

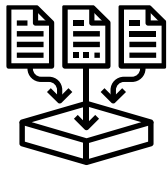
PSI

FAIR data pipelines

in atmospheric science



Thorsten Bartels-Rausch
Laboratory of Atmospheric Chemistry (LAC)



Versatile Data Collection – Field & Lab & Synchrotron



EPFL
Extreme Environments
Research Laboratory

Julia Schmale's laboratory brings in hands-on experience with Renku. Their science work for which ORD will be explored are international field studies in polar environment.

PSI
Laboratory of
Environmental Chemistry

Thorsten Bartels-Rausch has established openBIS as PSI-wide service. His team's science work for which ORD will be explored are laboratory studies at the large scale facility „Swiss Light Source“.

PSI
Laboratory of
Atmospheric Chemistry

Imad El Haddad's group brings in experience with openBIS. Their science work for which ORD will be explored are multi-diagnostic smog chamber studies.

CORE TEAM
Bartels-Rausch | Schmale | El Haddad

SOUNDING BOARD
Engaging the international community

Markus M. Frey, British Antarctic Survey, Cambridge, UK
Jennie Thomas, IGE, Grenoble, France
Jochen Stutz, University of California Los Angeles, USA
Megan Willis, Colorado State University, Fort Collins, USA
Jennifer G. Murphy, University of Toronto, Toronto, Canada
Paul Zieger, Stockholm University, Stockholm, Sweden
Katy Altieri, University of Cape Town, South Africa
Bruno Delille, Université de Liège, Belgium
Kerri Pratt, University of Michigan, USA
William Simpson, University of Alaska Fairbanks, USA

SERVICE PARTNER
Bringing in ORD expertise and ensuring compatibility with long-term ETH domain service development

ETH ZURICH SCIENTIFIC IT SERVICES
Caterina Barillari, openBIS data management

WSL
Ionut Iosifescu, envidat.ch repository

SWISS DATA SCIENCE CENTER
Fernando Perez-Cruz, Renku collaborative data tool

< > 2022_05__MayIssl

Ordner

- 📁 HidenMS
- 📁 Matlab
- 📁 NEXAFS
- 📁 Notes
- 📁 Photos
- 📁 Pressure
- 📁 RGA
- 📁 SES

Dokumente

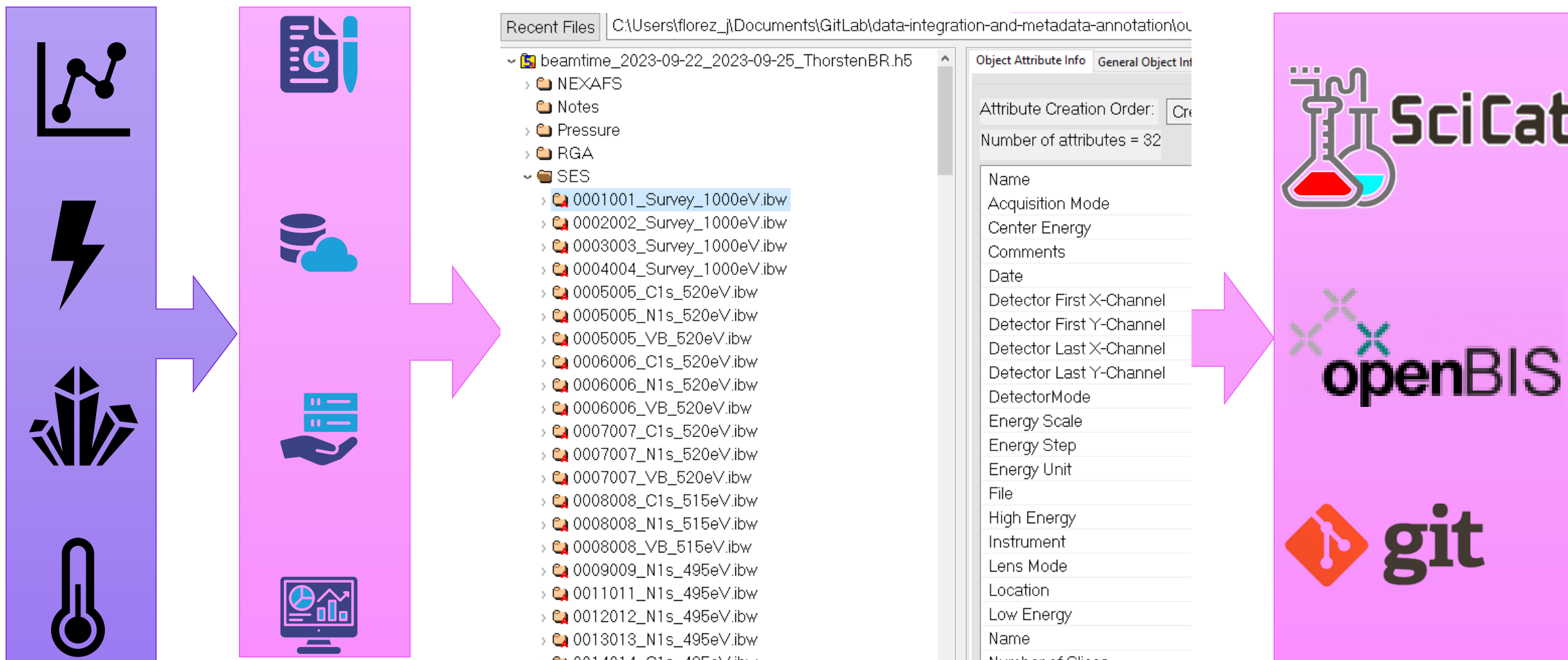
- 📄 May2022_DataList.csv

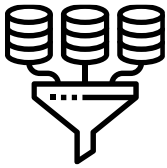
Andere

- 📄 May_2022.seq



Findable Data and Metadata





openBIS integration



Global Search

Default Experiment: 20230924_HCl on MgO ice_m20dC

+ New Edit Upload More ...

Objects

More ...

1-10 of 27 Rows per page: 10 COLUMNS FILTERS EXPORTS

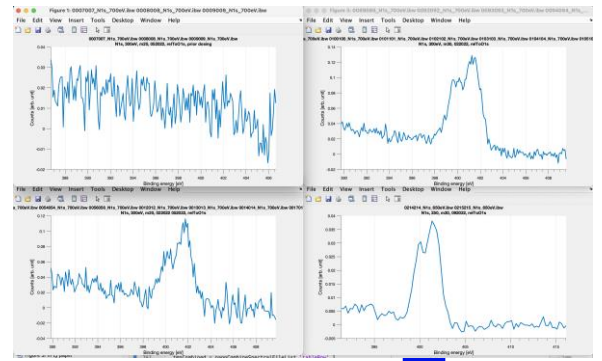
	Spectrum number	Results	Sample	Position x [mm]	Position y [mm]	Position z [mm]	Temperature reading [°C]	Pressure in sample cell [mbar]	Photon energy [eV]	Dwell time [s]	Pass Energy [eV]
						12.30	-22.89	1.42	395.0	0.80	20.00
						11.85	-22.98	1.40	750.0	0.52	20.00
						11.85	-23.00	1.40	750.0	0.52	20.00
						11.85	-22.85	1.41	750.0	0.52	20.00
						11.85	-23.13	1.40	750.0	0.52	20.00
						11.85	-23.31	1.40	395.0	0.80	20.00
						11.85	-22.88	1.42	750.0	0.52	20.00
	<input type="checkbox"/>	143	MgO powder,H2O,HCl	1.50	-3.00	11.80	-22.51	1.47	750.0	0.52	20.00
	<input type="checkbox"/>	144	MgO powder,H2O,HCl	1.50	-2.50	11.70	-23.00	1.44	750.0	0.52	20.00



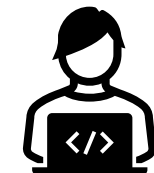
Modify Data with time

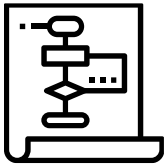
File Name	Date	SampleTemp_VV	SampleTemp_dC	Pressure_bar	SampleTemp_dC	Notes					
PHOENIX14032016_001.H5	15.03.16 02:23	100	200	NEXAFS	2340	2410	-10.01	1.14	-18.97	-19.03	NaCl solid 55% RH
PHOENIX14032016_002.H5	15.03.16 06:33	100	200	NEXAFS	2340	2400	-9.99	1.64	-15.12	-15.17	NaCl-water brine
									15.12	-15.16	NaCl-water brine
									15.08	-15.12	NaCl-water brine
									15.85		
									15.84	-15.88	NaCl solid 77% RH, actually
									15.86	-15.88	NaCl solid 77% RH, actually
									15.83	-15.9	-5.9
									15.83	-15.9	-5.9
									15.83	-15.9	-5.9
									15.83	-15.9	-5.9
									15.83	-15.9	-5.9
									15.84	-15.9	
									15.84	-15	
									15.9	-15	

```
tmpDataSelection = contains(FileList.name, '.ibw') ...
& contains(FileList.sample, 'Hexylamine ice') ...
& ~contains(FileList.sample, '(bad data)') ...
& ~contains(FileList.sample, '(excluded data)')...
& ~contains(FileList.sample, 'gas-phase')...
& ~contains(FileList.name, 'Survey')...
& ~contains(FileList.name, 'Auger')...
& FileList.xRayEkinRange_eV(:,1) == 700 ...
& contains(FileList.name, 'N1s')...
& month(FileList.lastModifiedDatenum) == 5 ...
& year(FileList.lastModifiedDatenum) == 2022 ...
& FileList.sampleTemp_dC >= -25 & FileList.sampleTemp_dC <= -15;
```



Project
Date
Experiment





Introducing well-defined data levels

EVOLUTION of a research project

Versatile data input and collaborative analysis



Issues	0	May 23, 2024
Merge requests	0	Add figure and data files bartels-rausch authored 1 month ago
Manage	>	
Plan	>	Added LJ and NEXAFS. WIP to restructure files bartels-rausch authored 1 month ago
Code	>	
Merge requests	0	Mar 05, 2024
Repository		Add the fig files bartels-rausch authored 3 months ago
Branches		Surface Concentration calculation now based on depth profile fitting. Also, a... ⋮
Commits		bartels-rausch authored 3 months ago

ACTRIS
Exploring the Atmosphere

Level 1
"Calibrated and quality assured data"

ACTRIS Data Centre

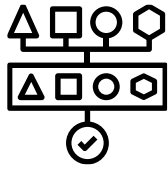
Home /

ACTRIS
Exploring the Atmosphere

Level 2
Approved and fully quality controlled data

ACTRIS Data Centre

Home /



Data Exchange and Archiving using structured H5 files



Data metadata

- Long name
- Short name
- Comment
- Unit

nexus v2024.02 documentation » User Manual and Reference Documentatio

NeXus

User Manual and Reference Documentation

<https://www.nexusformat.org/>

- [1. NeXus: User Manual](#)
 - [1.1. NeXus Introduction](#)
 - [1.2. NeXus Design](#)
 - [1.3. Constructing NeXus Files and Application Definitions](#)
 - [1.4. Strategies for storing information in NeXus data files](#)
 - [1.5. Verification and validation of files](#)
 - [1.6. Frequently Asked Questions](#)
- [2. Examples of writing and reading NeXus data files](#)
 - [2.1. Code Examples in Various Languages](#)
 - [2.2. Visualization tools](#)



CF MetaData

Conventions

Discussion

Governance

Training

Meetings

Vocabularies

CF Metadata Conventions

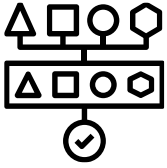
The CF metadata conventions are designed to promote the processing and sharing of files created with the [NetCDF API](#). description of what the data in each variable represents, and the spatial and temporal properties of the data. This enables quantities are comparable, and facilitates building applications with powerful extraction, regridding, and display capabilities. defines strings that identify physical quantities.

Conventions: Latest release (1.11) [HTML PDF](#) • Working draft [HTML PDF](#)

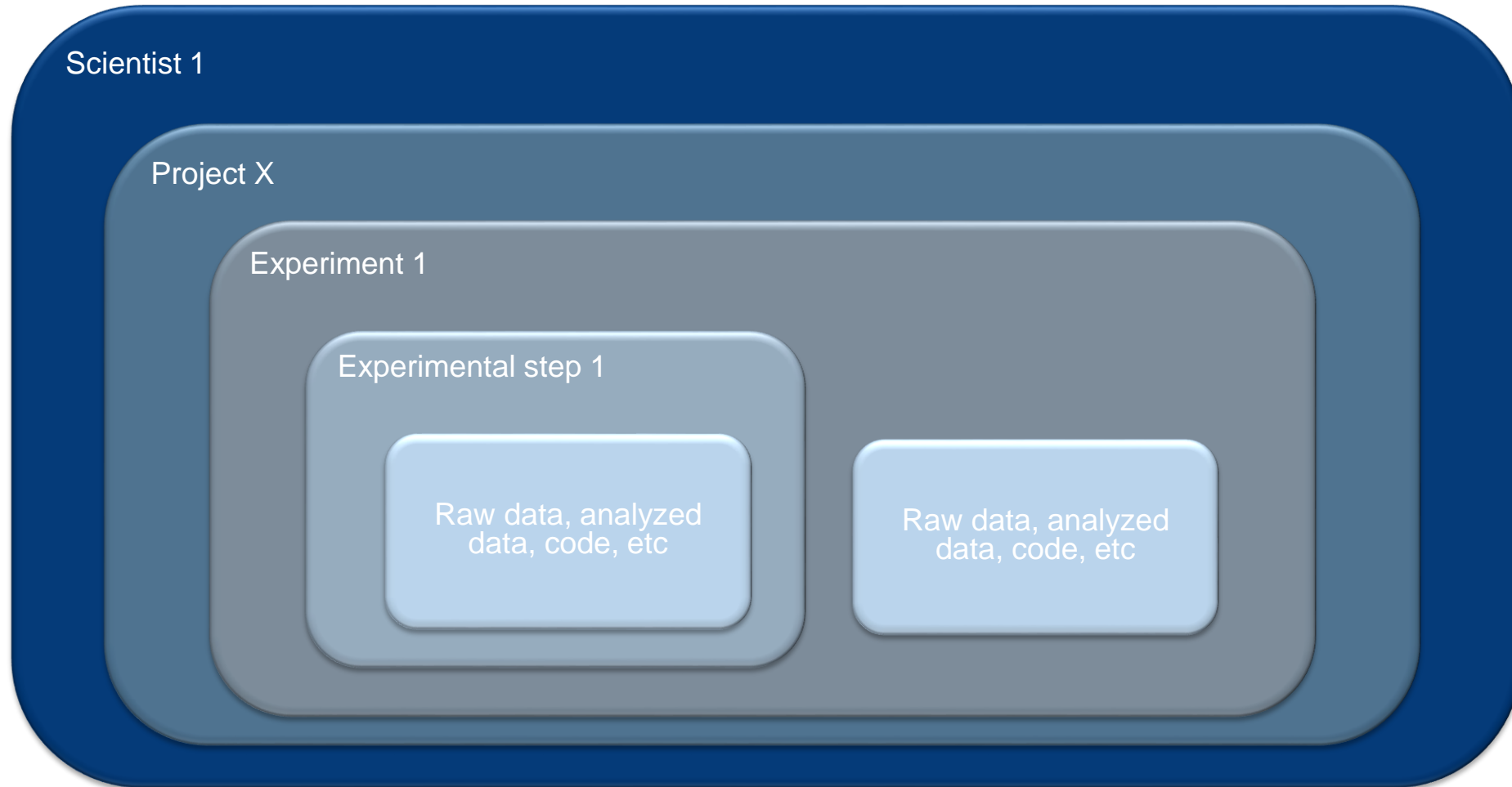
Vocabularies: [Standard names](#) • [Area types](#) • [Standardized regions](#)

Dataset metadata

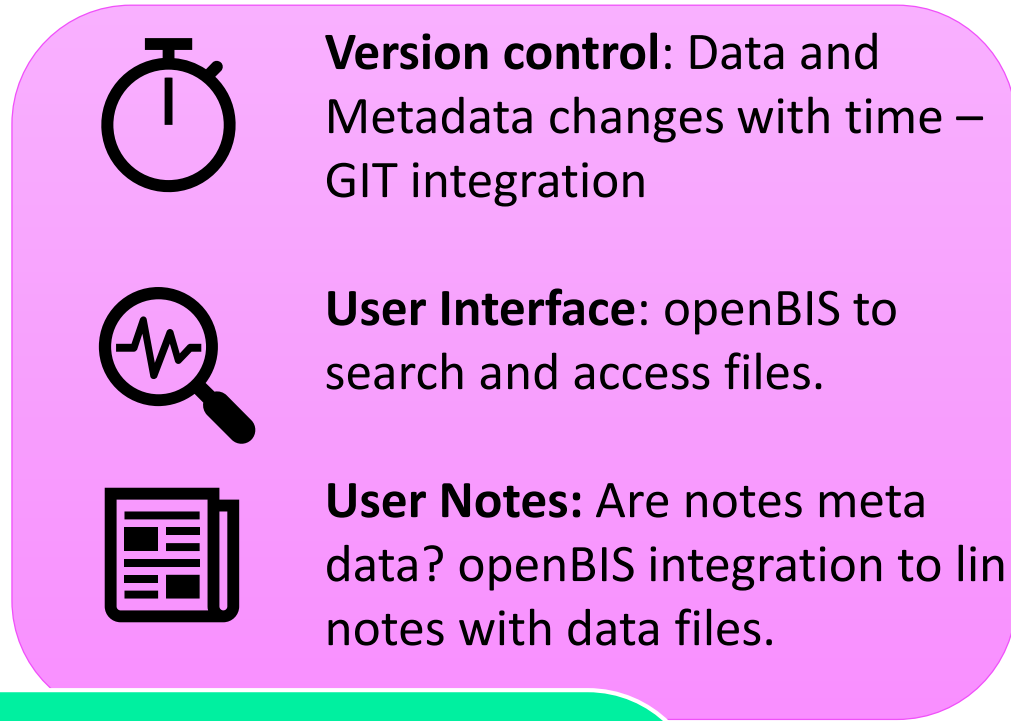
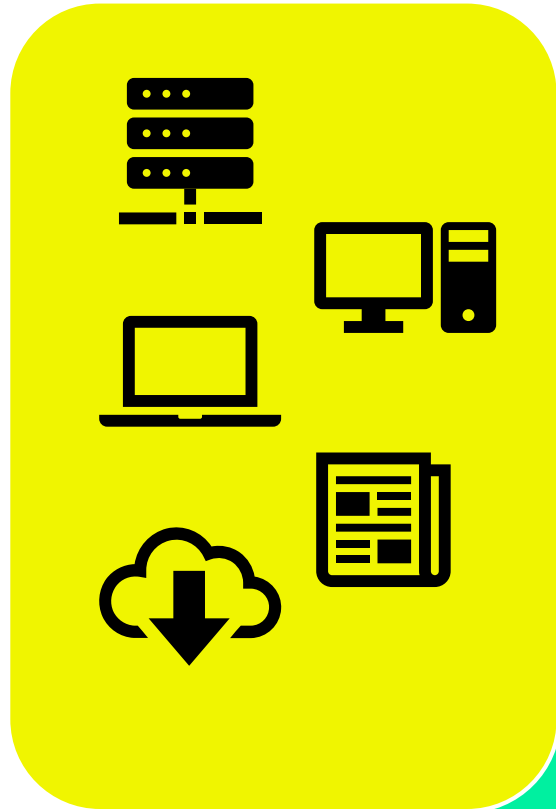
project	-
contact	contact (specifically E-mail address)
description	title (only info about content), comment (too broad in scope), source
experiment	-
actris_level	-
dataset_startdate	-
dataset_enddate	-
processing_filename	-
processing_date	-



Project and Experiment



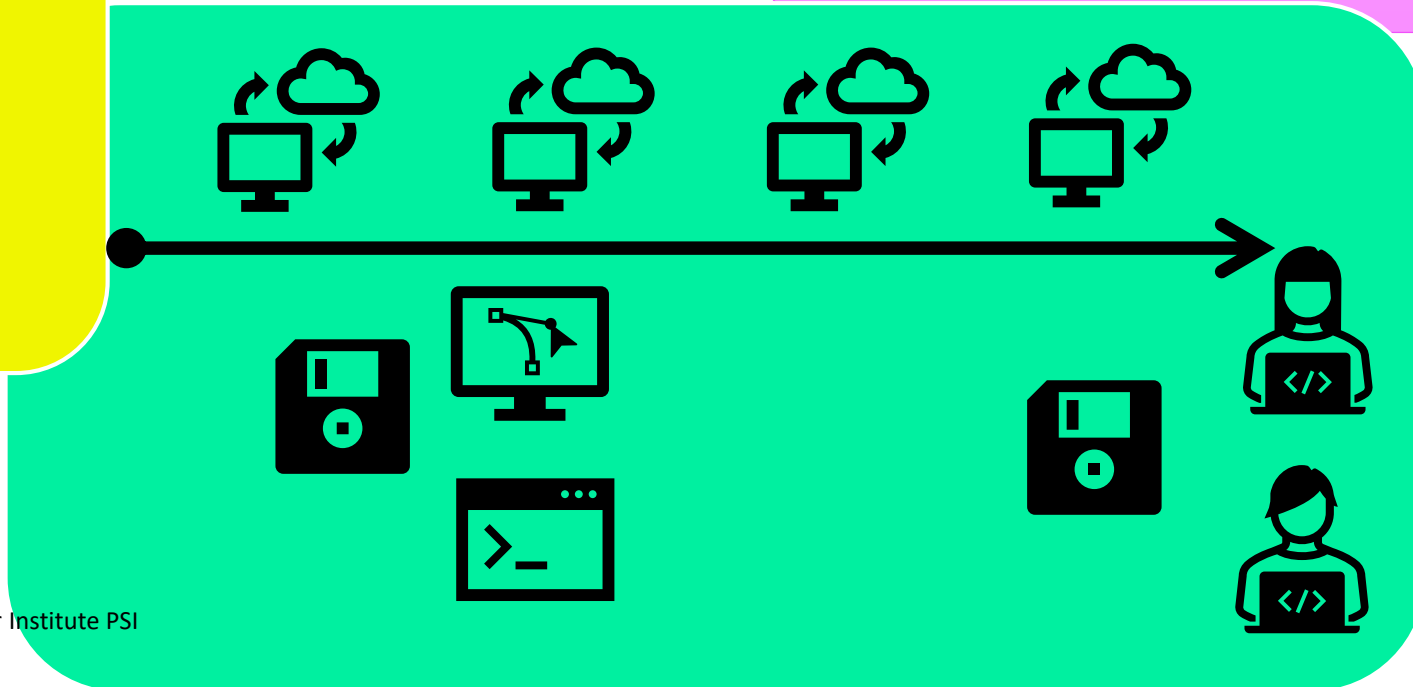
Summary & Questions



Version control: Data and Metadata changes with time – GIT integration

User Interface: openBIS to search and access files.

User Notes: Are notes meta data? openBIS integration to link notes with data files.



Thanks

- **Juan Felipe Florez Ospina**
- **ETH Domain for funding**
- **Alun Ashton, Carlo Minotti,**
- **Natasha, Lucia, Markus, Julia, Imad, Dave, Rob**

Bartels-Rausch, T., and Ammann, M. (2023). It is time to introduce the next generation of chemists to fair and open science: Chemical education, CHIMIA 77, 694-696, [10.2533/chimia.2023.694](https://doi.org/10.2533/chimia.2023.694)

