


Persistent Identifiers and the openBIS Research Data Management System

Other Conference Item

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Persistent Identifiers and the openBIS Research Data Management System

Henry Lütcke

Scientific IT Services, ETH Zurich

Persistent Identifiers for Research, ETH Library



Overview

1. Scientific IT Services & Research Data Management Support at ETH Zurich
2. Active Research Data Management with openBIS
3. Services based on openBIS
4. Persistent Identifiers in openBIS

Who is Scientific IT Services (SIS)?

- We are a section of ETH IT Services since 2013
- We are a team of experts in various areas of scientific computing
- SIS members have a background in different areas of science (Mathematics, Physics, Chemistry, Climate Science, Computer Science, Life Sciences)
- Most with research experience at least at PhD level

Who is Scientific IT Services?



Tools / Infrastructure

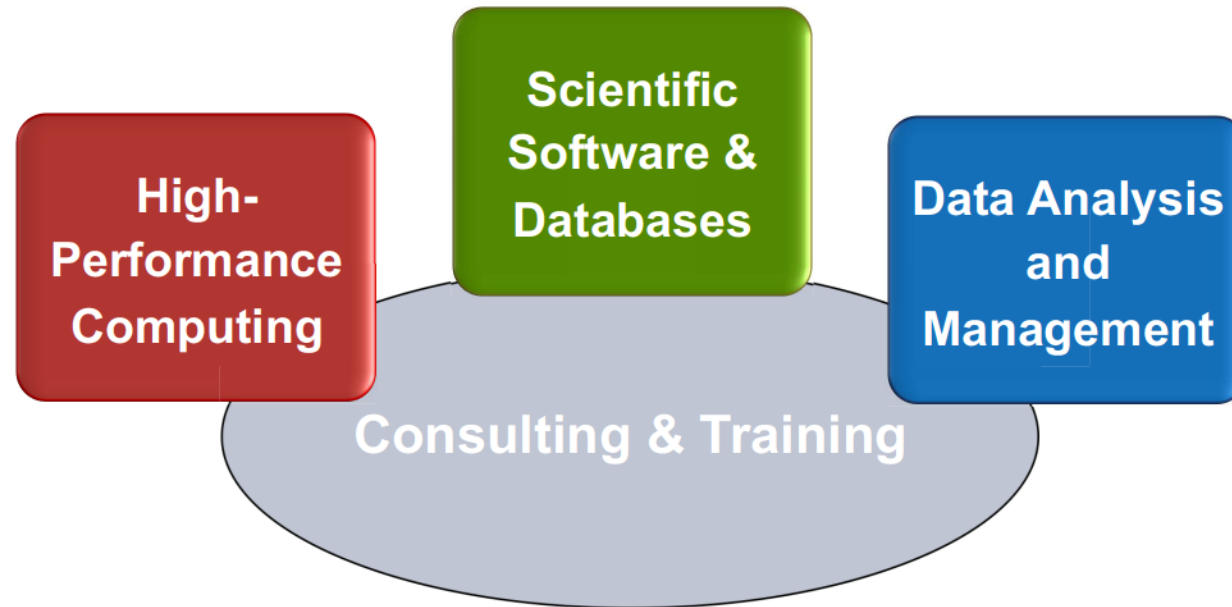


Support in using tools



Education

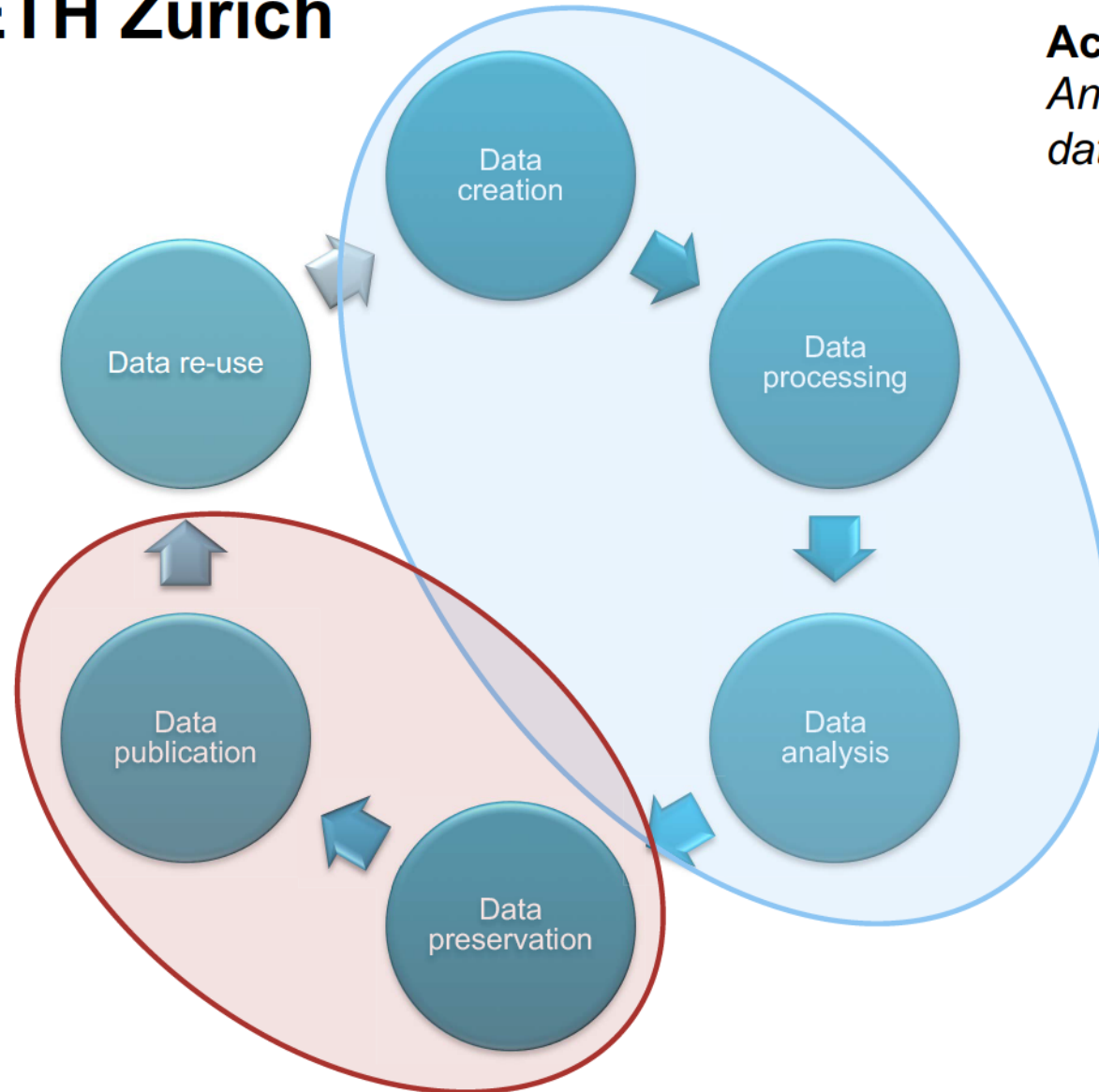
Who is Scientific IT Services?



- **Research Data Management**
- High Performance Computing and Big Data Analytics
- Writing, maintaining and optimizing scientific software
- Building computational pipelines (reproducibility)
- Training, Consulting and Triaging of computing needs in research labs / for research projects

RDM Support at ETH Zurich

Active data management
Annotate, store, backup data while it is produced

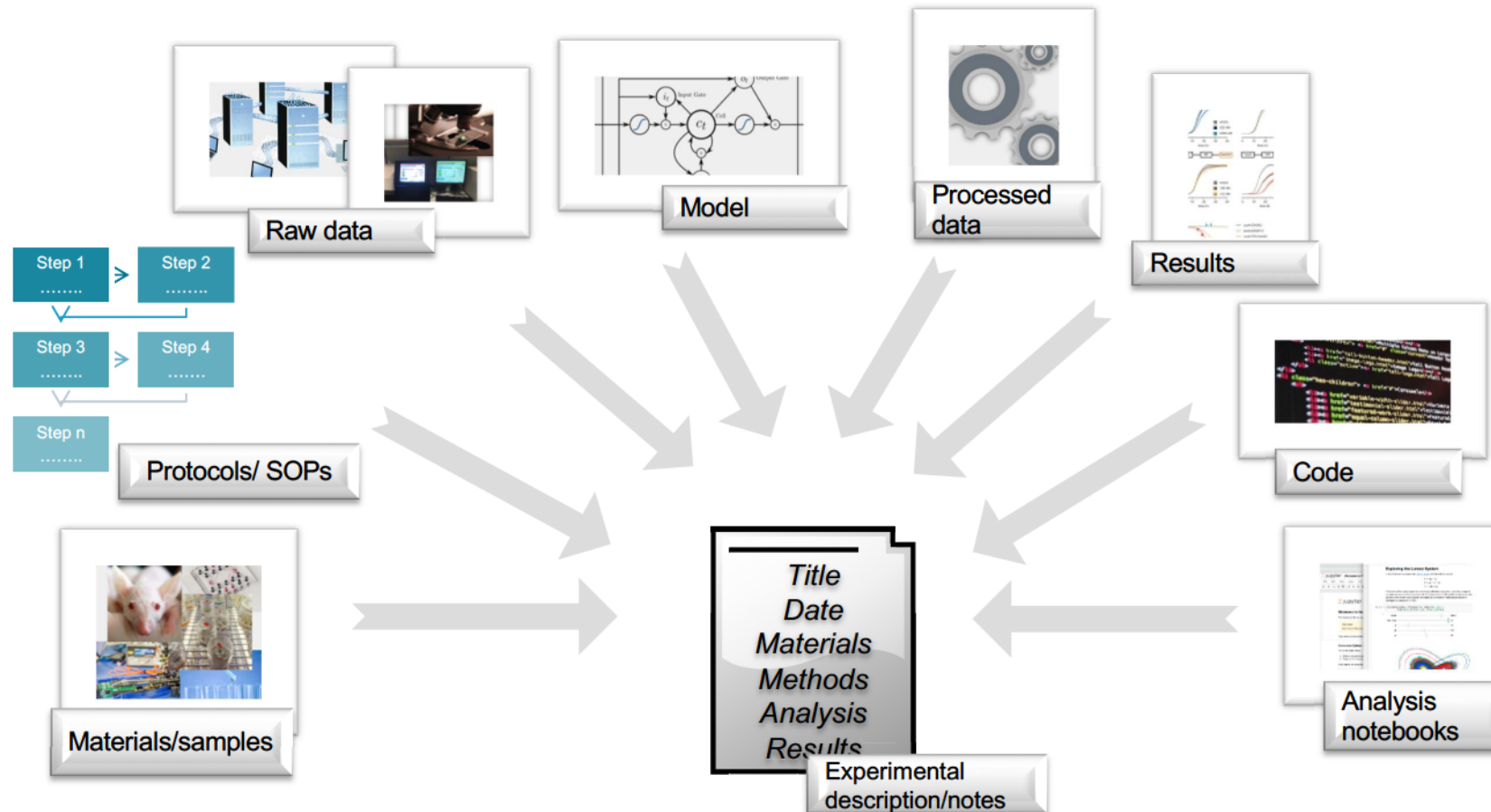


Long term data management
Annotate, share/publish, preserve data at the end of a project / publication

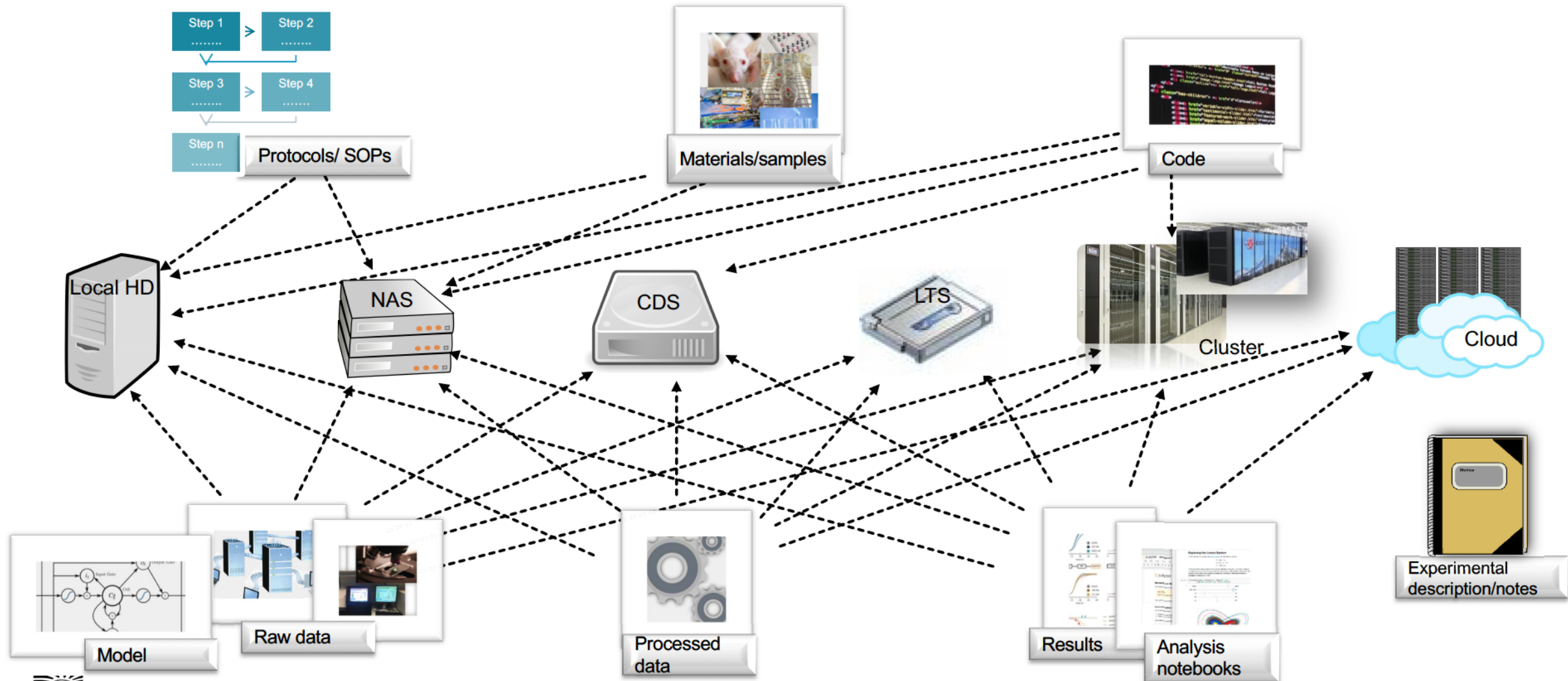


What does it take to manage research data?

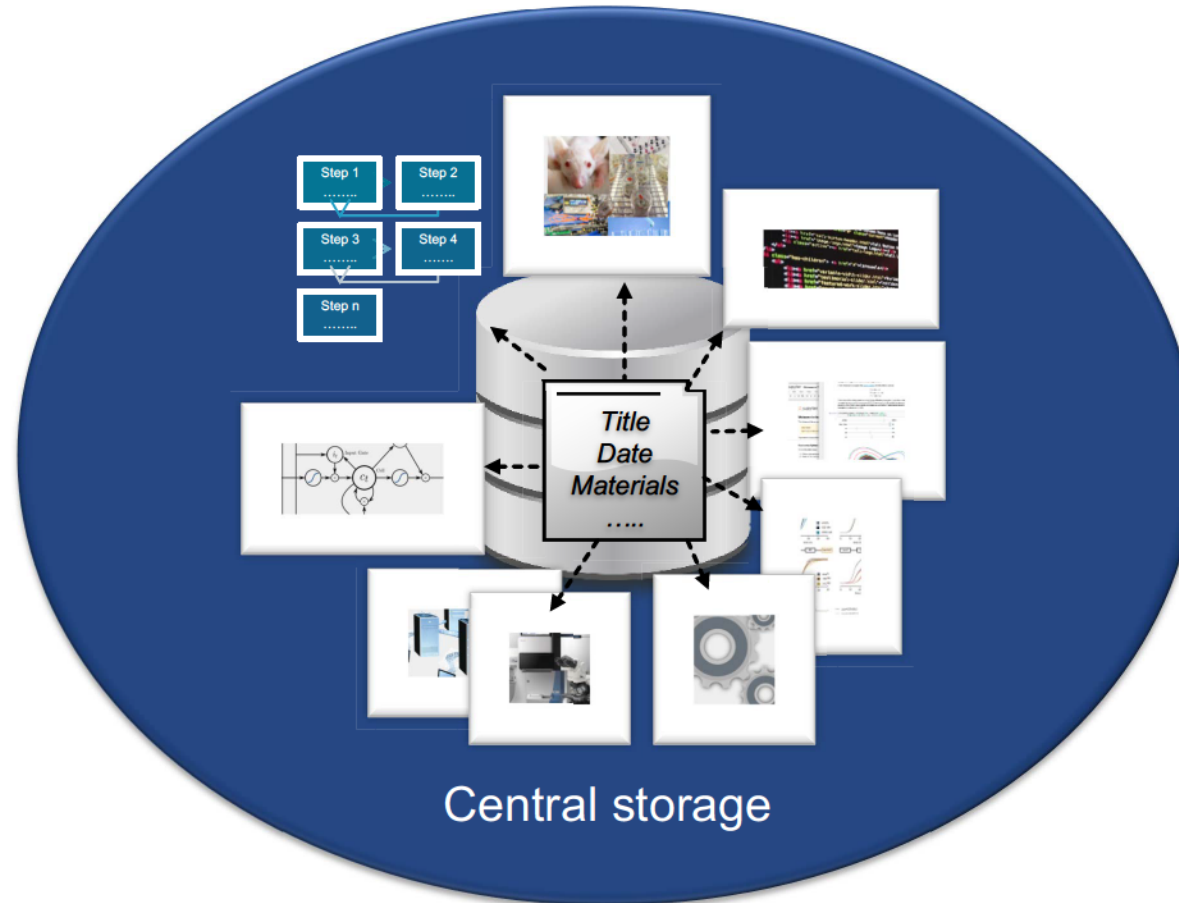
Complex process that requires tracking and linking different types of information



A common scenario at ETH

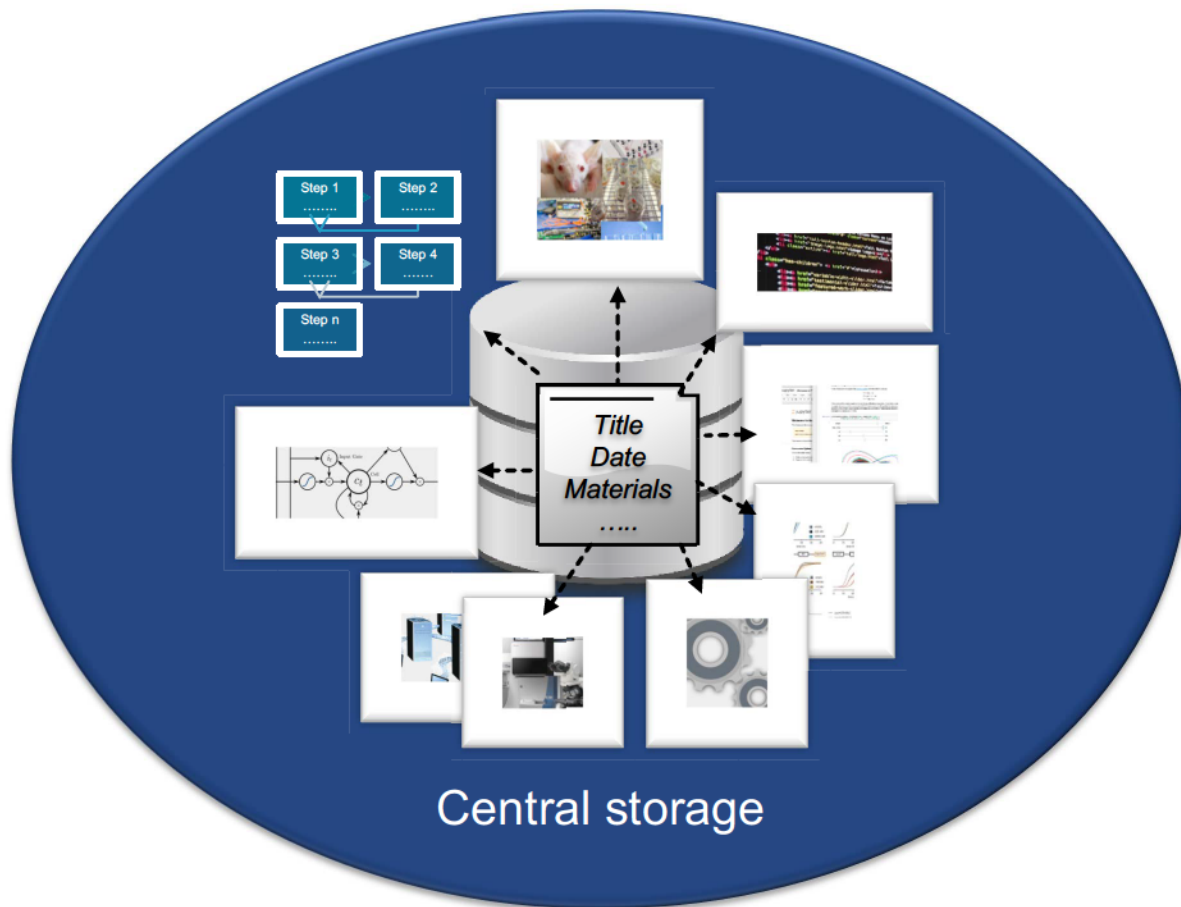


Our ideal scenario



Electronic Lab Notebook with Laboratory Information Management System (ELN-LIMS)

Our ideal scenario



Electronic Lab Notebook with Laboratory Information Management System (ELN-LIMS)

openBIS facts

Developed at ETH 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)

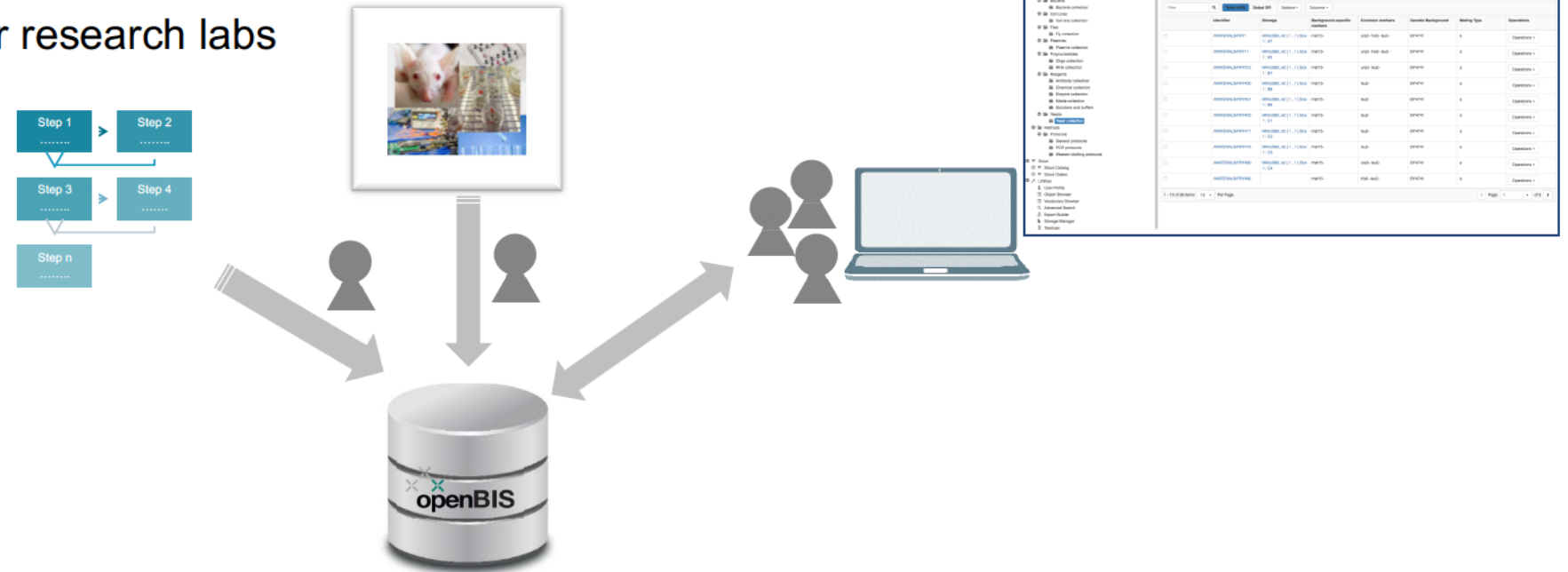


Used by research groups and facilities @ ETH, Swiss & European Universities, a few companies



openBIS in a nutshell

- openBIS is a solution for research labs



Collection: Yeast collection

/MATERIALS/YEASTS/YEAST_COLLECTION_1

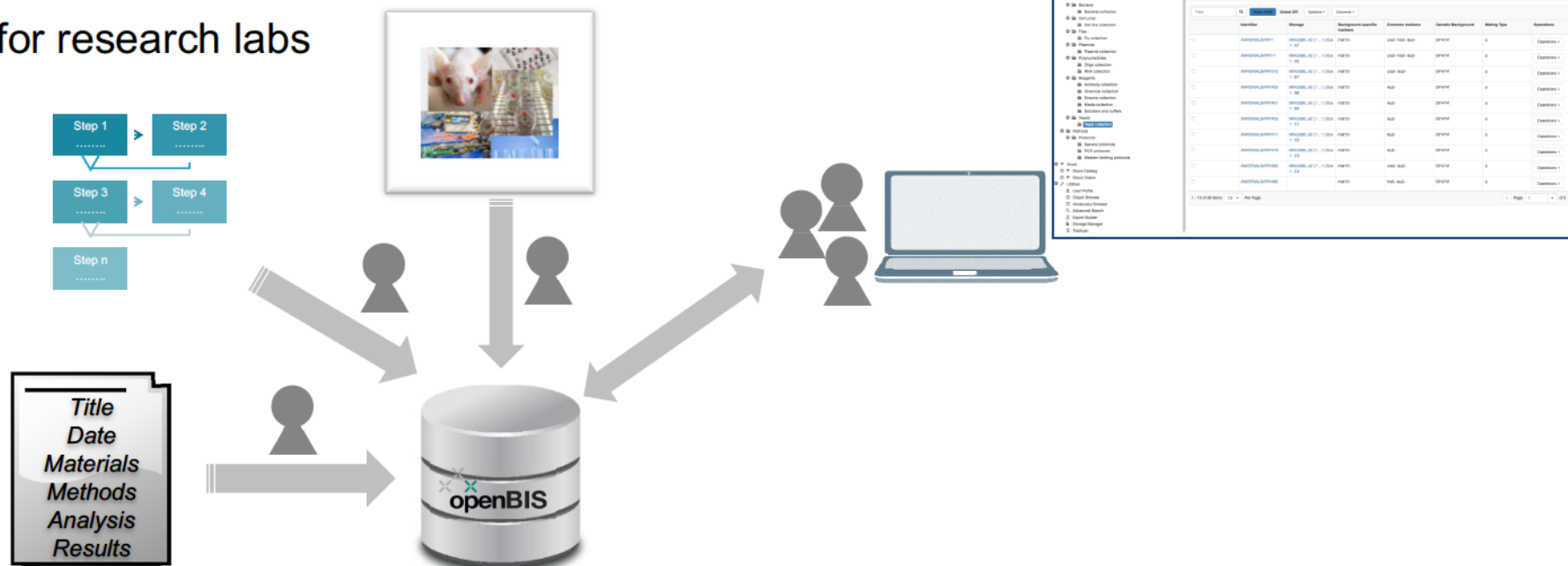
+ Operations

- Lab Notebook
- Others
- Inventory
 - Materials
 - Bacteria
 - Bacteria collection
 - Cell Lines
 - Cell line collection
 - Flies
 - Fly collection
 - Plasmids
 - Plasmid collection
 - Polynucleotides
 - Oligo collection
 - RNA collection
 - Reagents
 - Antibody collection
 - Chemical collection
 - Enzyme collection
 - Media collection
 - Solutions and buffers
 - Yeasts
 - Yeast collection**
 - Methods
 - Protocols
 - General protocols
 - PCR protocols
 - Western blotting protocols
- Stock
 - Stock Catalog
 - Stock Orders
- Utilities
 - User Profile
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - User Manager
 - Trashcan
 - Settings

Identifier	Storage	Endogenous 2micron plasmid in yeast	Genetic modifications	Mating Type	Origin	Publication	Source
/MATERIALS/FRY1		cir+		a		Brachmann, et al., Yeast, 1998	Euroscarf
/MATERIALS/FRY11		cir+	FRP235 INTEGRATION "ADH1 terminator"	a	negative selection	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY312	MINUS80_A2 [1 , 3] 3 - NoPos	cir+	FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY400	MINUS80_A2 [1 , 3] 3 - NoPos	cir+	FRP791 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY401	MINUS80_A2 [1 , 3] 3 - NoPos	cir+	FRP792 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY403	MINUS80_A2 [1 , 3] 3 - NoPos	cir+	FRP795 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY417	MINUS80_A2 [1 , 3] 3 - NoPos	cir+	FRP800 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY418	MINUS80_A2 [1 , 3] 3 - A2	cir+	FRP793 INTEGRATION "URA3" FRP718 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY460	MINUS80_A2 [1 , 3] 3 - NoPos	cir+	FRP467 INTEGRATION "HIS3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	
/MATERIALS/FRY482		cir+	FRP795 INTEGRATION "URA3" FRP235 INTEGRATION "ADH1 terminator"	a	transformation	Ottoz et al., Nucleic Acids Research, 2014	

openBIS in a nutshell

- openBIS is a solution for research labs



Projects
Experiments
Experimental
steps

Lab Notebook

- Others
 - Caterina
 - Diana Ottoz
 - Inducible Transcription Factor
 - Induction of the transcription factor
 - Detection of LexA-ER-B42 indu**

Object: Detection of LexA-ER-B42 induction by flow cytometry

/DIANA_OTTOZ/INDUCIBLE_TRANSCRIPTION_FACTOR/INDUCTION_OF_TF/FC_LEXA-ER-B42

+ ✎ 📄 🗑️ 🖨️ 👤 📄 ⌚ ⌚ 📄

General

Name: Detection of LexA-ER-B42 induction by flow cytometry

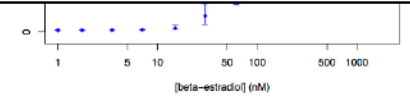
Owner: Diana Ottoz

Experimental goals:

Select a dataset type

Files Uploader

- RAW_DATA : Flow cytometry files
- ANALYSIS_SCRIPTS : scripts
- ANALYZED_DATA : Analysis results



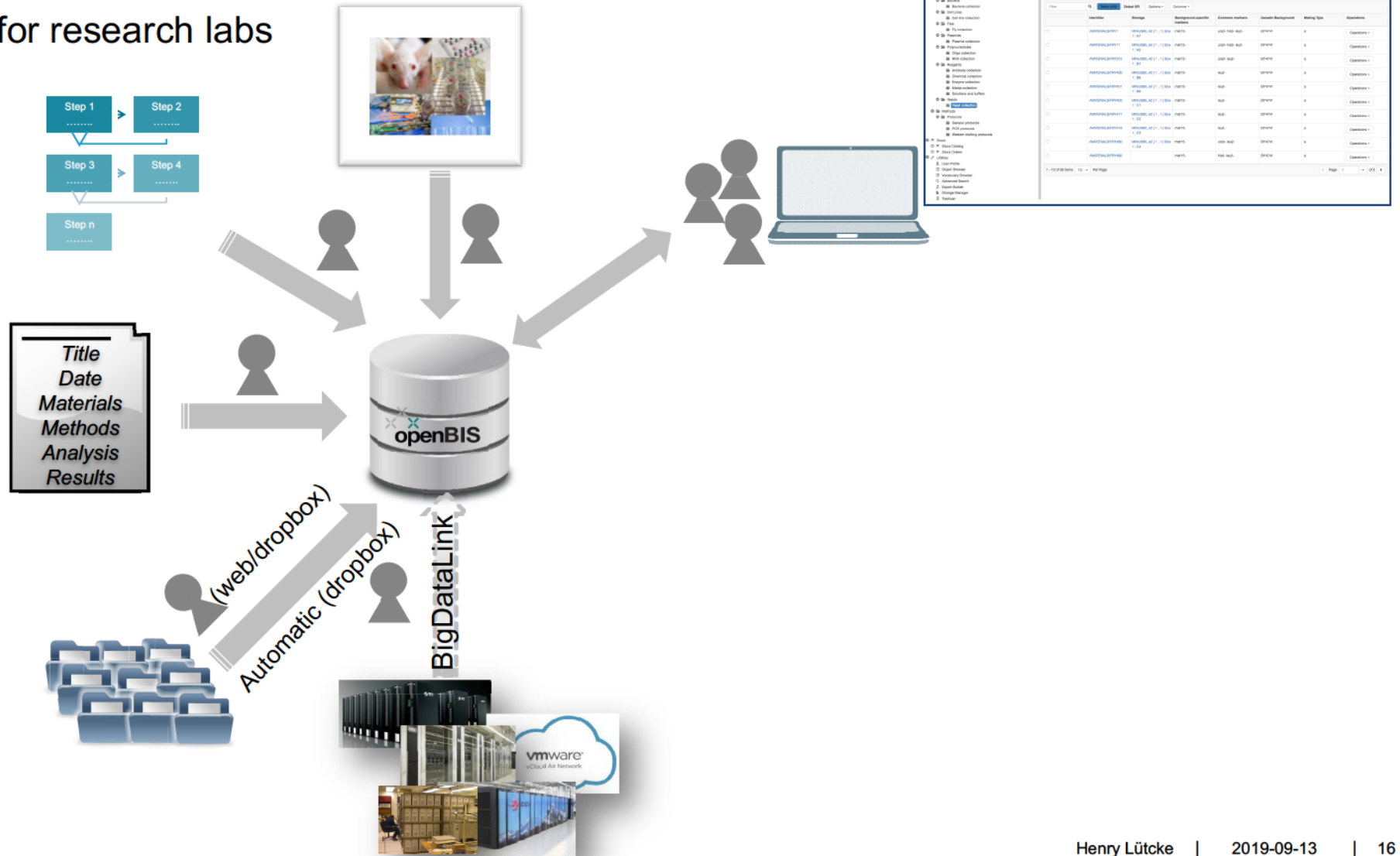
Links to materials & methods

Filter Q **AND** OR Options Columns

Code	Name	Comments	Details
FRM11	liquid S media	SDC at 25°C	
FRSOB34	1000X Cycloheximide	diluted 1/1000, treated for 1/2 hour	Dissolve in DMSO. Aliquot.
FRSOB37	beta-estradiol	1:2 concentration series with 2000 nM maximum for 24	Dissolve in EtOH.

openBIS in a nutshell

➤ openBIS is a solution for research labs



Object: Detection of LexA-ER-B42 induction by flow cytometry

/DIANA_OTTOZ/INDUCIBLE_TRANSCRIPTION_FACTOR/INDUCTION_OF_TF/FC_LEXA-ER-B42



- Lab Notebook
 - Others
 - Caterina
 - Diana Ottoz
 - Inducible Transcription Factor
 - Induction of the transcription factor
 - Detection of LexA-ER-B42 indu**
 - Flow cytometry files
 - scripts
 - Analysis results
 - Detection of LexA-ER-B42 indu
 - Detection of LexA-ER-B112 ind
 - Analysis of the abundance of the fc
- Inventory
 - Materials
 - Methods
- Stock
 - Stock Catalog
 - Stock Orders
- Utilities
 - User Profile
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - User Manager
 - Trashcan
 - Settings
- About

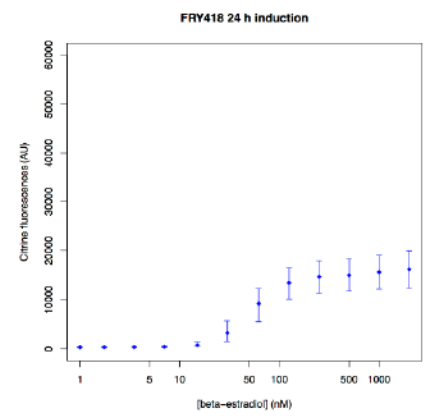
General

Name:
Detection of LexA-ER-B42 induction by flow cytometry

Owner:
Diana Ottoz

Experimental goals:
Analyze the induction of **LexA-ER-B42** in a concentration series of beta-estradiol using a fluorescence readout

Experimental results:
The LexA-ER-B42 induction can be measured by using a target gene encoding a fluorescence protein. *LexA-ER-B42 induction is different at different concentrations of inducer.*



Links to materials & methods

Code	Name	Comments	Details
FRM11	liquid S media	SDC at 25°C	
FRSOB34	1000X Cycloheximide	diluted 1/1000, treated for 1/2 hour	Dissolve in DMSO. Aliquot.
FRSOB37	beta-estradiol	1:2 concentration series with 2000 nM maximum for 24	Dissolve in EtOH.

- RAW_DATA : Flow cytometry files
 - FC_LEXA-ER-B42-raw
 - FC_LEXA-ER-B42-raw
 - 1.fcs (510.3Kb)
 - 10.fcs (510.4Kb)
 - 11.fcs (510.4Kb)
 - 12.fcs (510.3Kb)
 - 2.fcs (510.3Kb)
 - 3.fcs (510.3Kb)
 - 4.fcs (510.3Kb)
 - 5.fcs (510.3Kb)
 - 6.fcs (510.3Kb)
 - 7.fcs (510.3Kb)
 - 8.fcs (510.3Kb)
 - 9.fcs (510.3Kb)
 - ANALYSIS_SCRIPTS : scripts
 - FC_LEXA-ER-B42-script.R (2.9Kb)
 - ANALYZED_DATA : Analysis results
 - FC_LEXA-ER-B42-analyzed
 - FC_LEXA-ER-B42-analyzed
 - FRY418t24hCitrine.pdf (5.2Kb)
 - FRY418t24hmKate2.pdf (5.2Kb)

Select a dataset type

Files Uploader



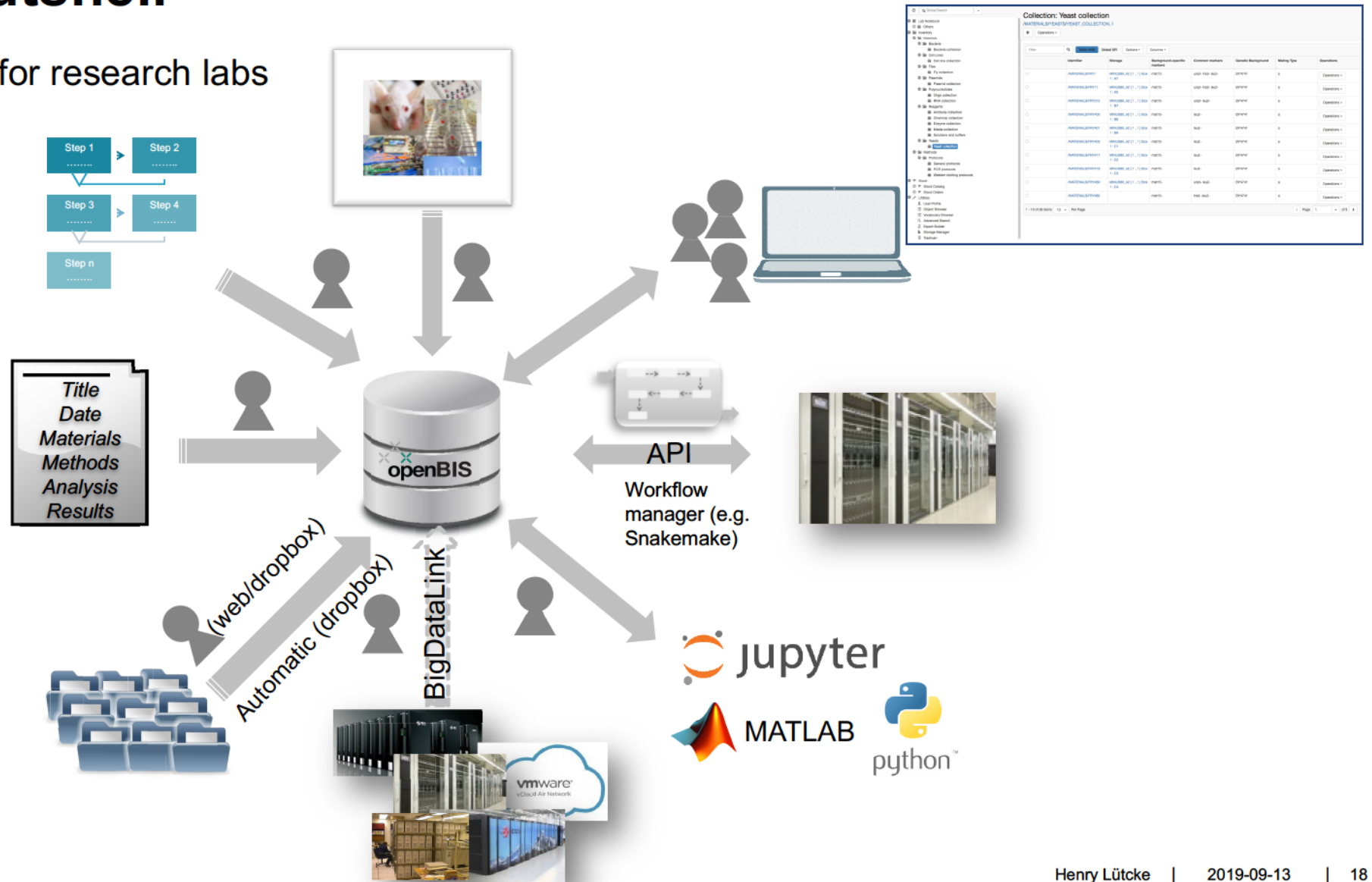
Select files to upload

Create

Auto upload on drop

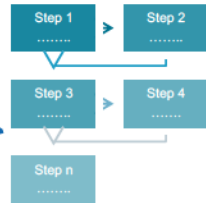
openBIS in a nutshell

➤ openBIS is a solution for research labs

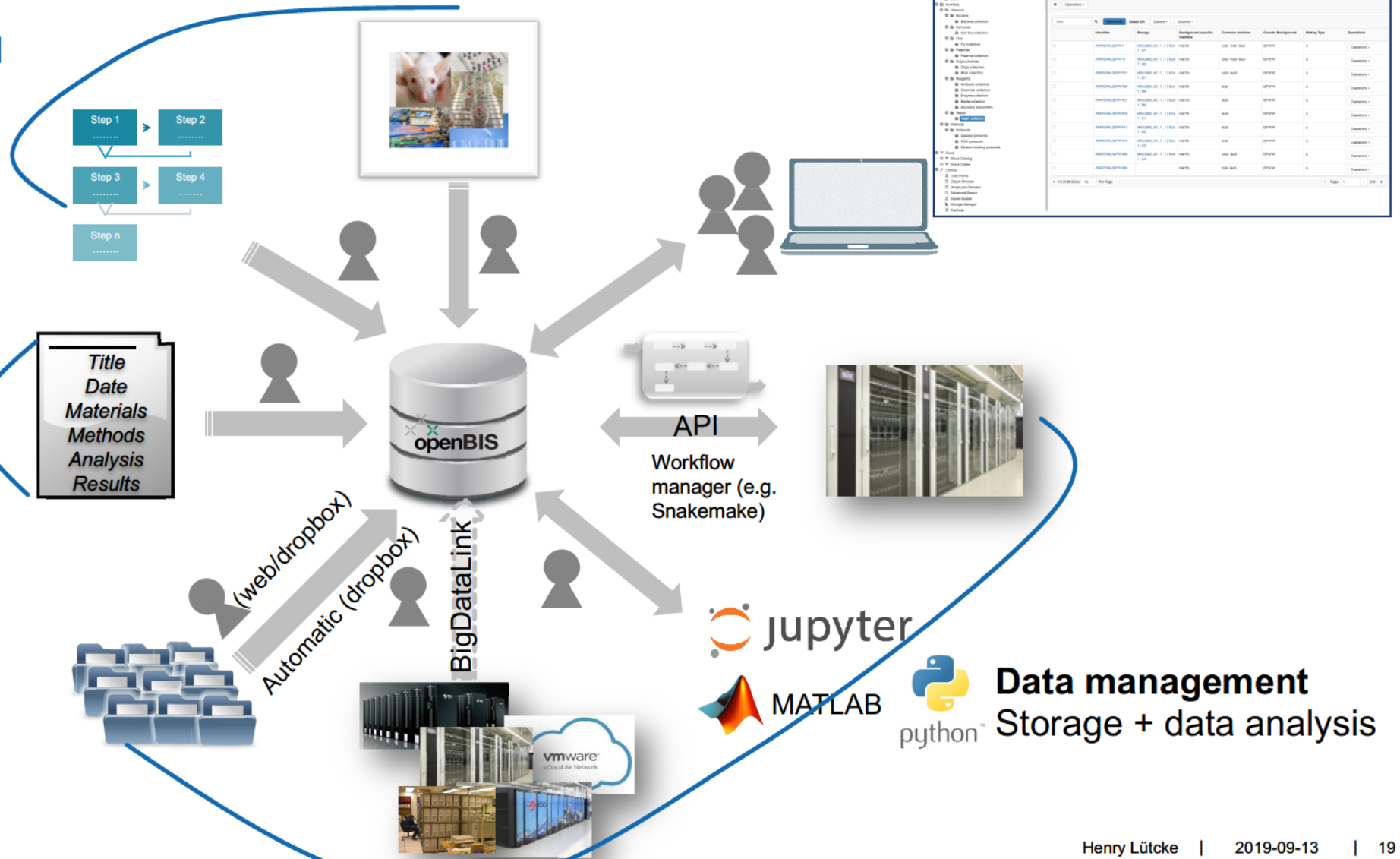
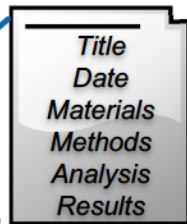


openBIS in a nutshell

Inventory of samples and protocols
Shared by all lab members



ELN
Personal folder. Can be shared with all lab members and collaborators



id	name	status	parent_id	parent_name	parent_status	parent_type	parent_permissions
1	Yeast collection	active					
2	Yeast collection	active	1	Yeast collection	active		
3	Yeast collection	active	1	Yeast collection	active		
4	Yeast collection	active	1	Yeast collection	active		
5	Yeast collection	active	1	Yeast collection	active		
6	Yeast collection	active	1	Yeast collection	active		
7	Yeast collection	active	1	Yeast collection	active		
8	Yeast collection	active	1	Yeast collection	active		
9	Yeast collection	active	1	Yeast collection	active		
10	Yeast collection	active	1	Yeast collection	active		



Services based on openBIS provided by SIS

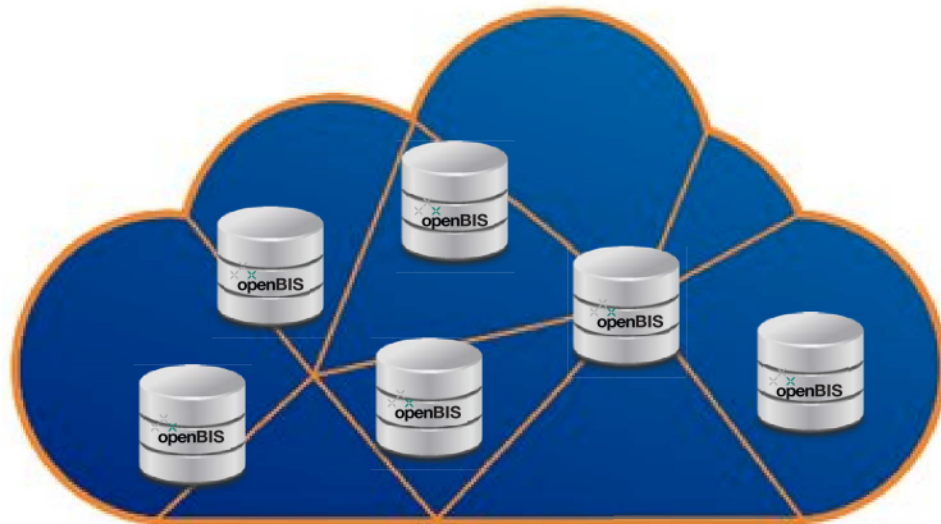
openBIS services at ETH Zurich

- Standard service for research groups:
 - **ETH Research Data Hub:** openBIS central server, all ETH research groups
 - **ETH Departmental Data Hub:** openBIS central server for department
 - **ETH Research Data Node:** openBIS group servers (single ETH research group)
- **Regular trainings & workshops**
- **Support & consulting**
- **Prefilled SNF DMP template** for openBIS users (<https://www.ethz.ch/services/en/service/a-to-z/research-data/data-management-planning.html>)
- **Advanced customization & development work:** separate support contract

openBIS services in Switzerland: openRDM.swiss



University of
Zurich^{UZH}



National service for RDM based on openBIS

- Build upon “lessons learned” in DLCM 1

Cloud-hosted openBIS

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

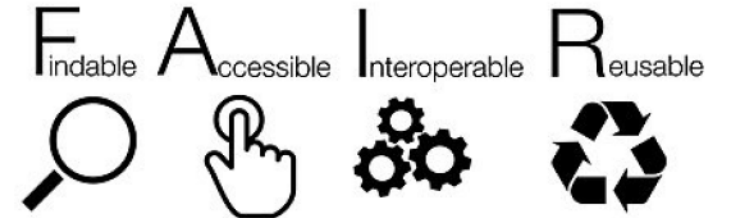
Self-hosted openBIS

- Support for set up on local IT infrastructure

Training & ‘best effort’ user support

- Optional: support contract with ETH SIS

SWITCHengines



Persistent Identifiers and openBIS

Native Data Identifiers in openBIS

Global Search

Lab Notebook

- My Space (Sis Hluetcke)
 - Demo
 - Demo Project
 - Demo experiment**
 - Step 1
 - Obit
 - Others
 - Others (disabled)
- Inventory
- Stock
- Utilities
 - Jupyter Workspace
 - New Jupyter Notebook
 - Object Browser
 - Vocabulary Browser
 - Advanced Search
 - Export Builder
 - Storage Manager
 - User Manager
 - Trashcan
 - Settings
- About

Experiment: Demo experiment ← **Name**

[/SIS_HLUETCKE/DEMO_PROJECT/DEMO_PROJECT_EXP_1](#) ← **ID**

General

Name:
Demo experiment


Show in project overview:
true

Start date:
2019-04-03 09:35:26 +0200

End date:
2019-04-03 10:35:26 +0200

Experimental details

Experimental Results:



Browse ▾ New ▾ Import ▾ Utilities ▾

Object JUPYTER-DEMO Collection Browser Collection DEMO_PROJECT_EXP_1

SIS_HLUETCKE » DEMO_PROJECT » Collection DEMO_PROJECT_EXP_1 [DEFAULT_EXPERIMENT]

Collection Properties

Collection	/SIS_HLUETCKE/DEMO_PROJECT/DEMO_PROJECT_EXP_1 ← ID
PermID	20190403103907141-571 ← Perm ID
Collection Type	DEFAULT_EXPERIMENT
Registrator	Lütcke, Henry
Registration Date	2019-04-03 10:39:07
Project	/SIS_HLUETCKE/DEMO_PROJECT
Name	Demo experiment ← Name
Show in project overview	true
Start date	2019-04-03 09:35:26 +0200
End date	2019-04-03 10:35:26 +0200
Experimental Results	<?xml version="1.0" encoding="UTF-8"?><html><head></head><body><p></p></body></html>

Objects Data Sets

Objects **ID**

Code

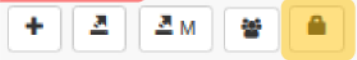
EXPS

PermID's can serve as **unique but non-persistent** identifiers **within an openBIS instance**

Native Data Identifiers in openBIS

It is now possible to “freeze” entities in openBIS:

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](#)



Native Data Identifiers in openBIS

Freezing creates truly persistent identifiers

Freeze Entity

Choose the entities to freeze (all by default):

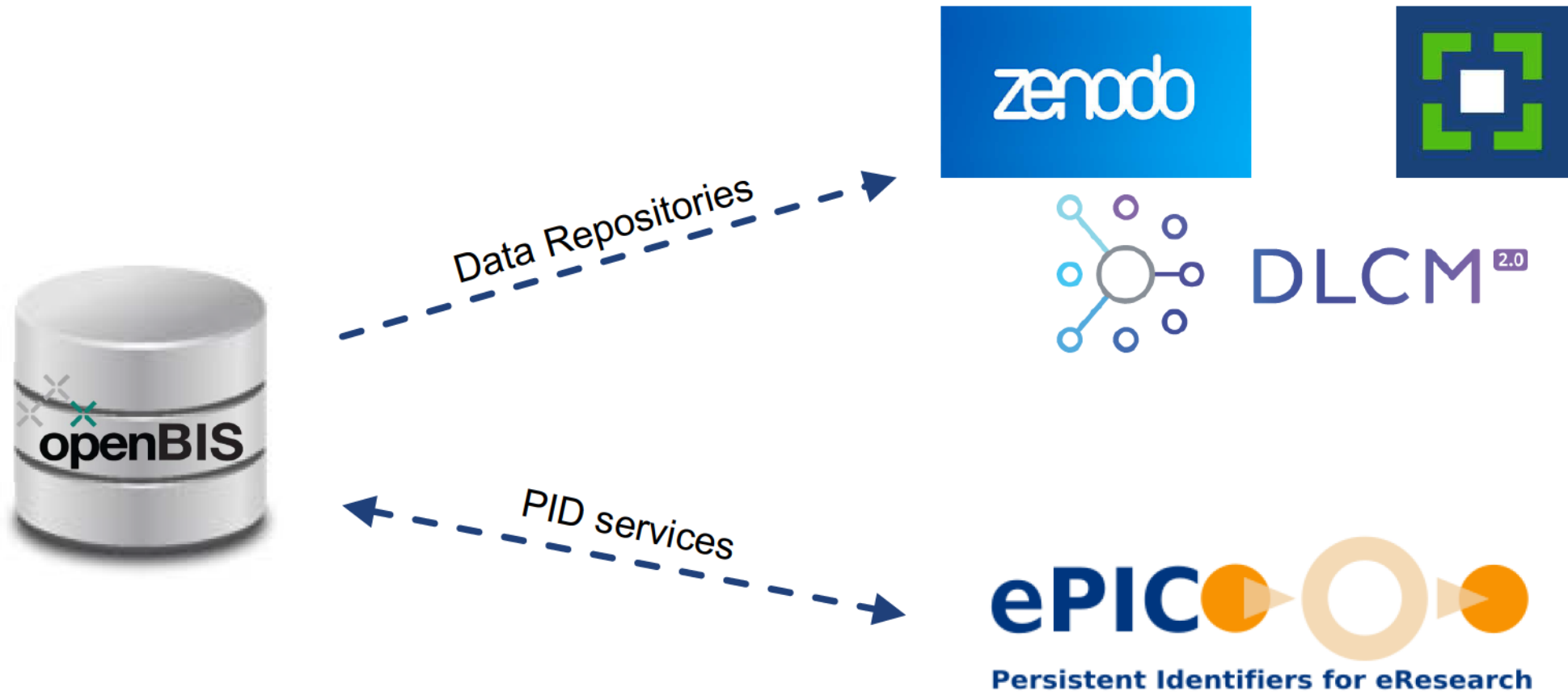
Selected	Type	Permid	Name
<input checked="" type="checkbox"/>	Space	DEFAULT_LAB_NOTEBOOK	DEFAULT_LAB_NOTEBOOK
<input checked="" type="checkbox"/>	Project	20190528221459905-1	DEFAULT_PROJECT
<input checked="" type="checkbox"/>	Project	20190611122038970-49	DEMO_PROJECT
<input checked="" type="checkbox"/>	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:

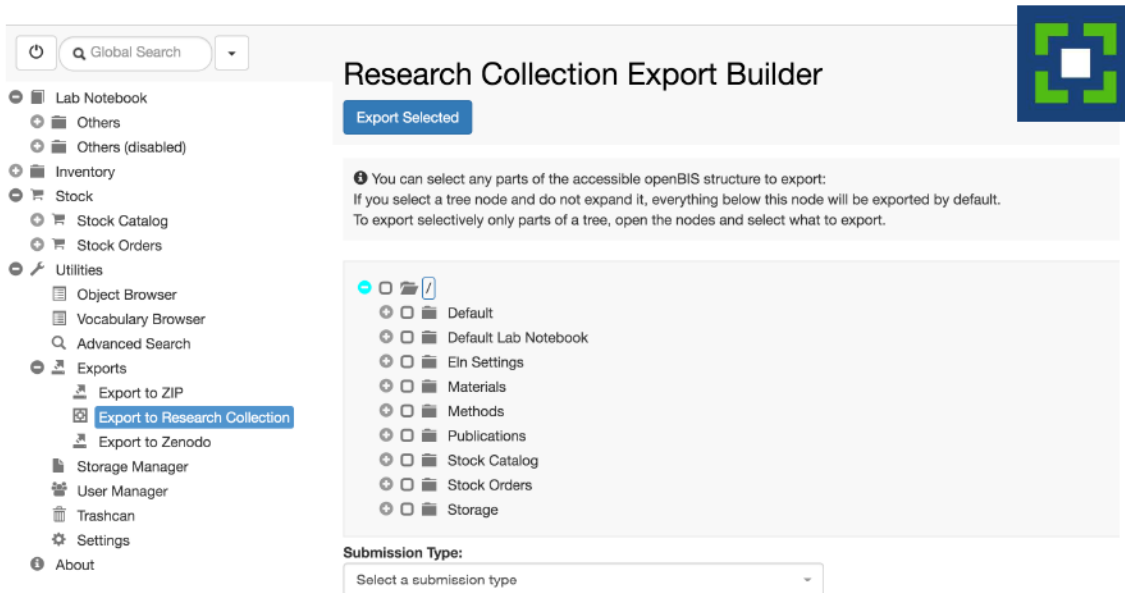
⚠ This operation is irreversible!

Password (*):

Integration with External Services



Integration with Data Repositories



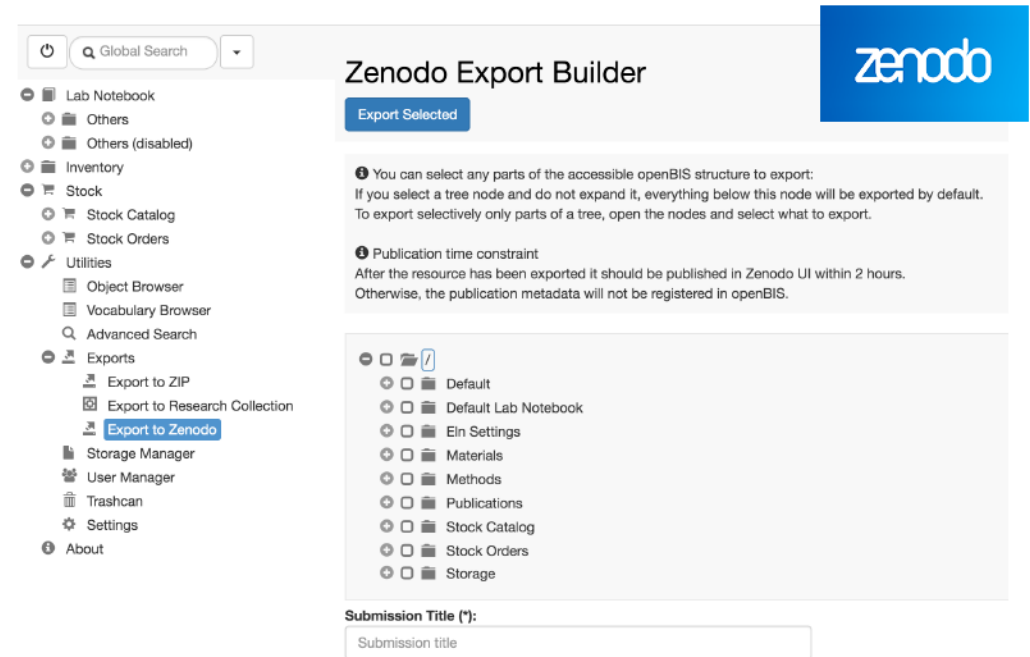
Research Collection Export Builder

Export Selected

You can select any parts of the accessible openBIS structure to export: If you select a tree node and do not expand it, everything below this node will be exported by default. To export selectively only parts of a tree, open the nodes and select what to export.

- Default
- Default Lab Notebook
- Ein Settings
- Materials
- Methods
- Publications
- Stock Catalog
- Stock Orders
- Storage

Submission Type:
Select a submission type



Zenodo Export Builder

Export Selected

You can select any parts of the accessible openBIS structure to export: If you select a tree node and do not expand it, everything below this node will be exported by default. To export selectively only parts of a tree, open the nodes and select what to export.

Publication time constraint
After the resource has been exported it should be published in Zenodo UI within 2 hours. Otherwise, the publication metadata will not be registered in openBIS.

- Default
- Default Lab Notebook
- Ein Settings
- Materials
- Methods
- Publications
- Stock Catalog
- Stock Orders
- Storage

Submission Title (*):
Submission title

- Published datasets receive a DOI and are preserved in the long-term
- Researchers comply with FAIR data principles
- Researchers comply with requirements (funders, institutions, journals)
- Easy data exchange with other researchers

Integration with PID Services

- Integration of ePIC PIDs in openBIS planned
- Provider: CSCS PID Service <https://pid.cscs.ch/services/>
- Implementation currently under consideration
- High-level workflow:
 1. Select openBIS object & get PermID URL



Collection Properties	
Collection	/SIS_HLUETCKE/DEMO_PROJECT/DEMO_PROJECT_EXP_1
PermID	20190403103907141-571
Collection Type	DEFAULT_EXPERIMENT
Registrar	Lütcke, Henry
Registration Date	2019-04-03 10:39:07
Project	/SIS_HLUETCKE/DEMO_PROJECT
Name	Demo experiment

<https://openbis-tst.ethz.ch/openbis/index.html?permId=20190403103907141-571>

Integration with PID Services

- Integration of ePIC PIDs in openBIS planned
- Provider: CSCS PID Service <https://pid.cscs.ch/services/>
- Implementation currently under consideration
- High-level workflow:
 1. Select openBIS object & get PermID URL
 2. Authenticate with CSCS ePIC PID service
 3. Generate PID
 - Suffix based on openBIS PermID; e.g. *21.17xxx / 20190403103907141-571*
 4. Resolve PID (requires authentication to openBIS)
 5. Optional: Update existing PID (e.g. when URL changes)



Challenges & Open Issues



- Integration with openBIS authentication and permissions
- Entity deletion → only create PIDs for frozen items?
- At which level of openBIS hierarchy should PIDs be granted?
- PID prefix administration (researchers / labs, university, service provider)
- Typical uses cases for PIDs vs. repositories
- Lack of user requests
- Training / education of researchers to raise awareness



Resources & Acknowledgements

Documentation & video tutorials:

<https://labnotebook.ch/>

SIS website:

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

Twitter:

https://twitter.com/ETH_SIS



Thanks to the entire SIS team!

