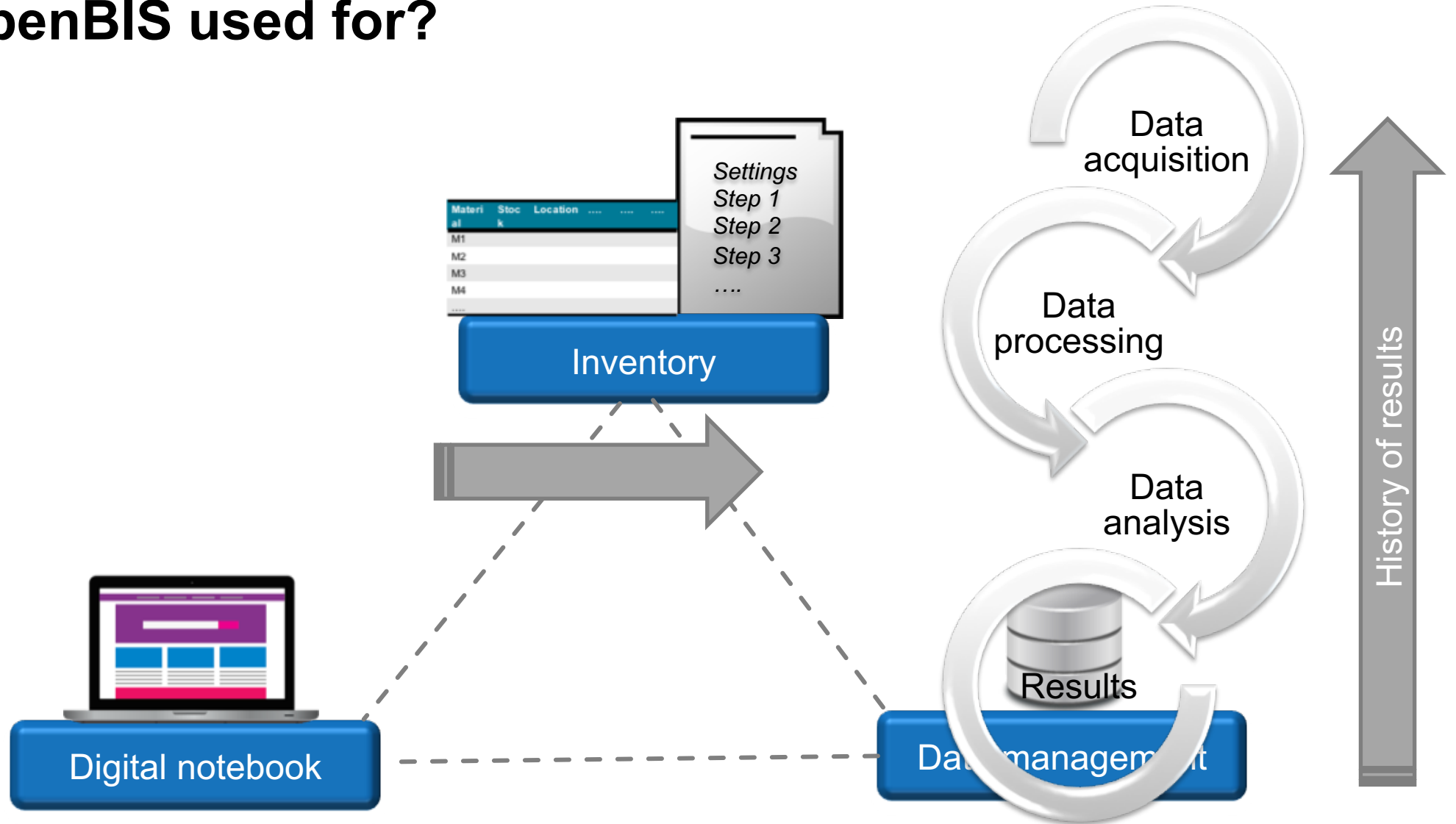
- ✓ Describing experiments



- ✓ Uploading data to experiments

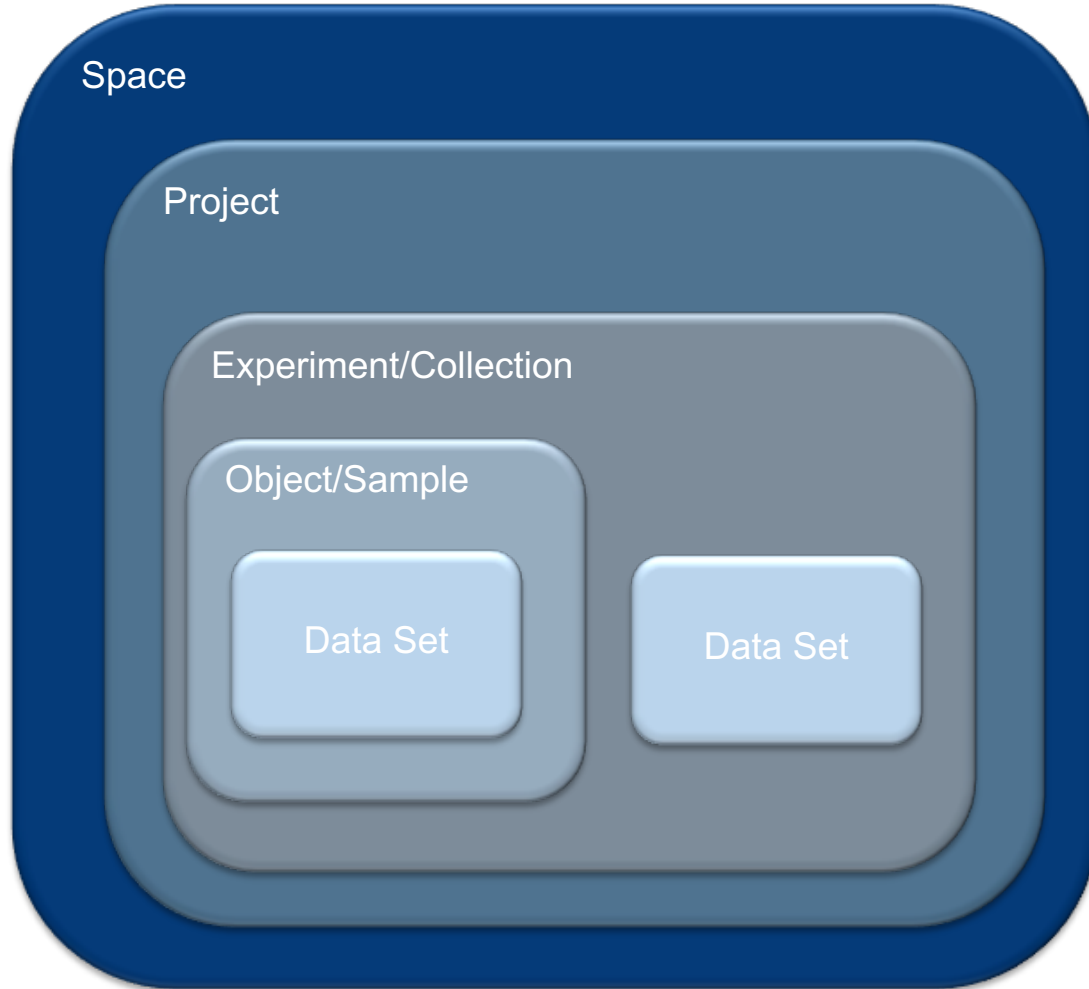


What is openBIS used for?



Basic openBIS concepts

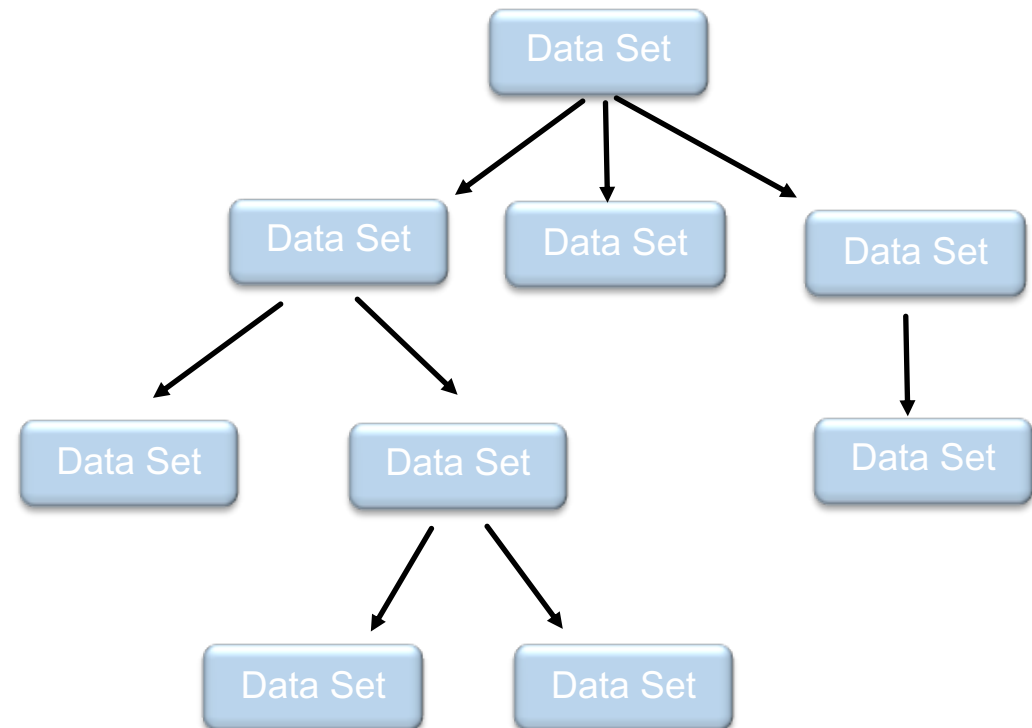
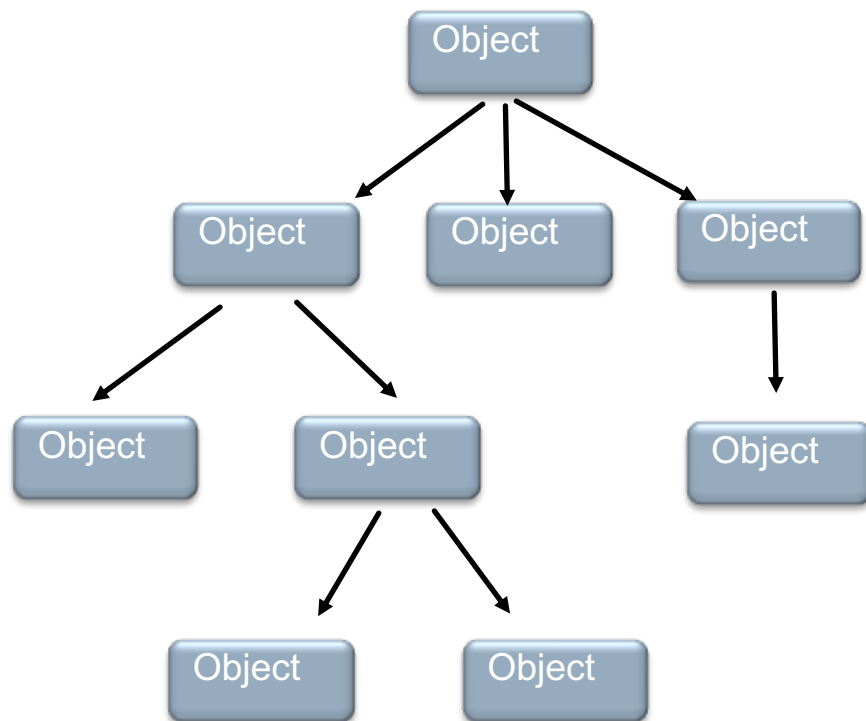
openBIS data structure



1. Folder with only code
2. Folder with code + description
3. Folder with code + user-defined properties. There can be several types of Experiment/Collection, each defined by different properties.
4. Basic entity with code + user-defined properties. There can be several types of Objects/Samples, each defined by different properties.
5. Folder for storing data files with code + user-defined properties. There can be several types of Data sets, each defined by different properties.

Linking objects and datasets

- Objects can be linked to other objects, datasets to other datasets with $N:N$ relationship
- In openBIS terms, these are “parent-child” relationships

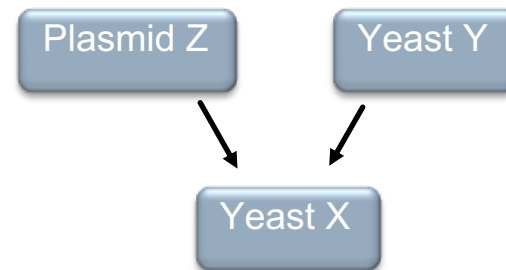


What are “parents” and “children”?

➤ They are a way of connecting entities together.

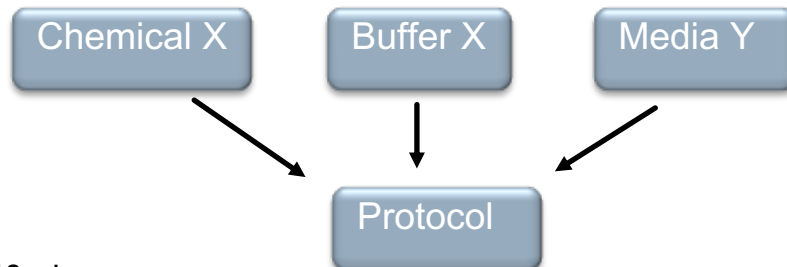
➤ Examples:

1. You make a sample from other samples.



***Yeast X** is made inserting **Plasmid Z** into **Yeast Y**. These are assigned as parents to **Yeast X**.*

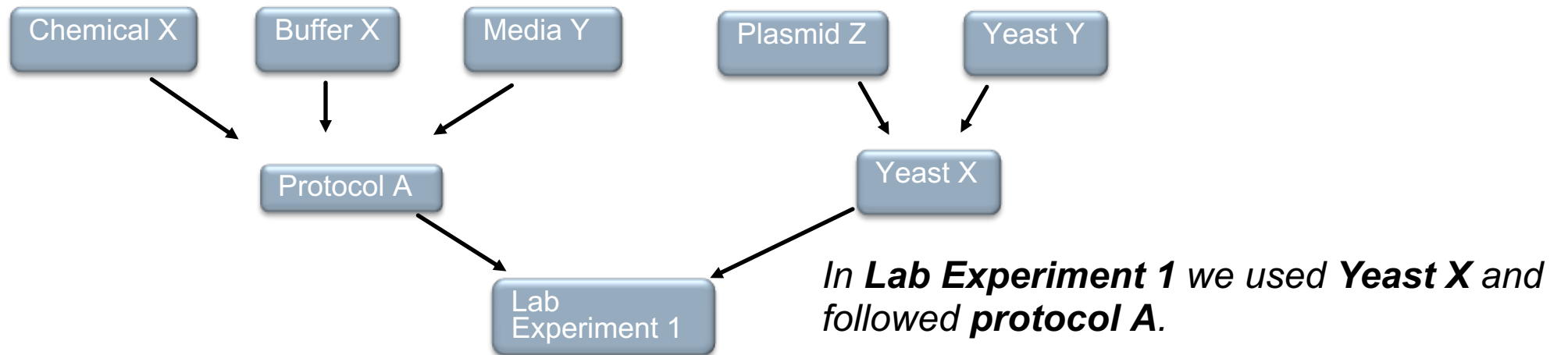
2. You write a protocol, and want to keep track of the samples used.



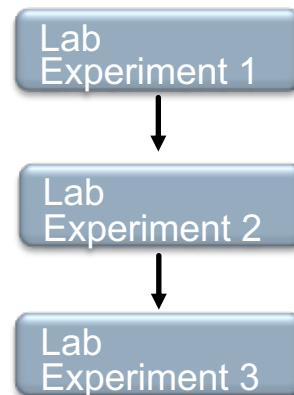
***Chemical X**, **Buffer X** and **Media Y** are needed to perform this protocol. They are parents of this protocol.*

What are “parents” and “children”?

3. You describe an experiment and you want to keep track of the protocol(s) and samples used



4. You make one experiment in several steps and you want to link each step to the previous one



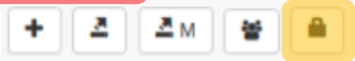
Roles

Role	Capabilities
Observer (Space or Instance)	Read-only access to given spaces or to the whole instance.
Space/Project user	Create + edit Object, Experiment. Edit Project .
Space/Project power user	User rights +create Projects . Delete object, experiment, project, datasets. Add, update vocabulary terms.
Space/Project admin	Power user rights+ list roles; create and delete space roles; edit datasets.
Instance admin	Space admin rights + create types. Has access to everything.

Freezing entities

- It is possible to “freeze” every level of the openBIS hierarchy.

Space: DEFAULT_LAB_NOTEBOOK



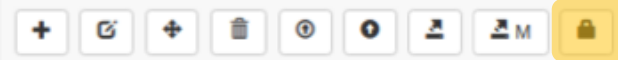
Project: DEMO_PROJECT

/DEFAULT_LAB_NOTEBOOK/DEMO_PROJECT



Experiment: Demo experiment 1

/DEFAULT_LAB_NOTEBOOK/DEMO_PROJECT/DEMO_PROJECT_EXP_1



Object: Step 1

/DEFAULT_LAB_NOTEBOOK/DEMO_PROJECT/DEMO_PROJECT_EXP_1/EXP3



Dataset: test data

/DEFAULT_LAB_NOTEBOOK/DEMO_PROJECT/DEMO_PROJECT_EXP_1/EXP3/20190611123601400-54



Freezing entities

- At every level, everything below is always selected to be frozen. Selection can be modified.

Freeze Entity

Choose the entities to freeze (all by default):

Selected	Type	Permid	Name
<input checked="" type="checkbox"/>	Space	DEFAULT_LAB_NOTEBOOK	DEFAULT_LAB_NOTEBOOK
<input checked="" type="checkbox"/>	Project	20190528221459905-1	DEFAULT_PROJECT
<input checked="" type="checkbox"/>	Project	20190611122038970-49	DEMO_PROJECT
<input checked="" type="checkbox"/>	Experiment/Collection	20190611122056078-50	Demo experiment 1
<input checked="" type="checkbox"/>	Experiment/Collection	20190528221459905-14	Default Experiment
<input checked="" type="checkbox"/>	Object	20190611122145679-52	Step 2
<input checked="" type="checkbox"/>	Object	20190611122213447-53	Step 3
<input checked="" type="checkbox"/>	Object	20190611122127059-51	Step 1
<input checked="" type="checkbox"/>	Object	20190528221828470-42	test
<input checked="" type="checkbox"/>	DataSet	20190611123601400-54	test data

Enter your password to freeze the entities, after they are frozen no more changes will be allowed:

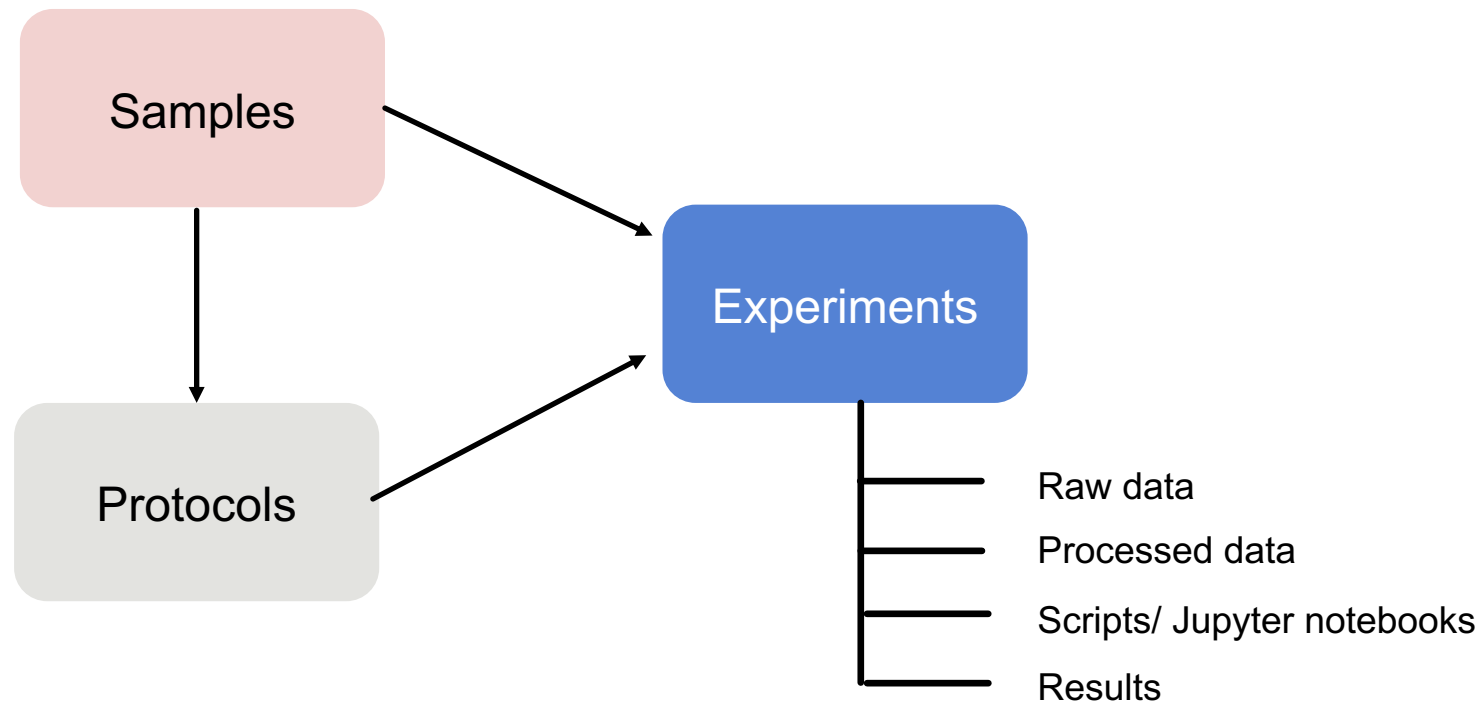
⚠ This operation is irreversible!

Password (*):

How to use the openBIS Inventory & Lab Notebook

Inventory

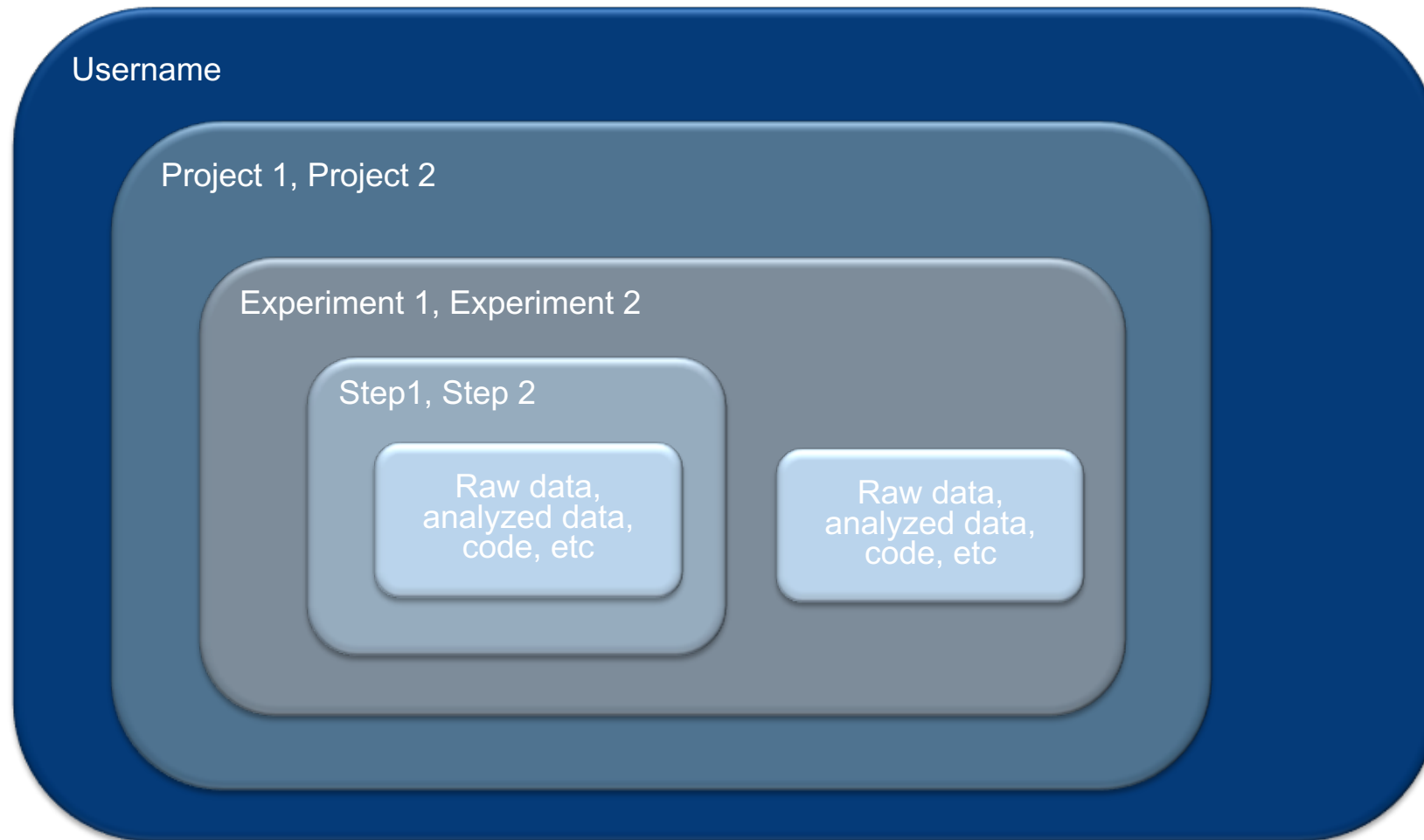
Lab Notebook



How to use the openBIS Lab Notebook

- In the Lab Notebook part of openBIS, usually each user has a **personal Space** where to organize **projects** and **experiments**
- Experiments can be divided in **Experimental Steps**
- **Experimental Steps** can be linked to samples, protocols, other Experimental Steps
- Data (raw, processed, analysed, final results) can be attached to Experiments or Experimental steps in **Datasets**

openBIS Lab notebook



Experiments and Experimental Steps

- An openBIS Experiment is a specific scientific question. The single attempts to answer this question can be modelled as Experimental Steps.
- Example 1:

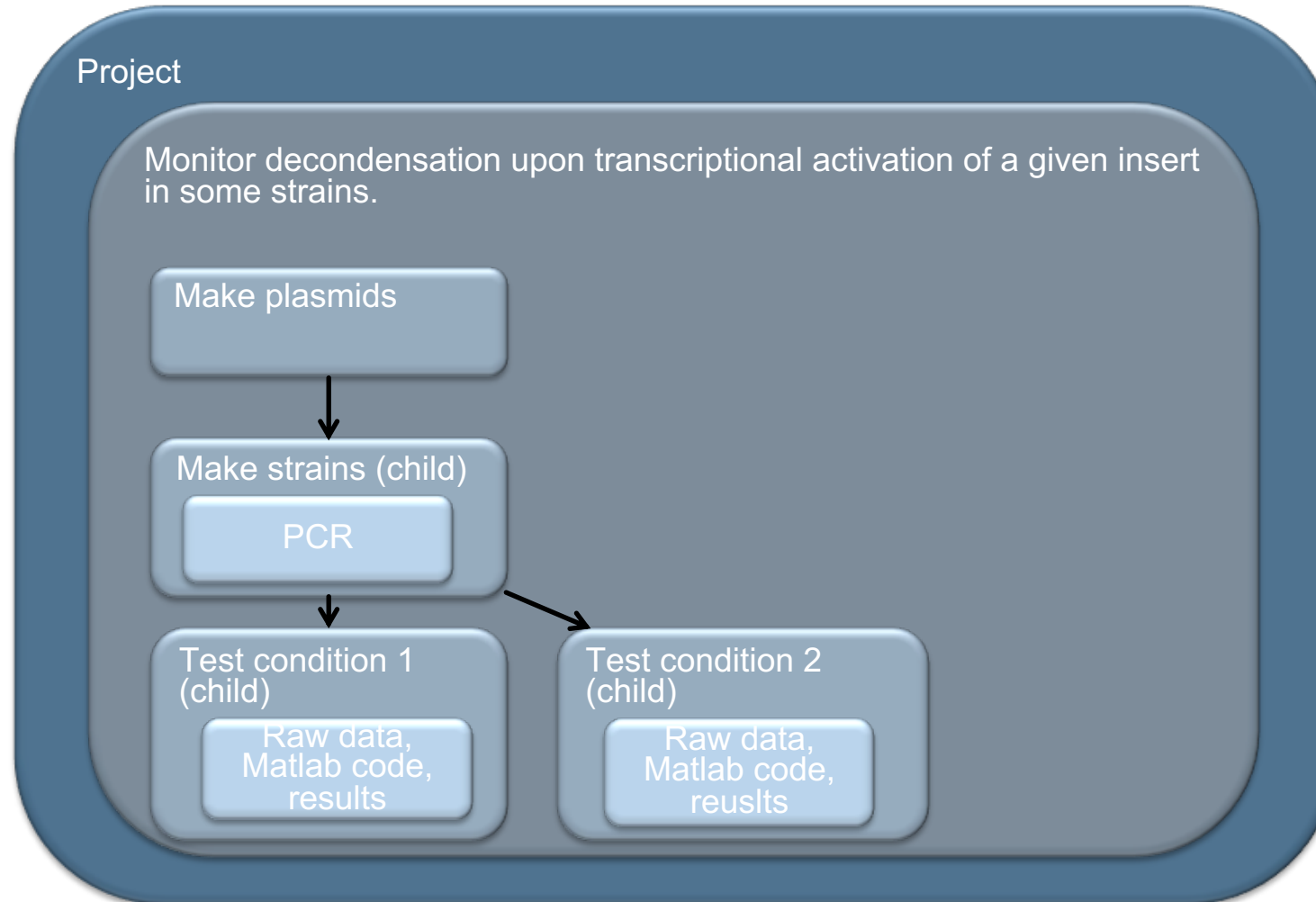
Monitor de-condensation upon transcriptional activation of a given insert in some strains.

This experiment involves 3 different steps:

1. Make some plasmids
2. Make reporter strains for de-condensation using plasmids made before—> PCR results
3. Test strains made before in different conditions -> raw data, MATLAB code

Each step depends on the previous one. It is possible to model this in openBIS by establishing connections between the steps.

openBIS data model for Example 1



Experiments and Experimental Steps

- Example 2:

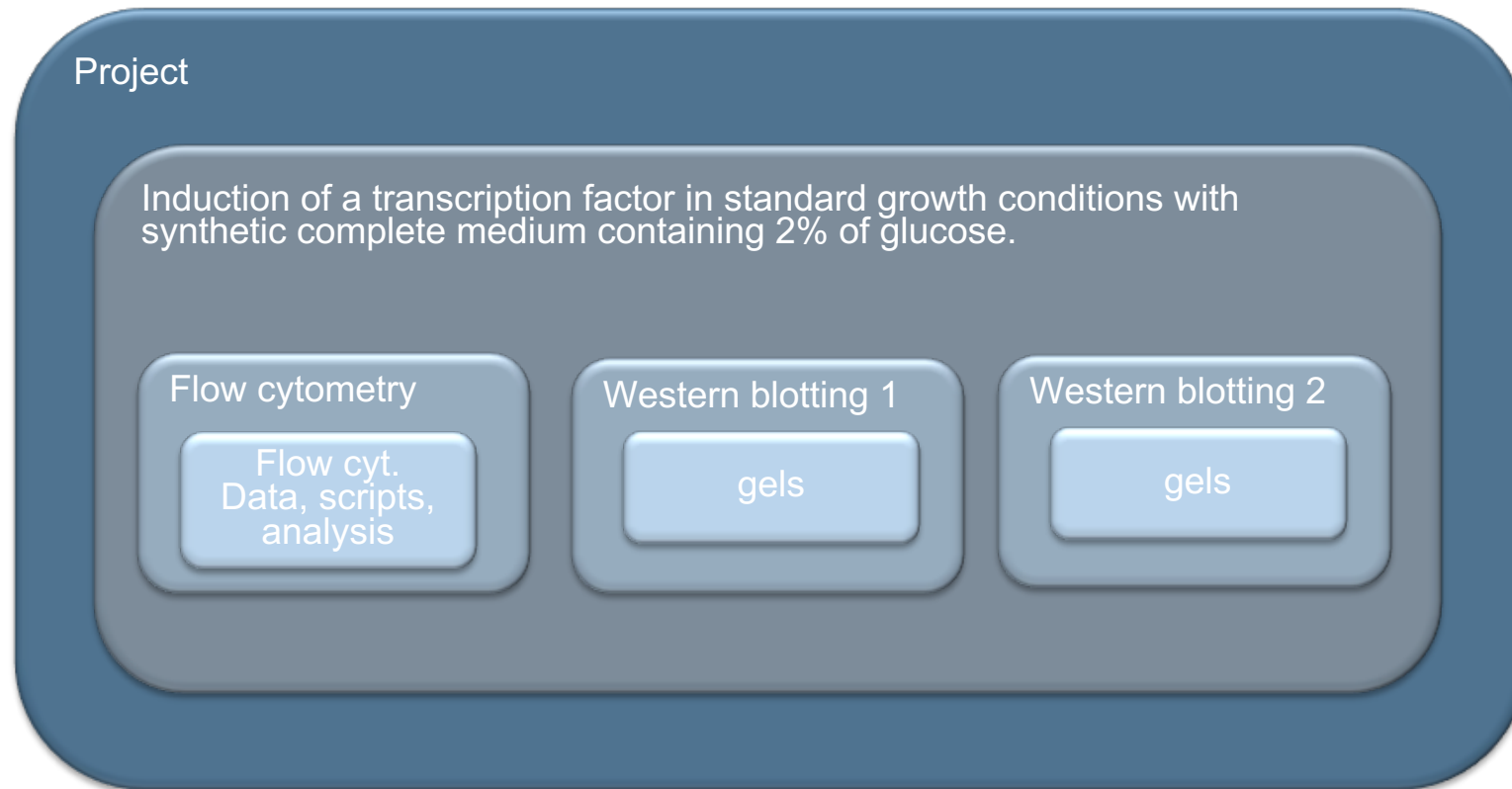
Induction of a transcription factor in standard growth conditions with synthetic complete medium containing 2% of glucose.

This experiment involves 3 different steps:

1. Detection of transcription factor induction by flow cytometry
2. Detection of transcription factor induction by Western blotting
3. Detection of transcription factor induction by Western blotting

Each step is independent of the previous one.

openBIS data model for Example 2



Overview of openBIS tutorial

Use-case example

Experimental yeast biology lab

- Lab that uses fission (*Schizosaccharomyces pombe*) and budding (*Saccharomyces cerevisiae*) yeast, as model systems with the aim to understand how a network performs its function in a cellular setting. They focus on the metabolism and effects on the physiological state of the cell.

Examples of samples used	Examples of exp. techniques used
Chemicals	PCR
Yeasts	Microscopy
Plasmids	Flow cytometry
Oligos	Western blotting
Enzymes	Etc...
Etc..	

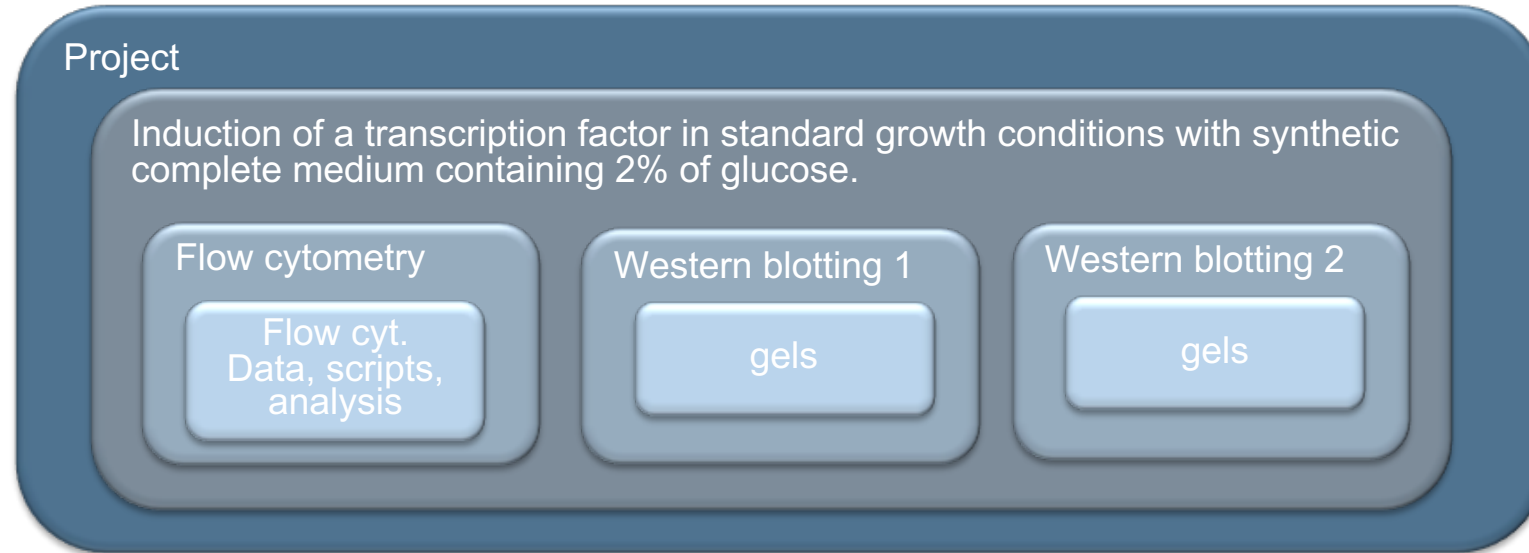
Management of samples and protocols

We will register a few samples and one protocol in the inventory, covering different topics:

1. Single sample registration
2. Batch registration of samples
3. Batch modification of samples
4. How to assign storage positions
5. How to establish relationships between samples
6. How to establish relationships between samples and protocols

Lab notebook

- In this tutorial, we will use Example 2 seen before:



- We will create **1 Project, 1 Experiment and 1 Flow Cytometry Experimental Step** in your personal space.
- We will see how we can **link** samples and protocols stored in the Inventory to the Experimental Step.
- We will **upload data** to the Experimental Step.

Go to tutorial
(p. 8-14)

Data analysis with Jupyter notebooks and MATLAB

Contacts & useful info

Documentation & video tutorials: <https://labnotebook.ch/>

SIS website: <https://sis.id.ethz.ch/>

Twitter: https://twitter.com/ETH_SIS

SIS helpdesk

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