



# openBIS Training

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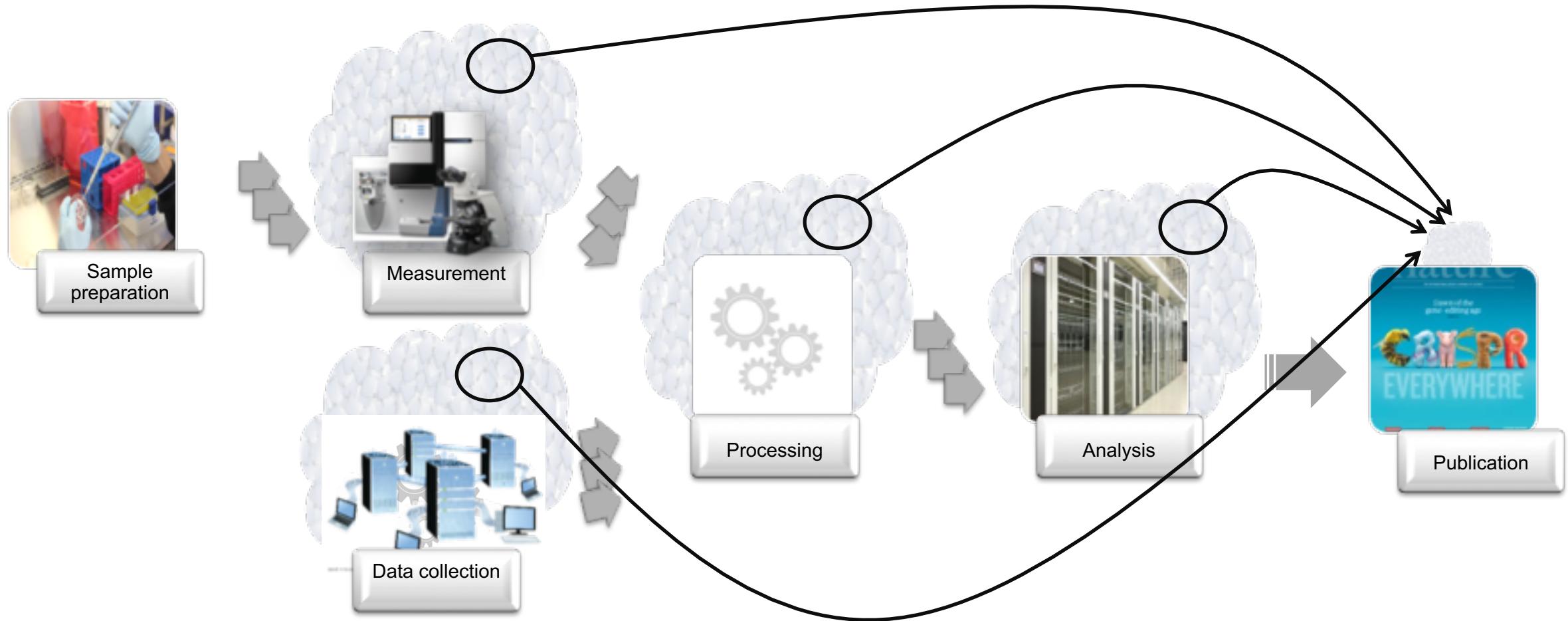
<https://openbis-training.ethz.ch/openbis/webapp/eln-lims/?>



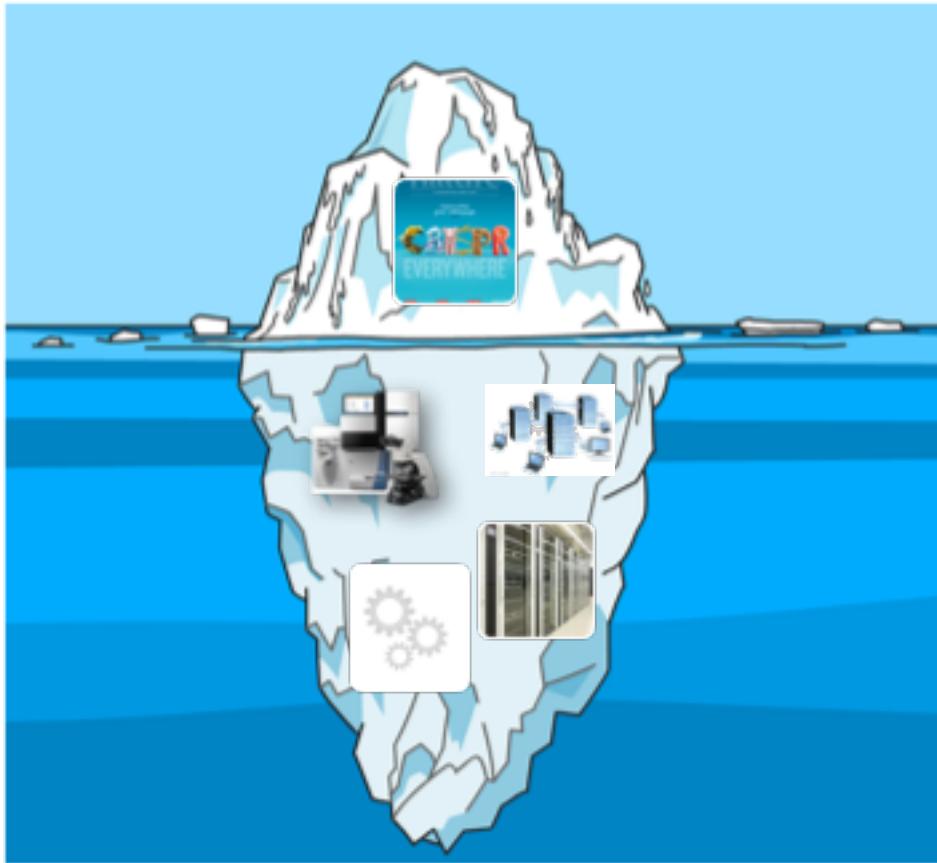
# Overview

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



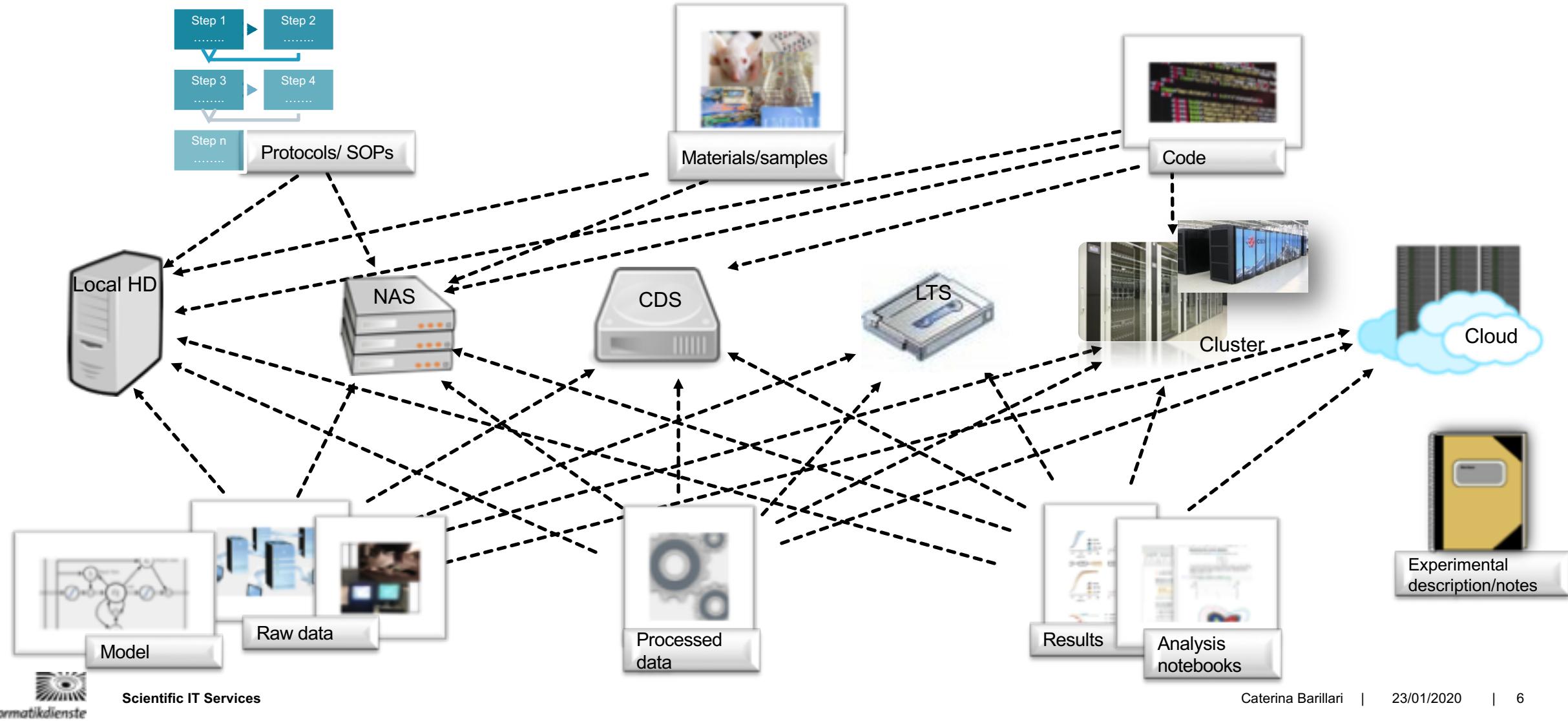
# The “Data Iceberg”



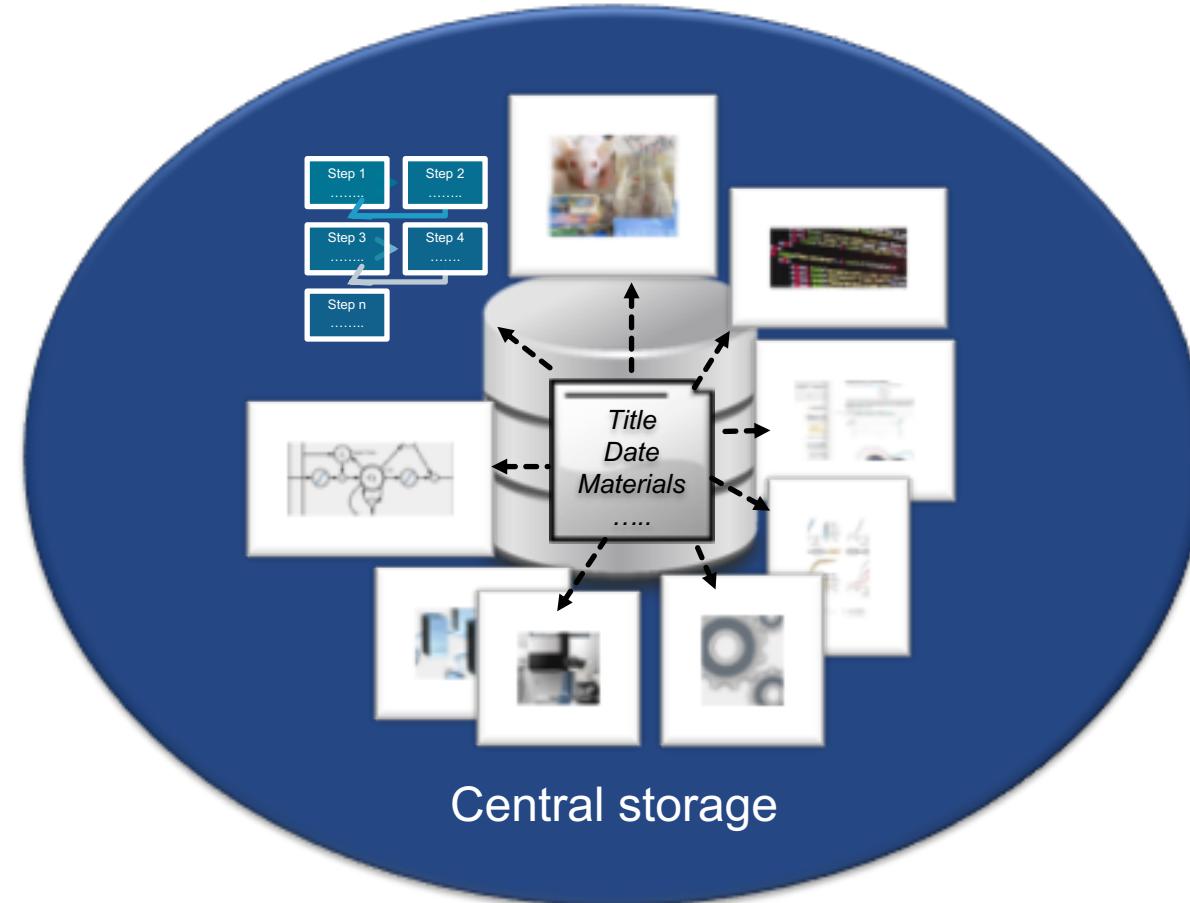
- Funding agencies and journals increasingly demand that data is published according to the **FAIR<sup>1</sup>** data principles (**F**indable, **A**ccessible, **I**nteroperable, **R**eusable).
- Published data is only the “tip of the iceberg”.
- Published data can be FAIR only if **all collected data** 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](https://doi.org/10.1038/sdata.2016.18).

# A common scenario @ ETHZ



# The ideal scenario

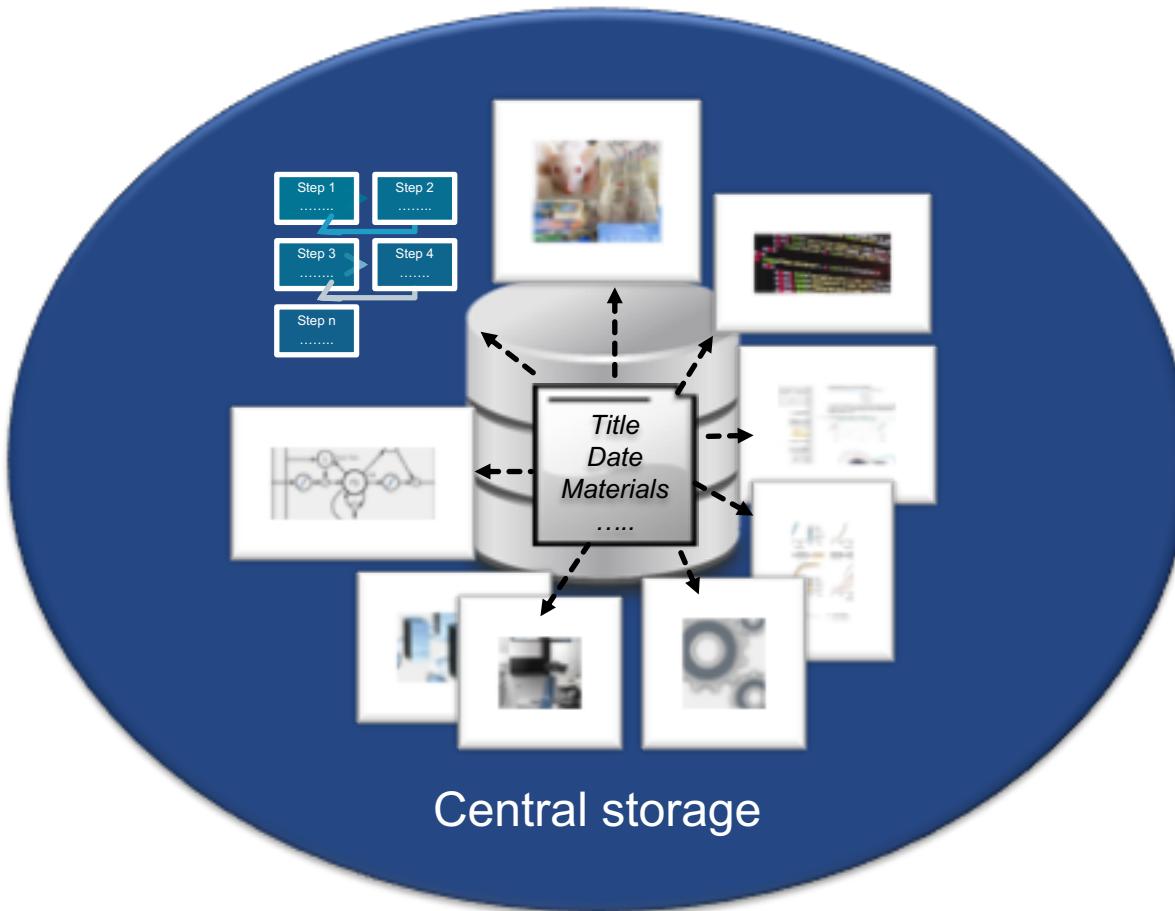


A combined ELN/LIMS can provide such solution

*ELN= Electronic Lab Notebook*

*LIMS= Laboratory Information Management Systems*

# 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 <sup>UZH</sup>



## SWITCHengines



Scientific IT Services

## swissuniversities



## 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

## Current users

- University of Bern, EMPA, University of Zurich, ZHAW

# What is openBIS used for?

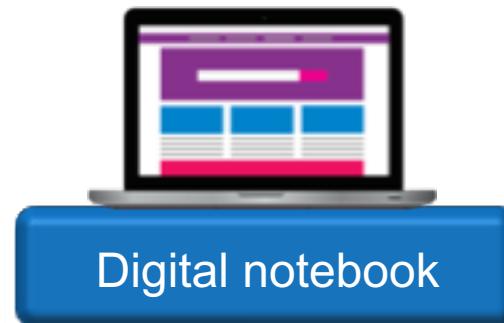
- openBIS is a software for:

✓ Keeping track of lab materials



✓ Keeping track of lab methods

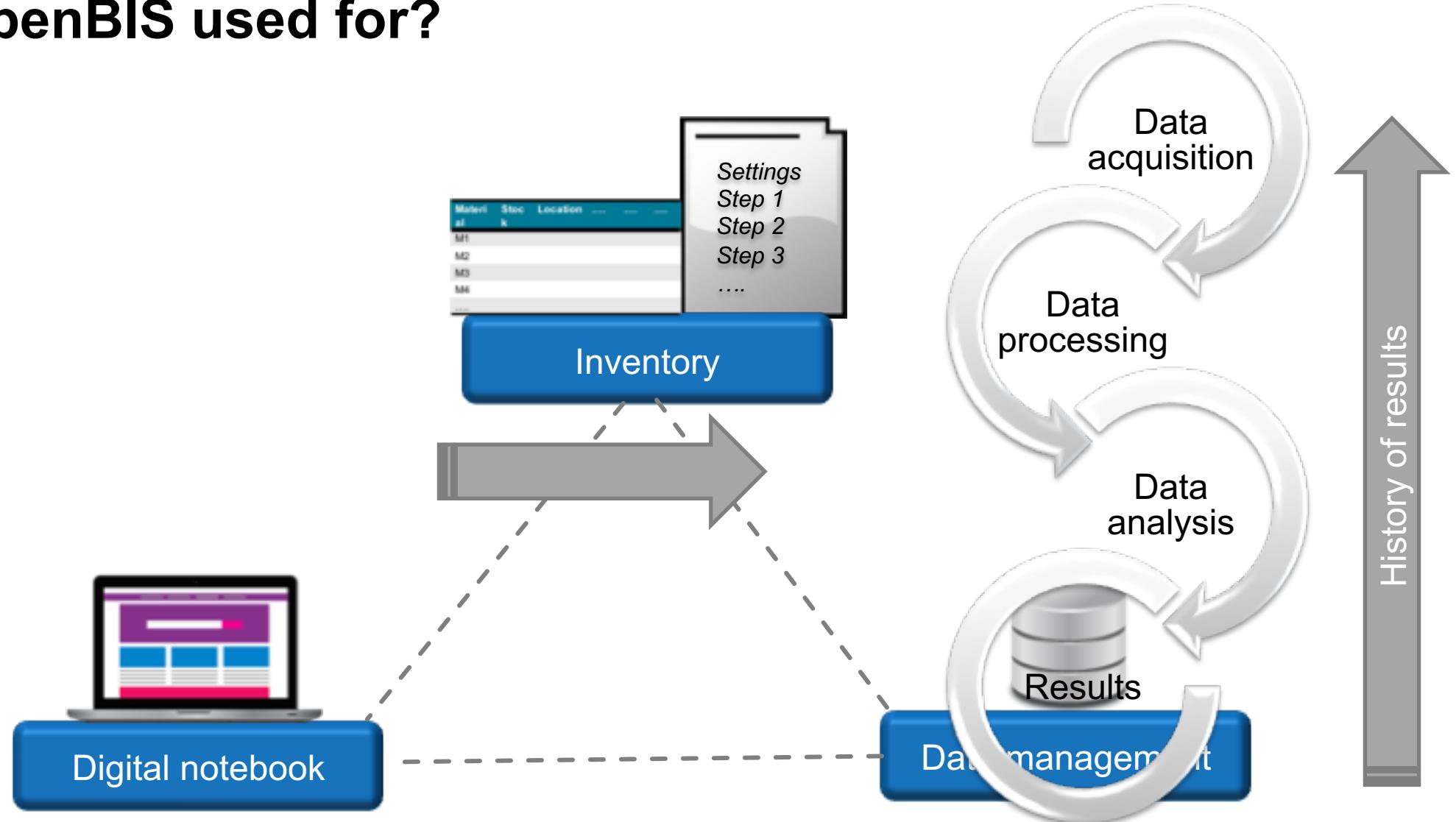
✓ Describing experiments



✓ Uploading data to experiments



# What is openBIS used for?



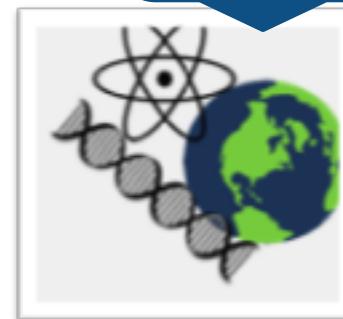
# openBIS facts

- Developed at ETHZ since 2007

Platform for managing scientific information and supporting research data workflows from “bench” to publication



Can be used in most quantitative science fields (e.g. life sciences, physics, env. sciences, etc)

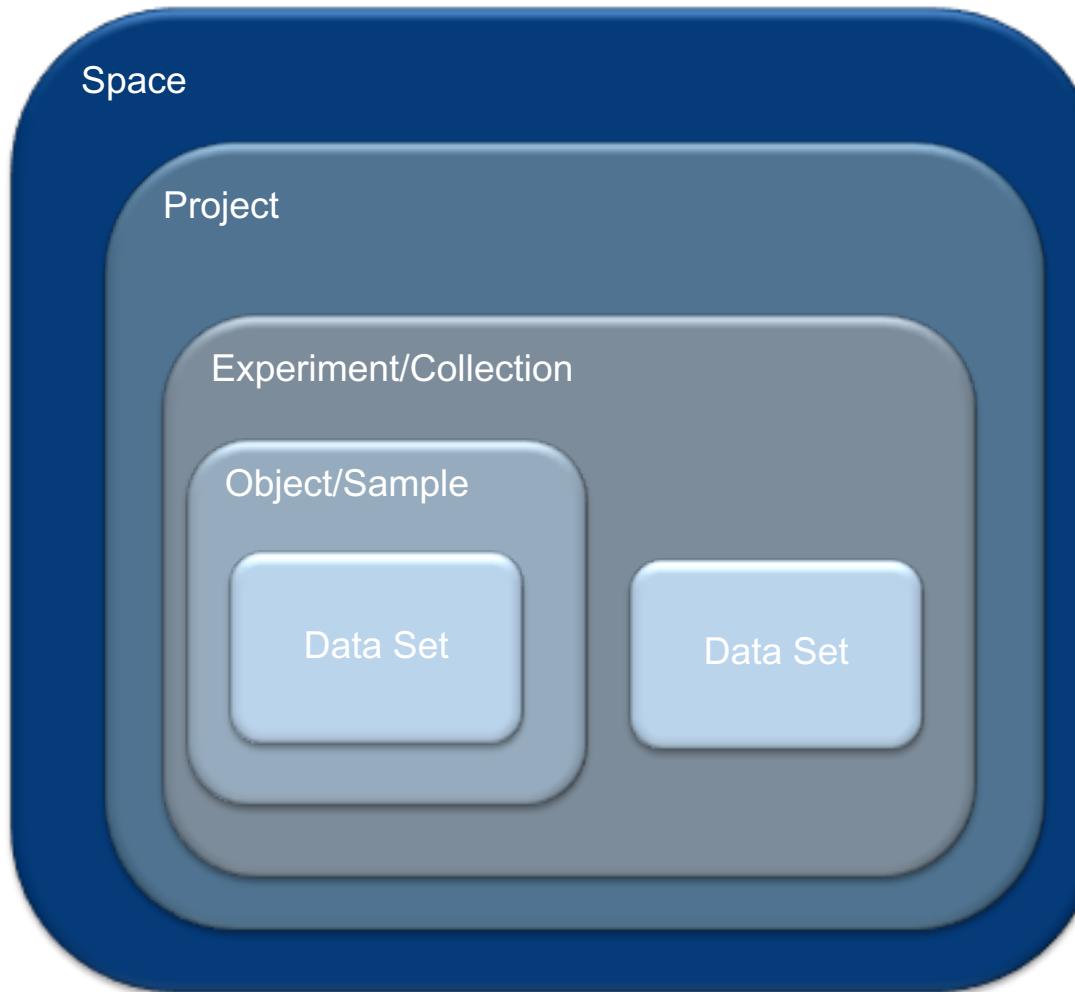


Used by research groups and facilities @ ETH, Swiss & European Universities, a few companies



# Basic openBIS concepts

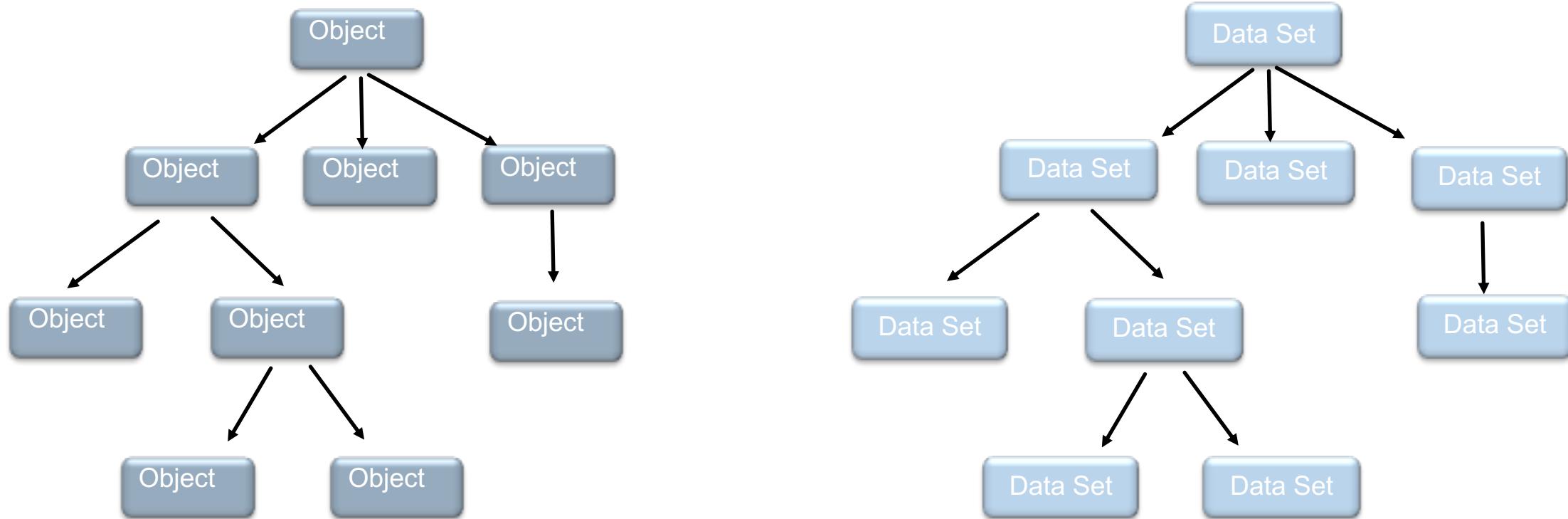
# openBIS data structure



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. Examples: *Antibody, Chemical, Sensor, Chip, General protocol, Experimental Step...*
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

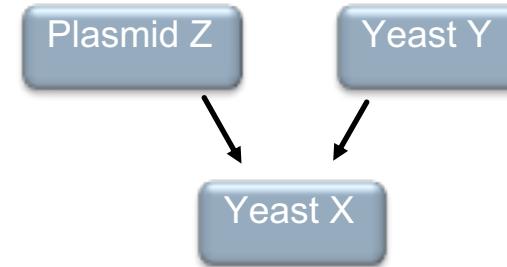
- Objects can be linked to other objects, datasets to other datasets with  $N:N$  relationship
- In openBIS terms, these are “parent-child” relationships



# What are “parents” and “children”?

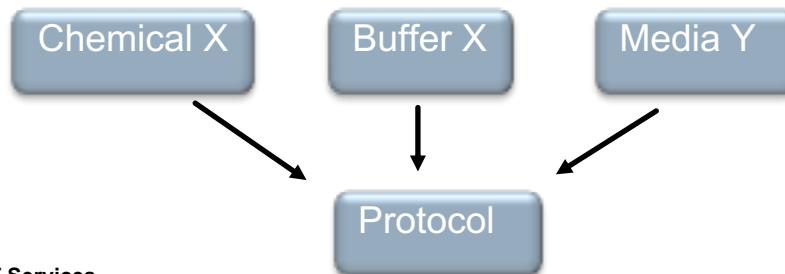
- They are a way of connecting entities together.
- Examples:

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**.

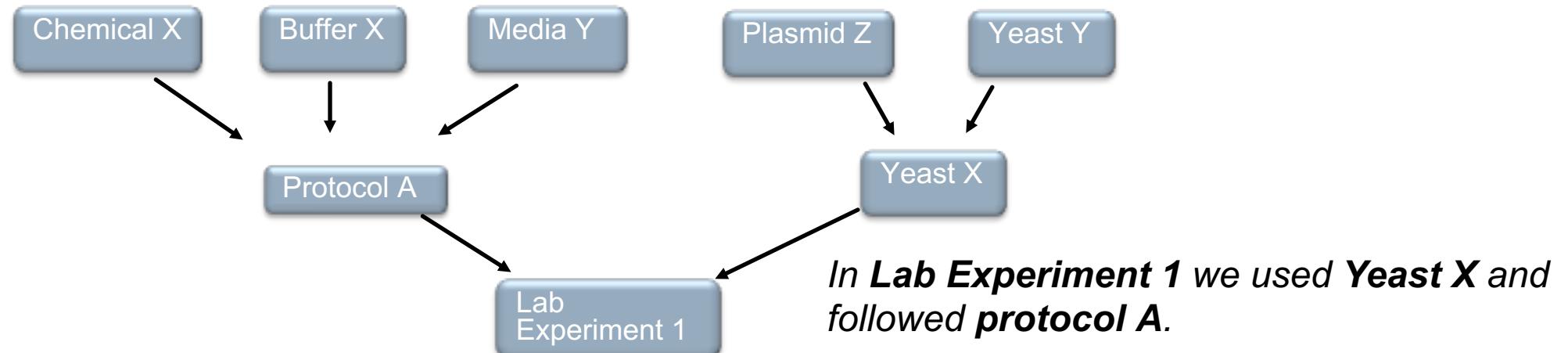
2. You write a protocol, and want to keep track of the samples used.



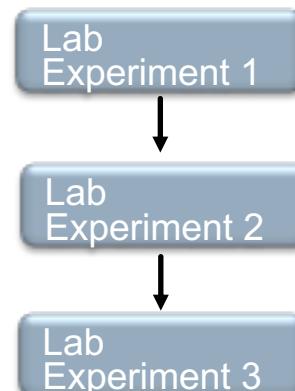
**Chemical X**, **Buffer X** and **Media Y** are needed to perform the steps described in this protocol. They are parents of this protocol.

# 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  
Experiment: Demo experiment 1  
Object: Step 1  
Dataset: test data

The screenshot displays a vertical hierarchy of openBIS entities. Each entity is represented by a card with a red header containing the entity name and a blue URL below it. A yellow box highlights the lock icon (a padlock) in the toolbar of each card. The entities are:

- Space:** DEFAULT\_LAB\_NOTEBOOK
- Project:** DEMO\_PROJECT
- Experiment:** Demo experiment 1
- Object:** Step 1
- Dataset:** test data

The URL for each entity is shown in blue text below the entity name. The toolbar icons include standard file operations (Create, Open, Copy, Paste, Delete, Move, Lock) and additional options like Operations.

# 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 type="checkbox"/>	Project	20190528221459905-1	DEFAULT_PROJECT
<input type="checkbox"/>	Project	20190611122038970-49	DEMO_PROJECT
<input type="checkbox"/>	ExperimentCollection	20190611122056078-50	Demo experiment 1
<input type="checkbox"/>	ExperimentCollection	20190528221459905-14	Default Experiment
<input type="checkbox"/>	Object	20190611122145679-52	Step 2
<input type="checkbox"/>	Object	20190611122213447-53	Step 3
<input type="checkbox"/>	Object	20190611122127059-51	Step 1
<input type="checkbox"/>	Object	20190528221828470-42	test
<input 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 (\*):



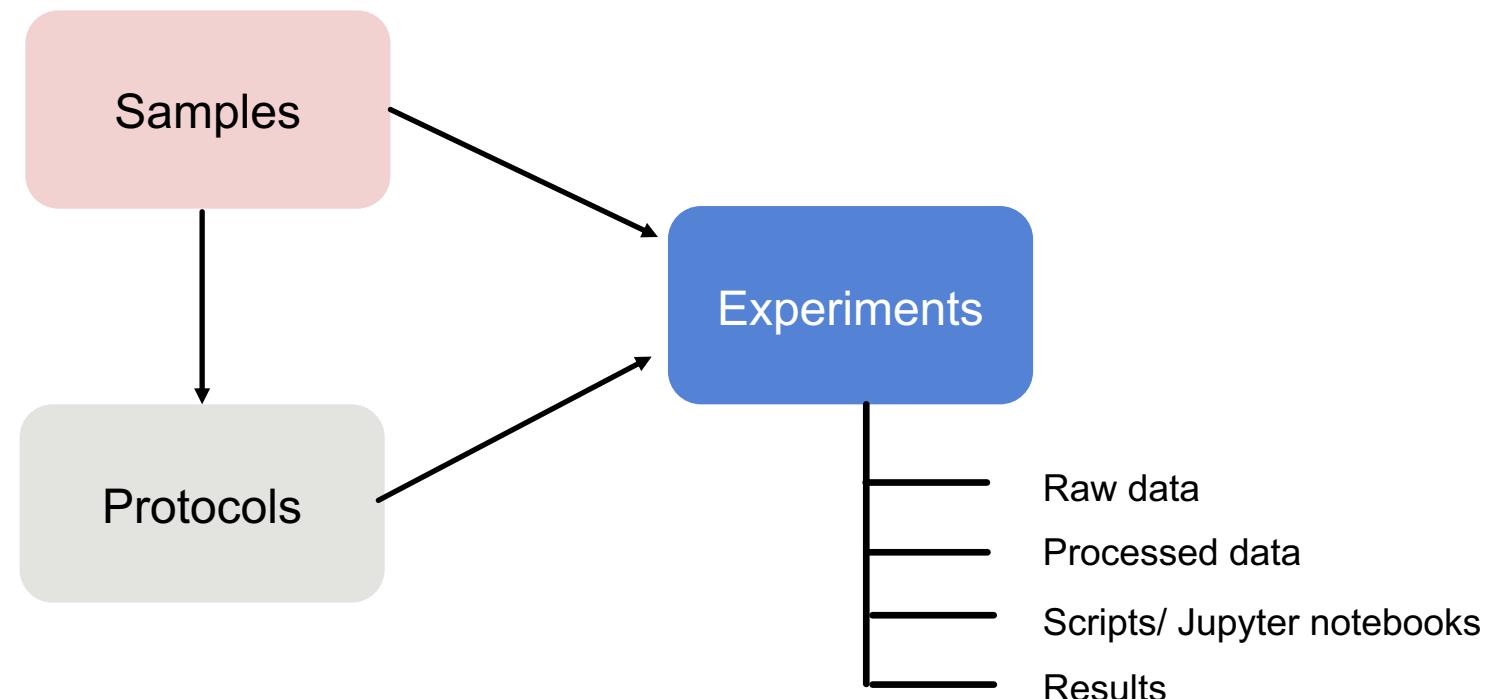
# How to use the openBIS Inventory & Lab Notebook

## Inventory

*Shared by all lab members.*

## Lab Notebook

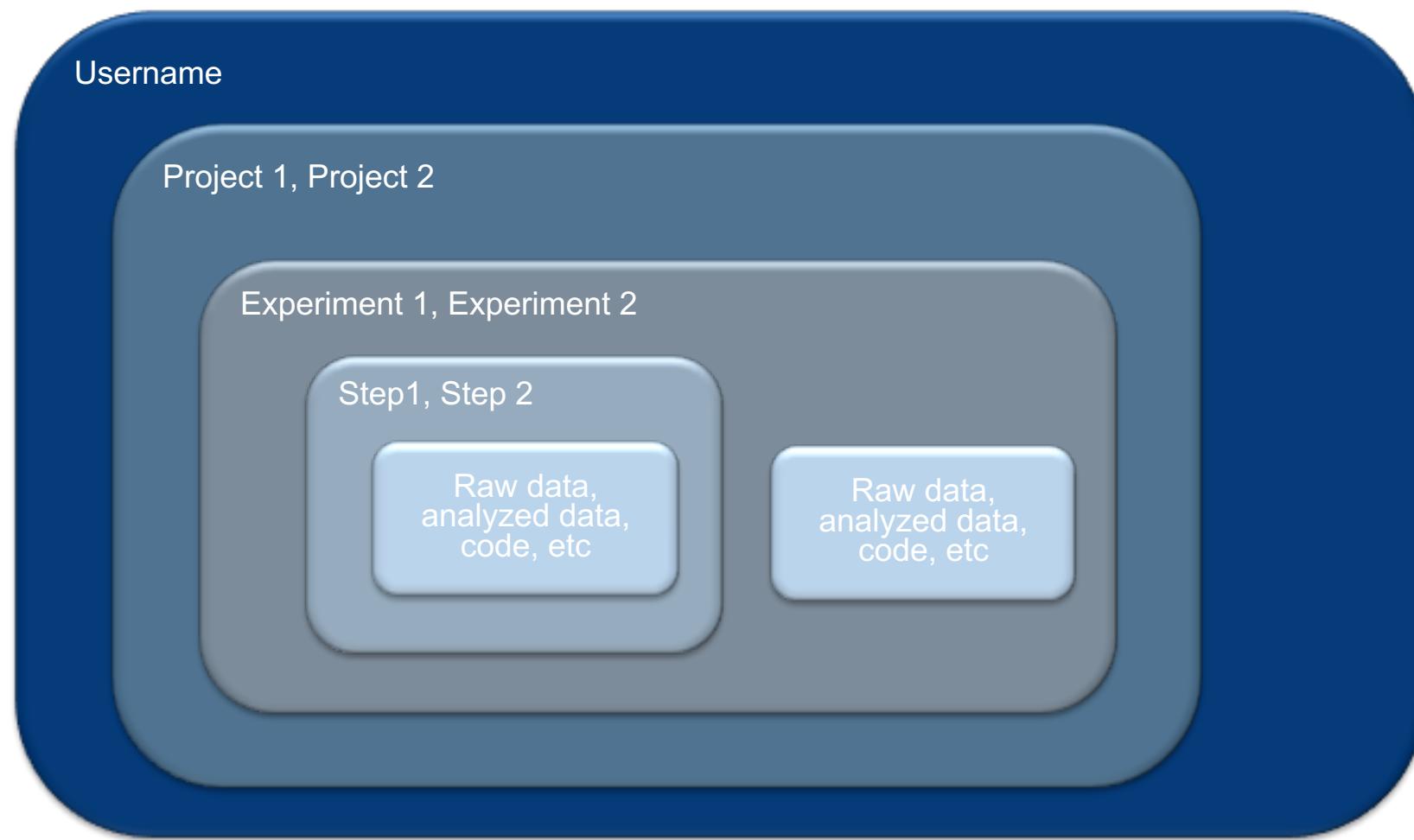
*Personal space. Can be shared.*



# Organization of openBIS Lab Notebook

- In the Lab Notebook part of openBIS, usually each user has a **personal Space** where to organize **Projects** and **Experiments**
- An openBIS **Experiment** is a specific scientific question. The single attempts to answer this question can be modelled as **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**

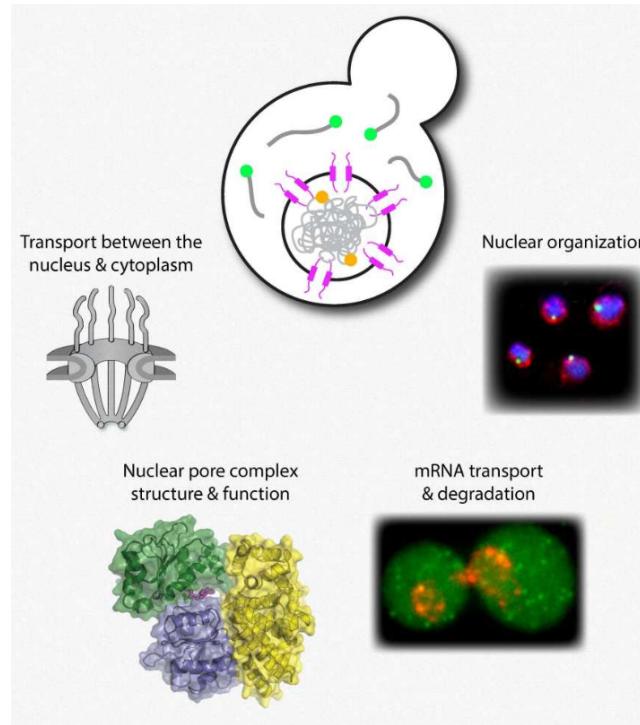
# openBIS Lab notebook





## Example use-cases

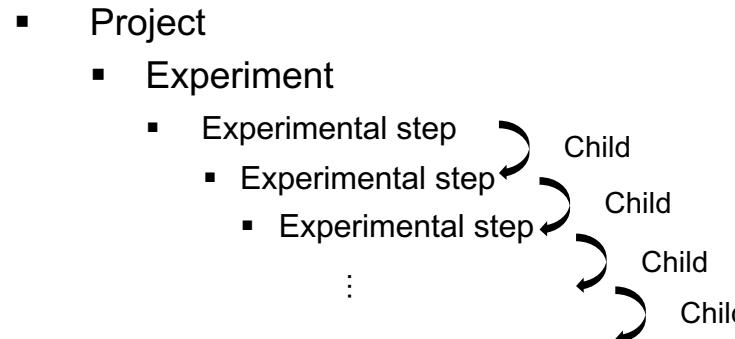
# 1. Cellular dynamics lab @ETHZ (prof. K. Weis)



- **Light microscopy:** Single particle tracking, single molecule live cell microscopy, FRAP, FCS
- **RNA biology:** qPCR, next generation sequencing, nanopore sequencing
- **Protein biochemistry:** *in vitro* liquid-liquid phase separation, mass spectrometry
- **Electron microscopy:** Cryo-electron tomography, FIB-SEM

# openBIS use in Weis lab

- Introduced in 2016. Mandatory for all group members since 2017.
- Inventory used for samples (imported from pre-existing db) and protocols
- Parent-child relationships used:
  - reagents used to create a new one → parents
  - reagents or protocols used during an experiment → parents
  - reagents generated as a result of an experiment → children



- + Lab Notebook
- Inventory
- Materials
- + Cell Lines
- + Plasmids

Object: 181029 colony PCR tetrades Mex67 fusion 1  
 /EDULTZ/MISCELLANEOUS/MISCELLANEOUS\_MEX67\_CARINA/SUBEXP\_

General

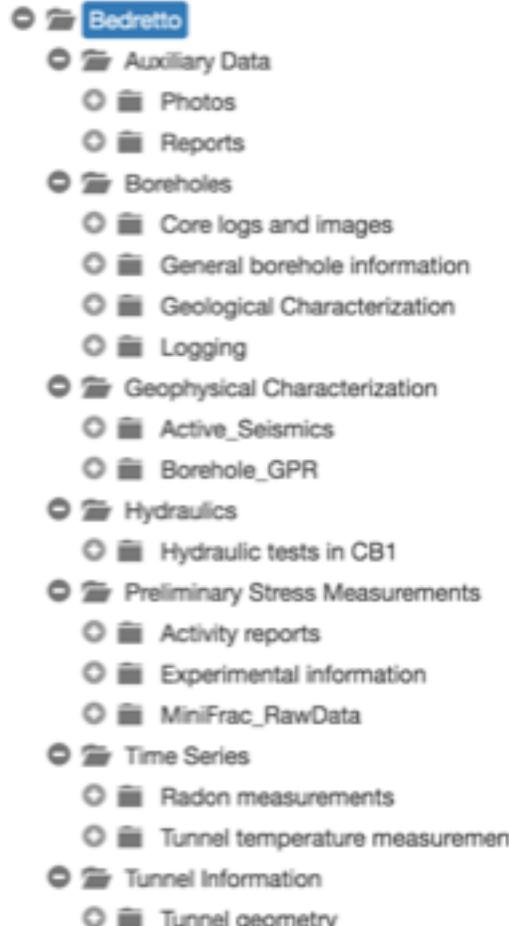
Name: 181029 colony PCR tetrades Mex67 fusion 1  
 Experiment Status: Finished good  
 Experimental goals: find spore clones that have genotype Δmex67 Nup-Mex67  
 Experimental results: good clones:  
 Nup100-Mex67: spores 5D, 6B  
 Nup159-Mex67: spores 9B, 9C, 16C

Parents

Identifier	Code	Type	Name	Notes
/EDULTZ/EXP1137	EXP1137	EXPERIMENTAL_STEP	Mex67 fusion to Nups	

Select files to upload

## 2. Bedretto project @ETHZ

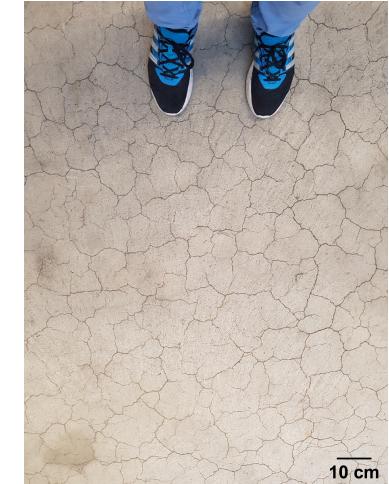


- The Swiss Energy Strategy 2050 aims at increasing the share of renewable energies by 2050. The goal of the Bedretto project is to study techniques and procedures for a safe, efficient, and sustainable use of geothermal heat => Heat captured underground can be re-used to electricity and heat production
- Several boreholes have been drilled in the Bedretto tunnel (connecting Ticino with the Furka tunnel)
- Sensors are placed in boreholes and data collected from these sensors are stored in openBIS
- Lab notebook organized by project, rather than by user
- Currently inventory is not used, only lab notebook + data management
- Data stored in openBIS is analyzed with Python via pyBIS

<http://www.bedrettolab.ethz.ch/home/>

# 3. Concrete/Construction Chemistry Laboratory @Empa

- Studies on concrete properties, e.g. measurements of shrinkage
- Shrinkage := (relative) length change ( $\frac{\Delta L}{L}$ )
- Total shrinkage := autogeneous shrinkage + drying shrinkage
- 1 datum set of (time-lapse) measured variables on 1 type of specimens prepared according to the same mix design

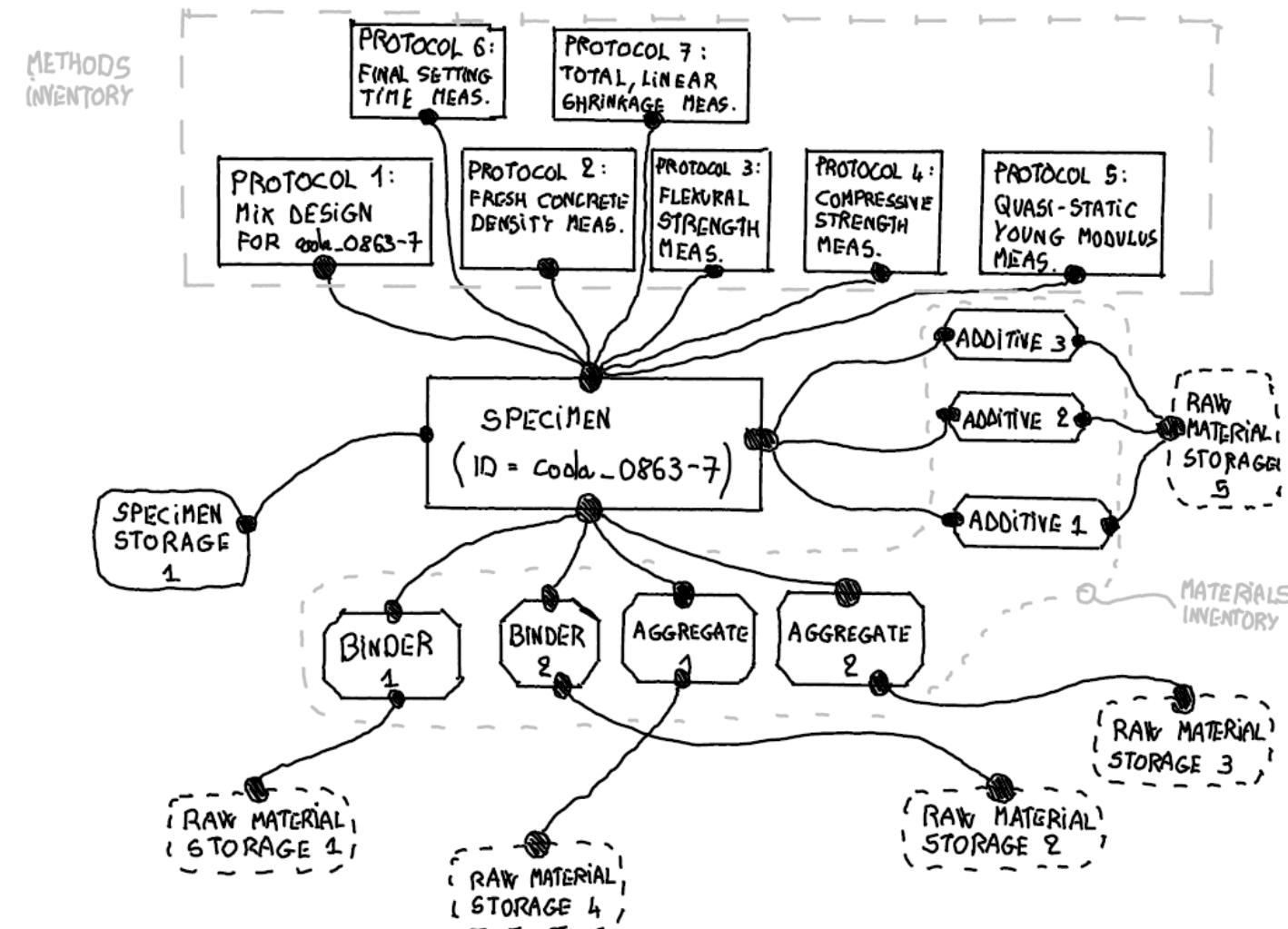


An example of drying shrinkage cracks in a concrete pavement at <undisclosed>.

Photo by Nik Toropovs (Empa).



# Mapping of workflow to openBIS



**One project (= OpenBIS project)**

Experiment: 30/70+G  
/TON/CODA/CODA\_0863

General info

Name:  
30/70+G

Default object type:  
CODA\_0863\_40

Objects

Identifier	Code	Type	Operations
/TON/CODA/S1	S1	CODA_0863_40	Operations
/TON/CODA/S2	S2	CODA_0863_40	Operations

Identification Info

Type: COLLECTION  
Project: /TON/CODA  
Code: CODA\_0863  
Registrar: ton  
Registration Date: 2020-01-21 14:49:09  
Modifier: ton  
Modification Date: 2020-01-21 14:59:33

**One set of measurements (= OpenBIS collection of objects of a given type): data from time-lapse measurements of a given type on distinct specimens cast with the same mix design**

**One specimen, two time points (= 2 instances of an object of a given type)**

**Collections of raw materials for the mixing, one collection for each raw material type**

**Collection of protocols/ways of measuring shrinkage**

**Collection of mix designs used to cast specimens in a specific project**

# 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
<i>Chemicals</i>	<i>PCR</i>
<i>Yeast</i>	<i>Microscopy</i>
<i>Plasmids</i>	<i>Flow cytometry</i>
<i>Oligos</i>	<i>Western blotting</i>
<i>Enzymes</i>	<i>Etc...</i>
<i>Etc..</i>	

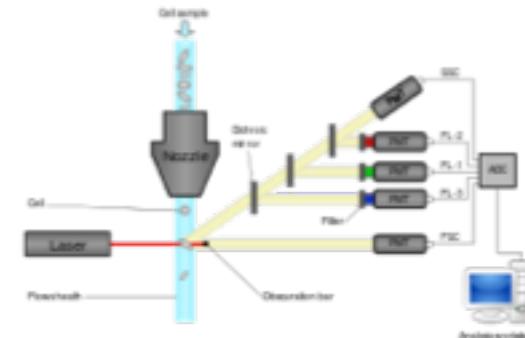
# Use-case example

- **Inducible, tightly regulated and growth condition-independent transcription factor in *Saccharomyces cerevisiae*, Nucleic Acids Research, 2014, 42(17).**
- Paper describes the construction of a transcription activator to control gene expression in yeasts in different growth conditions without toxic side effects. The activity of this transcription factor is regulated by the hormone beta-estradiol.
- They made different variants of their construct and monitored activity by **flow cytometry** and **western blotting**. They then selected one of these variants and evaluated induction in different growth conditions by flow cytometry and western blotting.

# Experimental techniques

## Flow cytometry

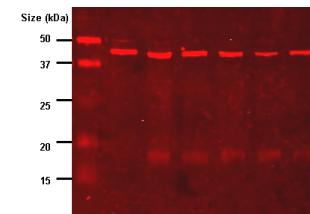
Flow cytometry is a technique used to measure physical and chemical characteristics of a population of cells. A sample with cells is suspended in a fluid and injected in the flow cytometer. Cells flow one at a time through a laser beam and the scattered light is characteristic to the cells and their components.



Source: [https://en.wikipedia.org/wiki/Flow\\_cytometry](https://en.wikipedia.org/wiki/Flow_cytometry)

## Western blotting

Technique used to detect single proteins in samples.



Source: [https://en.wikipedia.org/wiki/Western\\_blot](https://en.wikipedia.org/wiki/Western_blot)

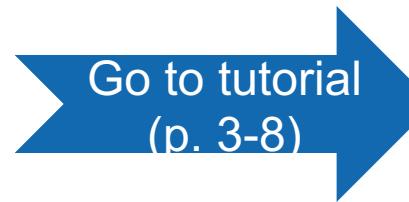
# Tutorial overview

- We will focus on the flow cytometry experiment done to monitor the activity of the transcription factor.
- For this experiment we use a few samples stored in the **Materials Inventory** (*plasmid, yeast, chemical, buffer, media*) and we follow a protocol stored in the **Methods Inventory** (flow cytometry protocol).
- We will start by building the **Inventory** part and we will then move to the **ELN** and see how we can link different parts of the system.

# Management of samples and protocols

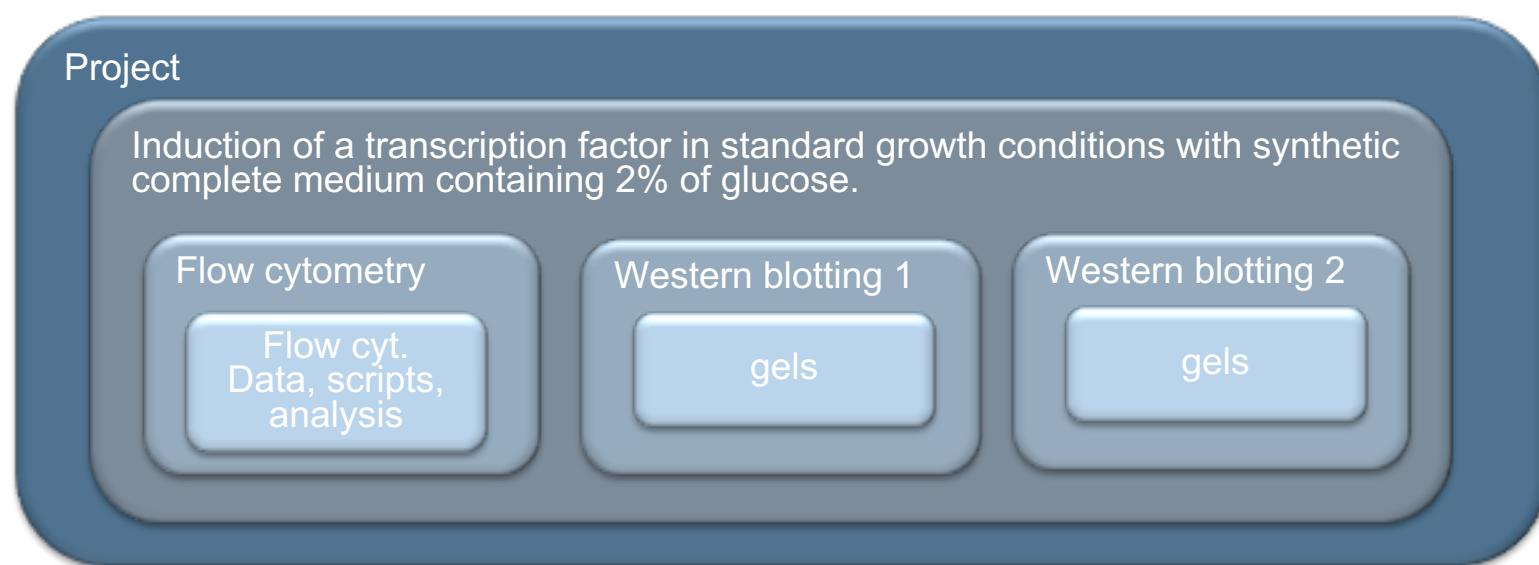
We will register a few samples and one protocol in the inventory, covering different topics:

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 register a standard lab protocol
7. How to establish relationships between samples and protocols



Go to tutorial  
(p. 3-8)

# Lab notebook



- 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. 9-15)

# Data analysis with Jupyter notebooks and MATLAB

Henry Lütcke

# Contacts & useful info

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

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

**Twitter:** [https://twitter.com/ETH\\_SIS](https://twitter.com/ETH_SIS)

**SIS helpdesk**

[sis.helpdesk@ethz.ch](mailto:sis.helpdesk@ethz.ch)

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