



openBIS & ETH RDH Training

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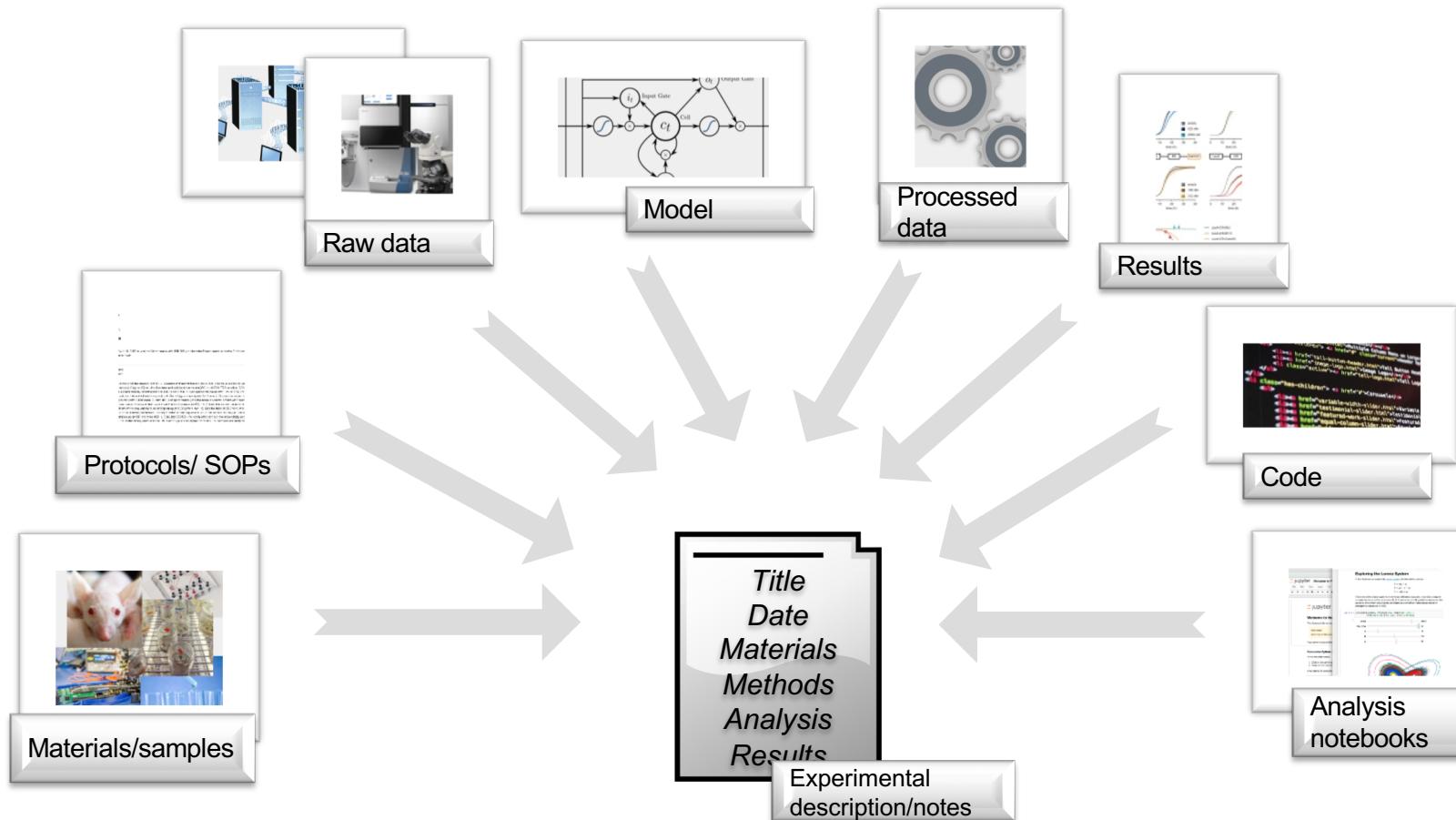
ETH Zurich, 13.05.2019

Overview

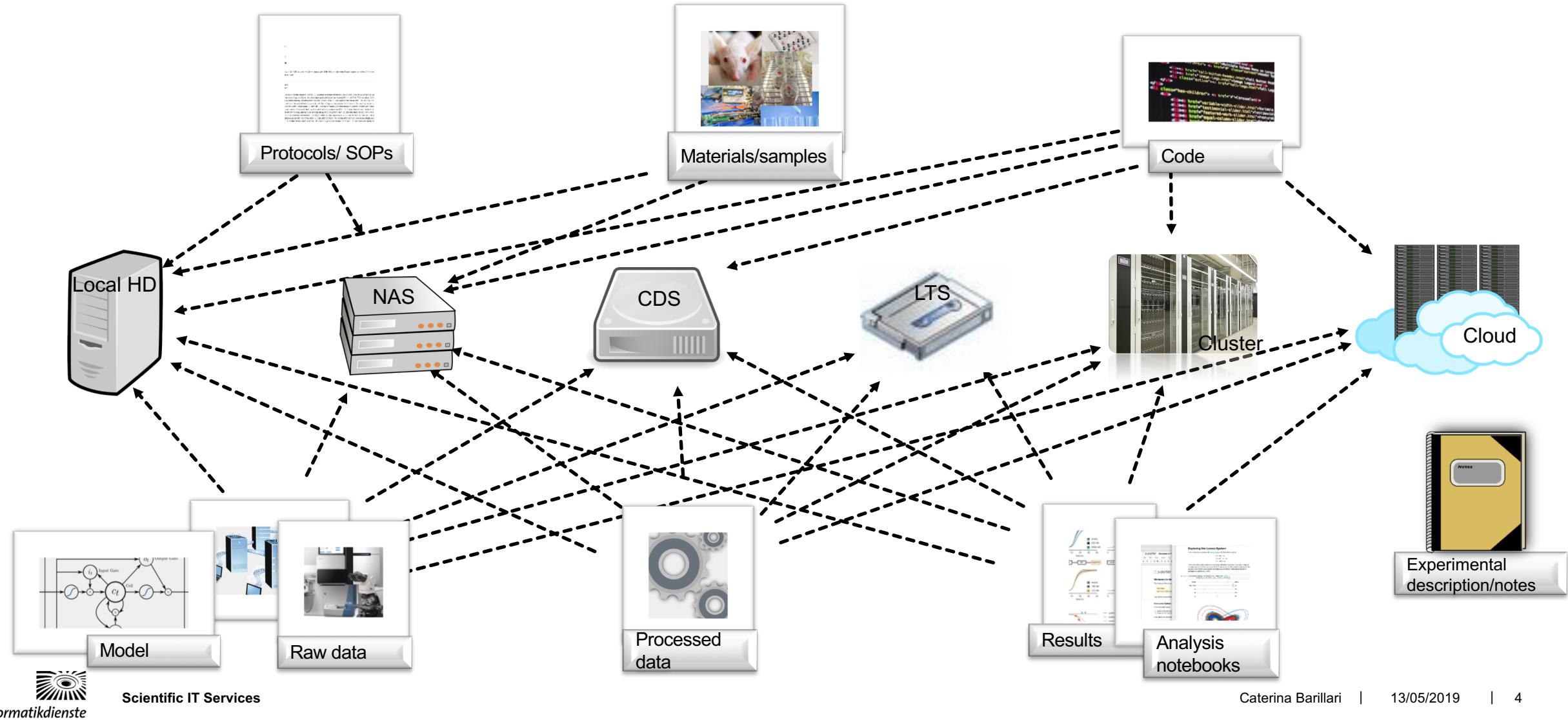
1. Overview of research data management with openBIS & ETH RDH
2. Introduction to basic openBIS concepts
3. Customization of inventory
4. Registration of samples
5. Registration of protocols
6. Recording experiments and uploading data
7. Data analysis with Jupyter notebooks
8. Data analysis with MATLAB

What does it take to manage research data?

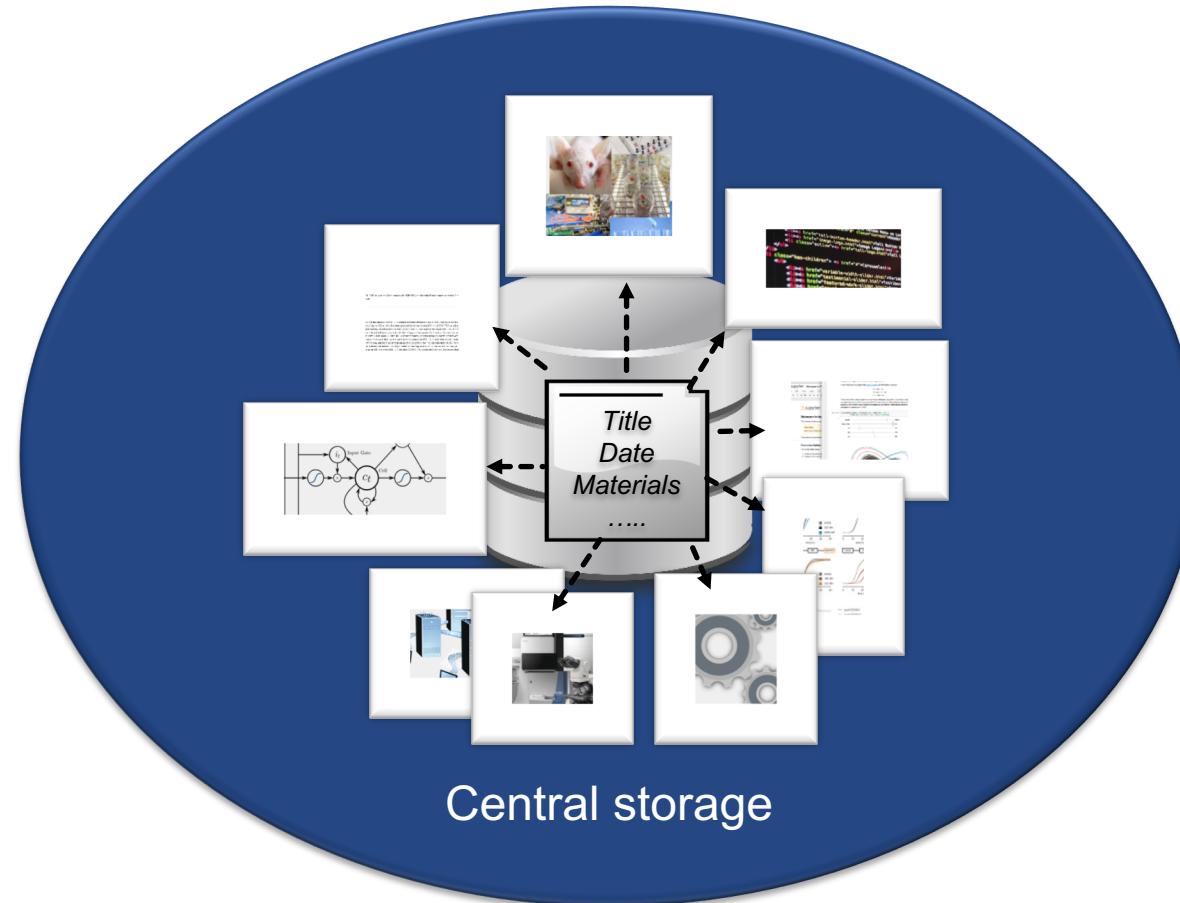
Complex process that requires tracking and linking different types of information



A very common scenario @ ETH Zurich



The ideal scenario



 **openBIS**

 **ETH RDH**

openBIS vs ETH RDH

- openBIS is a software developed by SIS.
- ETH RDH is a platform that uses openBIS. It is offered as a service to all ETH research groups.
- It is possible to have a departmental instance of ETH RDH (e.g. CHAB RDH).

What is openBIS used for?

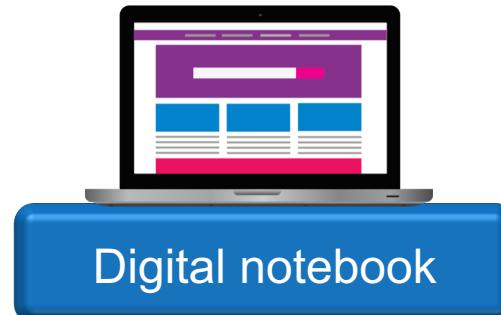
- openBIS is a software for:

✓ Keeping track of lab materials



✓ Keeping track of lab methods

✓ Describing experiments



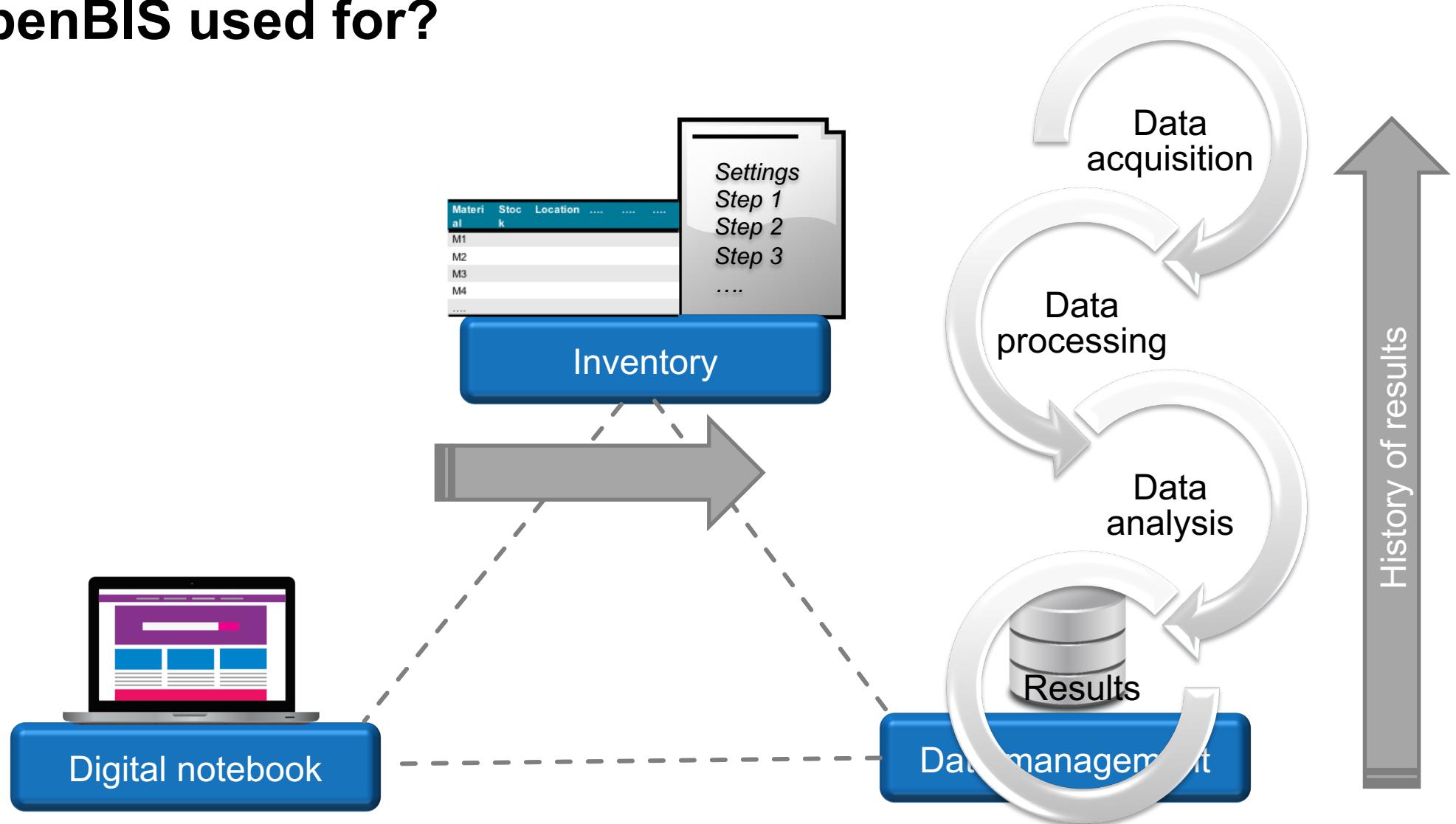
Digital notebook

✓ Uploading data to experiments

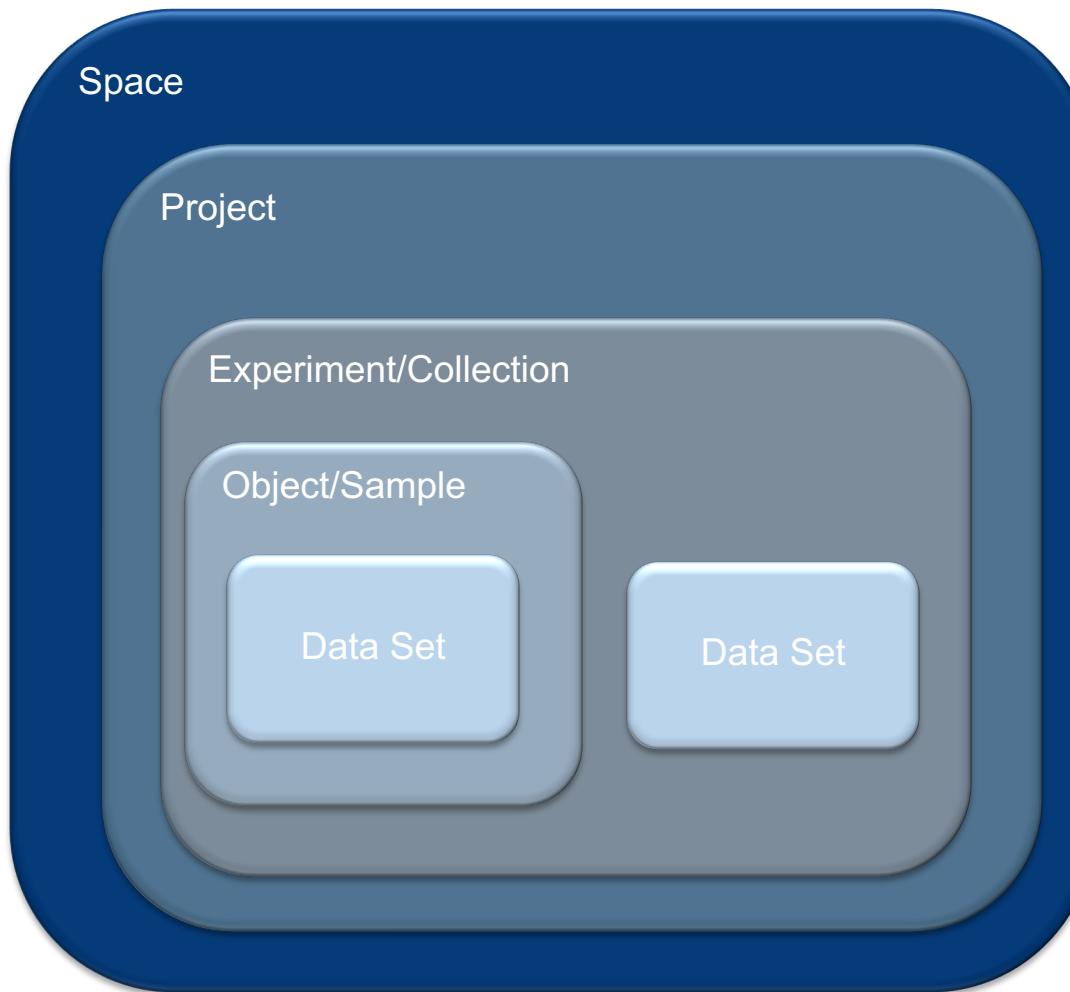


Data management

What is openBIS used for?



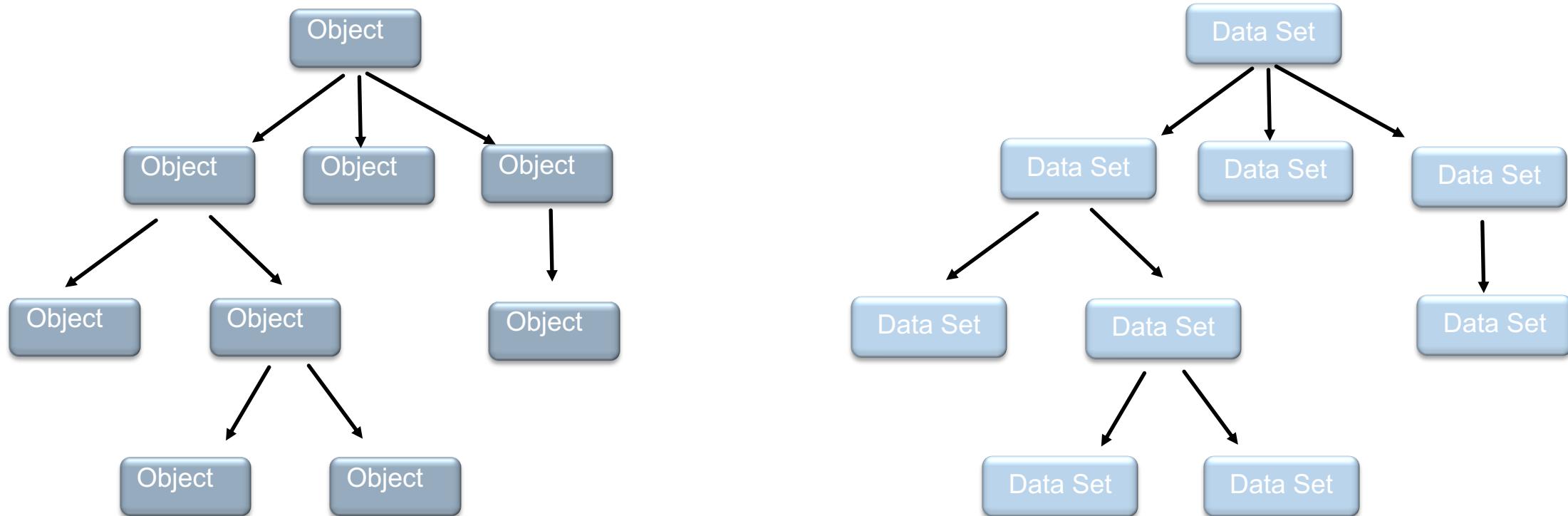
openBIS data structure



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
Datasets, 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



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.
Space/Project admin	Power user rights+ list roles. Create & delete space/project roles.

How can we create a data model in openBIS?

1. Think about your workflows
2. Start from the inventory:
 1. Materials
 2. Methods
 3. Equipment (if needed)
3. Lab notebook:
 1. Do you need to record info in specific fields for your experiments, or are generic fields (e.g. “description”, “goal”, “results” good enough?)
 2. What type of data do you generate?
 3. How do you want to organize these data?

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.
- Some experimental techniques used:
 - PCR
 - Microscopy
 - Flow cytometry
 - Western blotting

Inventory we want to have for our use-case

MATERIALS

1. Cell line
2. Plasmid
3. Chemical
4. Media
5. Solution/Buffer
6. Yeast

METHODS

1. Western blotting protocols
2. Flow Cytometry protocols

Inventory organization

- All samples, materials and protocols need to be organized in *Collections*.
- *Collections* are contained in a “first-level”, “container” folder.



Data structure mapping

Materials

Reagents, Cell Lines, Plasmids, Yeasts

Media Collection, Buffers Collection,
Chemicals Collection, Cell Lines
Collection, Plasmids Collection, Yeasts
Collection

Media 1-n, Buffer 1-n, Chemical 1-n, Cell
line 1-n, Plasmid 1-n, Yeast 1-n

Methods

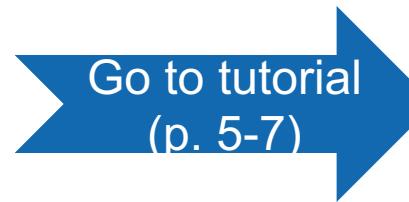
Protocols

Western Blotting Protocols, Flow
Cytometry Protocols

WB Protocol 1-n, FC protocol 1-n

Customization of Inventory of Materials for our use-case

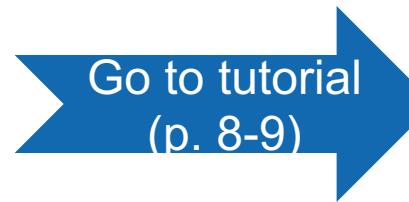
- We want to create 6 new Collection folders: *Media Collection*, *Buffers Collection*, *Chemicals Collection*, *Cell Lines Collection*, *Plasmids Collection*, *Yeasts Collection*.
- Each collection is contained in another folder: *Reagents*, *Cell Lines*, *Plasmids*, *Yeasts*.
- Steps:
 1. Create “container” folder
 2. Create Collection folder



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Customization of Inventory of Methods for our use-case

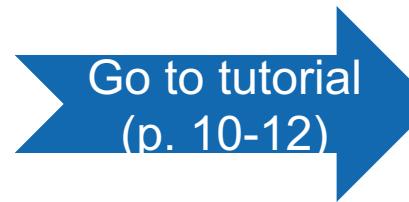
- We want to create 2 new Collection folders: *Western Blotting Protocols*, *Flow Cytometry Protocols*.
- Each collection is contained in another folder: *Protocols*.
- Steps:
 1. *Create “container” folder*
 2. *Create Collection folder*



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Customizing the ELN settings

- It is possible to customize some parts of the ELN by modifying the **Settings** in the ELN interface.
- What can be customized:
 - What is shown in the main menu
 - Lab storages
 - Templates for orders
 - Fields with Rich text editor
 - Inventory Spaces
 - Object types forms:
 - Object is a protocol
 - Object should shows storage
 - Pre-defined parents/children
- In the tutorial we will customize some lab storages and we will customize the form for the Experimental Step Object type.



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Summary of creating a data model for Materials

1. Which materials do you use?

Make a list

2. What do you want to record about these materials in a database?

For each material, make a list of fields

3. Do you already have Excel files of materials/samples?

The same fields have to be created in openBIS. openBIS-generated templates can then be used for upload

4. Do you already have information in a separate database?

The same fields have to be created in openBIS. openBIS-generated templates can then be used for upload

Summary of creating a data model for Methods

1. Do you have standard protocols in the lab?

Make a list

2. Which fields do you need in a protocol form? (e.g. *procedure*, *T requirement*, *P requirement*, *time*, etc)

Make a list

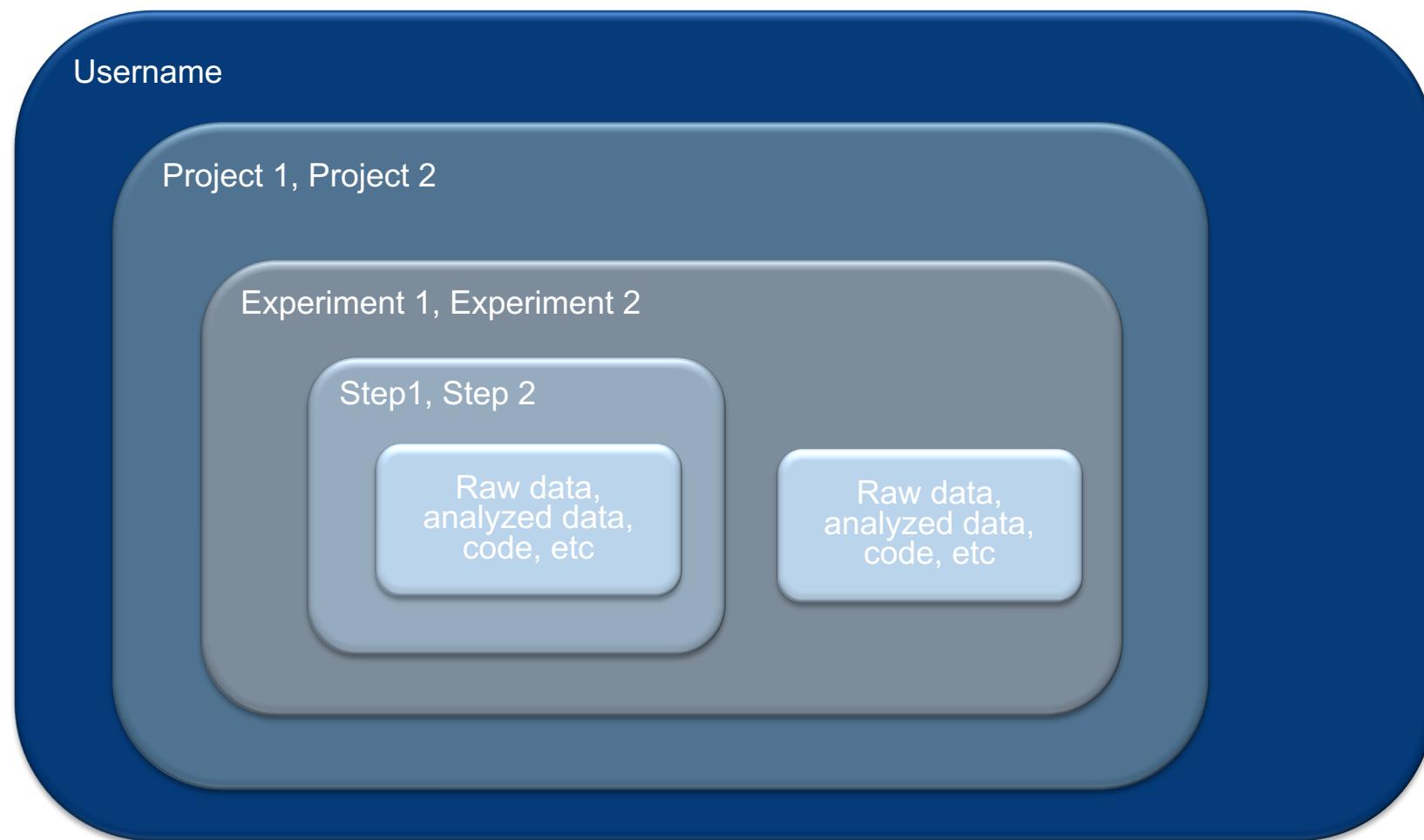
3. Do you need different types of protocols for different things, or is a generic template ok for everything?

Make a list of protocol types you need and the fields needed for each type

Data model for 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**
- Data 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:

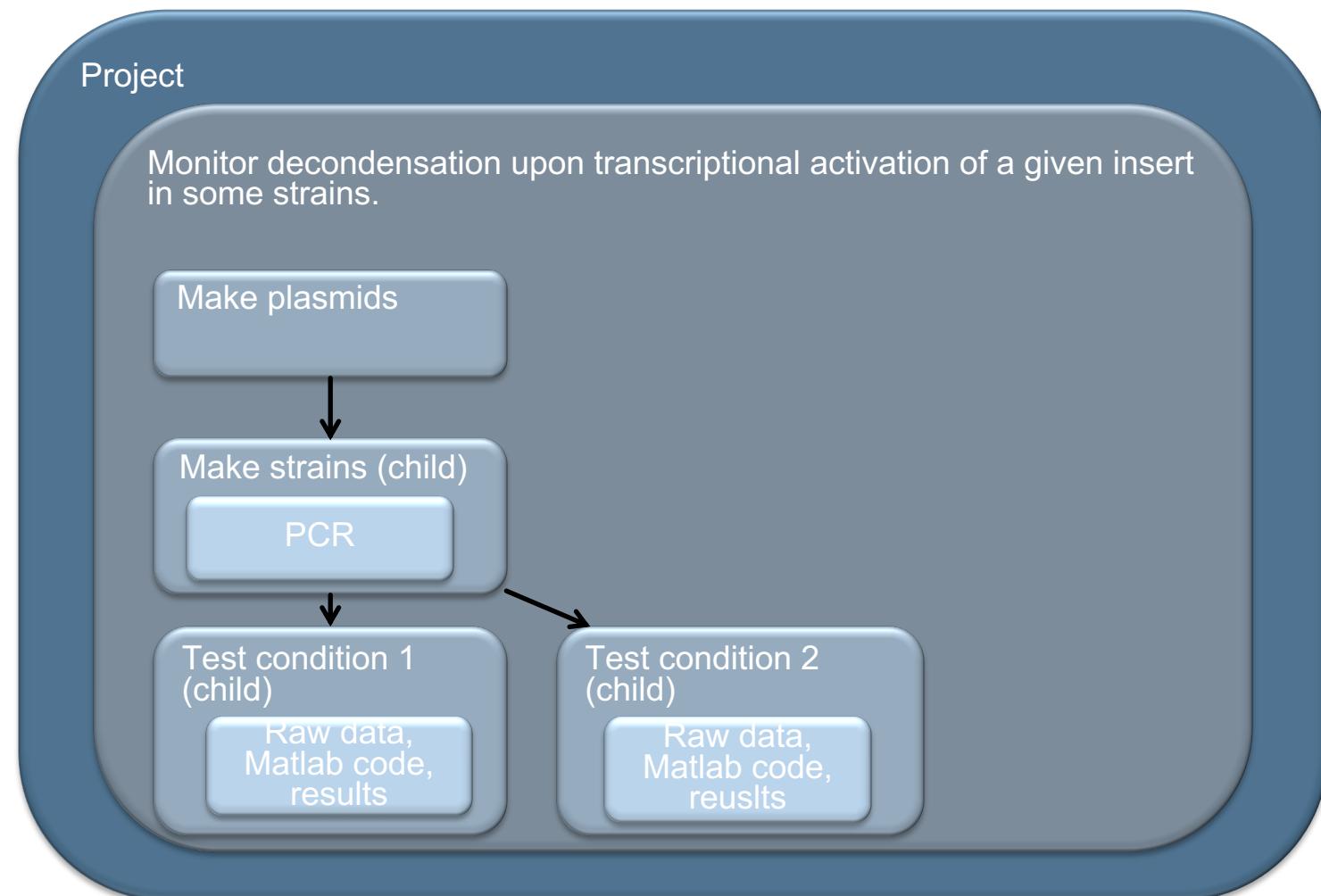
Monitor de-condensation upon transcriptional activation of a given insert in some strains.

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:

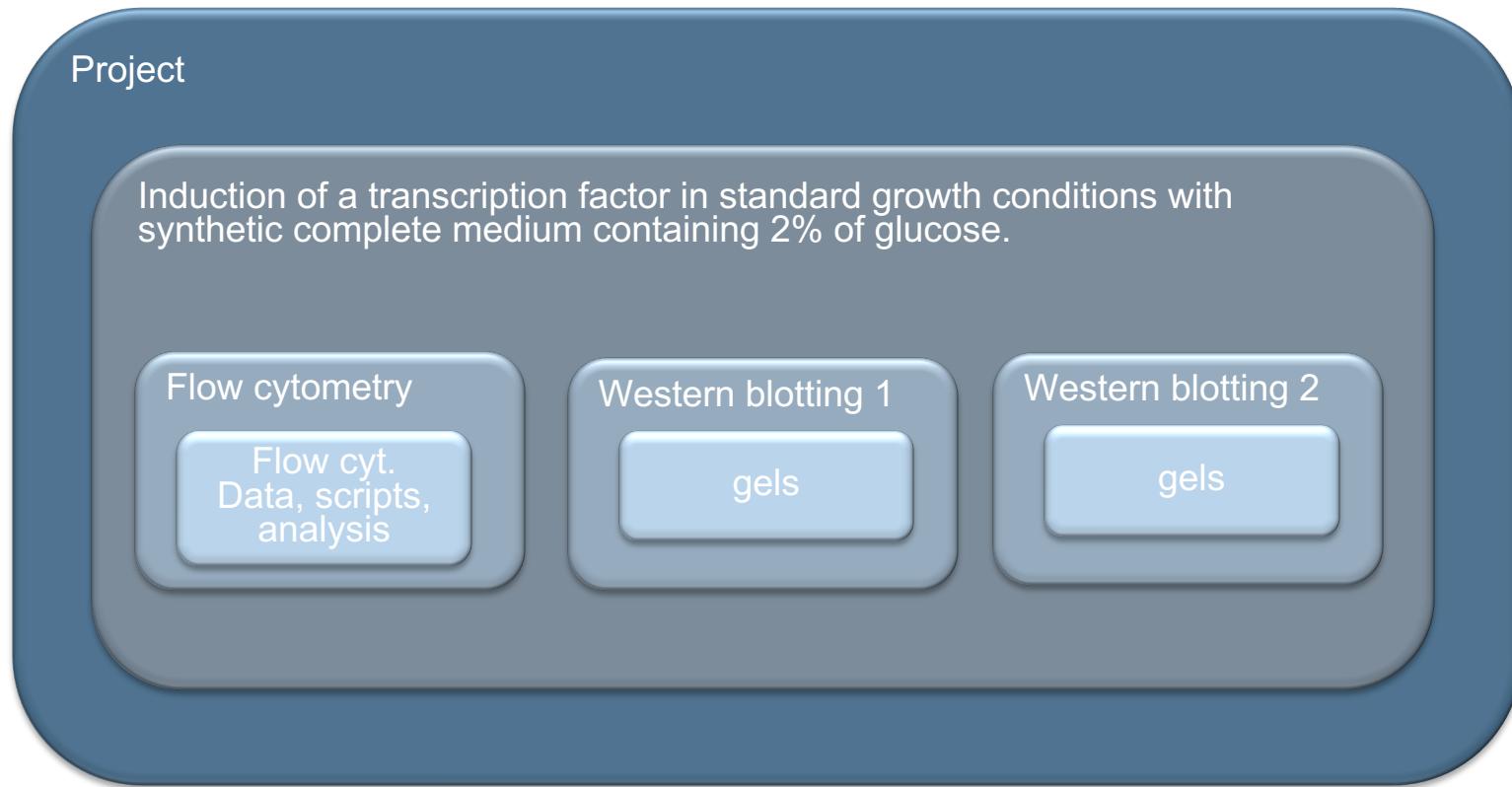
Induction of a transcription factor in standard growth conditions with synthetic complete medium containing 2% of glucose.

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



Defaults for lab notebook

- openBIS provides **defaults** that are suitable for the vast majority of use-cases:
 - **DEFAULT EXPERIMENT:** *Name, show in project overview, is finished, grant, start date, end date, experimental goals, experimental description, experimental results, references, publication, notes, comments*
 - **EXPERIMENTAL STEP:** *Name, show in project overview, is finished, start date, end date, experimental goals, experimental details, experimental results, references, publication, notes, comments*
 - **Data set types:** *ANALYZED_DATA, ATTACHMENT, ELN_PREVIEW, RAW_DATA, SEQ_FILE, UNKNOWN.*
 - All data set type have the *Name* and *Notes* fields.

Information and data management with openBIS

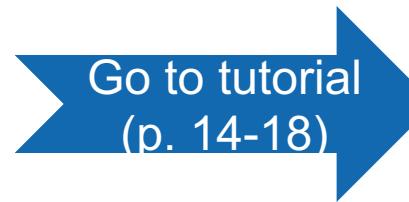
Overview

- After defining the data model and customizing openBIS for our needs, we can start filling the database with information relevant for our work.
- We will start by filling in the inventory and then we will register experiments and upload data to the lab notebook.
- We will see how we can link samples and protocols stored in the inventory to Experimental Steps. This is important for data history tracking.

Inventory

We will register the following samples and protocols in the inventory:

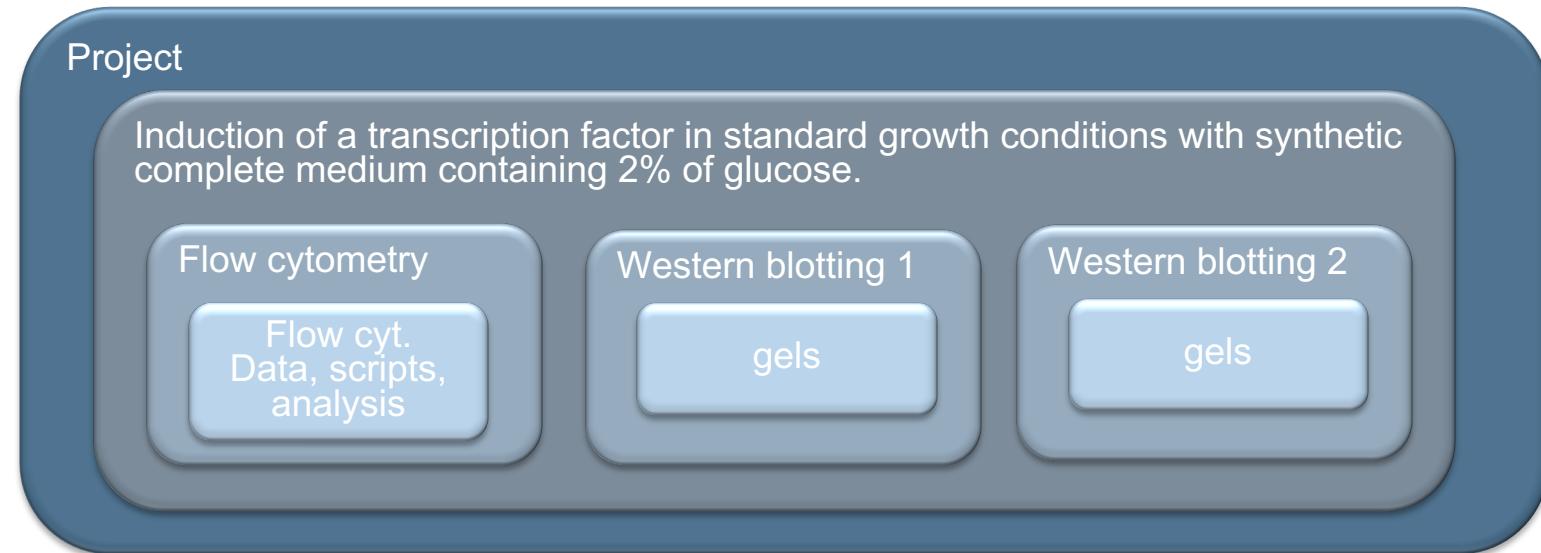
- Media
- Chemicals
- Plasmid
- Yeasts
- Buffers
- Flow cytometry protocol
- Western blotting protocol



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Lab notebook

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



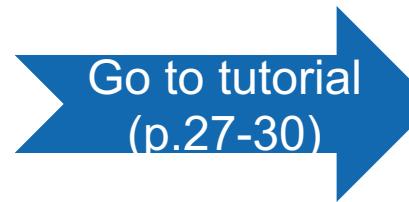
- We will create **one Project, one Experiment and 2 Experimental Steps.**
- We will see how we can **link** samples and protocols stored in the Inventory to the Experimental Steps.
- We will **upload data** to the Experimental Steps.

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Using the openBIS ordering system

Managing lab orders with openBIS

- The ordering functionality of openBIS can be used to keep track of products, suppliers and to manage requests and orders.
- Everyone in the lab can create requests for products. Only the lab admin can process the requests and create orders from them.
- We will:
 - Create a collection of suppliers
 - Create a collection of products
 - Create a request
 - Generate an order from the request



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Upcoming event

openBIS User Group Meeting

18th & 19th June 2019

ETH Zürich, Zentrum

<https://bit.ly/2Jf6niM>



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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