Scicat for Powder Diffraction at ESS

Point of view of Instrument Data Scientist

Céline Durniak
IDS for Diffraction (DREAM, BEER)

Agenda

1 Description of DREAM

2 Using Scicat for Powder Diffraction at ESS

3 Examples from other facilities

DREAM

Diffraction **R**esolved by **E**nergy and **A**ngle **M**easurements

One of the Tranche 1 instruments

Instrument features

- bi-spectral: thermal + cold
- pulse-shaping: high flux vs high resolution
- polarized (cold) neutrons
- 3D ^{10}B detectors

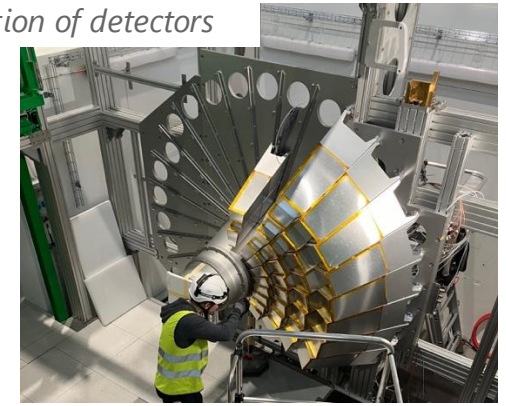
Science cases

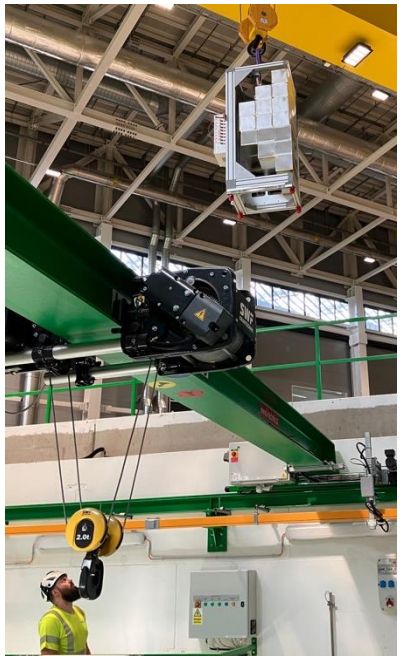
- Powder Diffraction
- Single Crystal Diffraction
- Pair Distribution Function
- SANS

Sample vessel

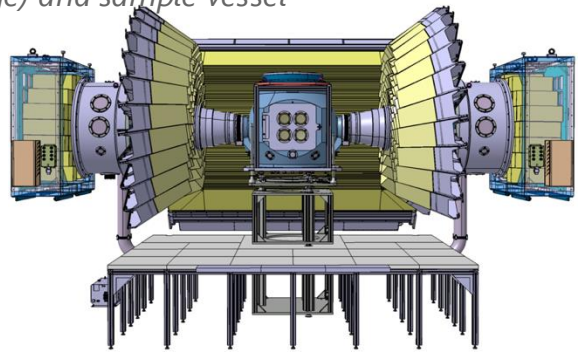
Experimental caves & control hutches

Installation of detectors





DREAM detector configuration (full coverage) and sample vessel



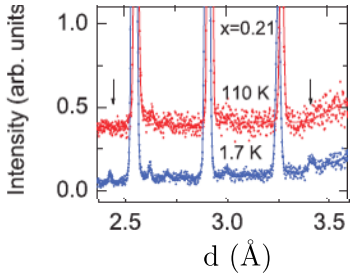
DREAM

Science Cases

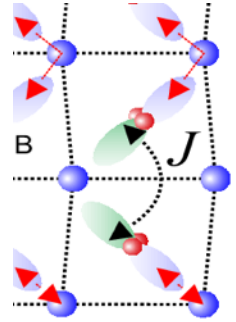
powders
single-crystals
nanoparticles
alloys
liquids

Magnetism

$Ba_{1-x}K_xFe_2As_2$

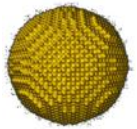


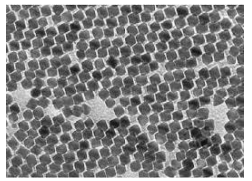
weak moments
phase diagrams of
superconductors
multiferroics



orbital ordering
charge ordering
distortion
magnetic exchange

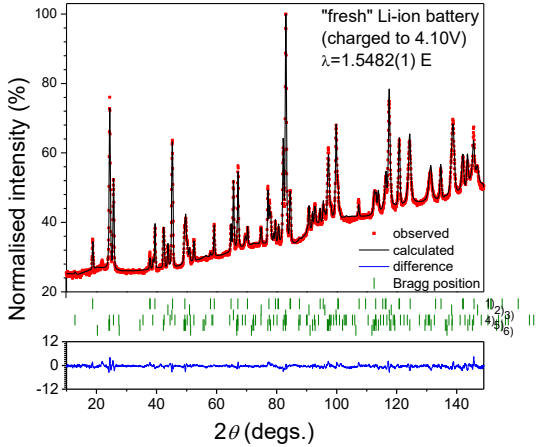
Nanostructures





magnetic nanoparticles
core-shell structures
self-assembly
synthesis

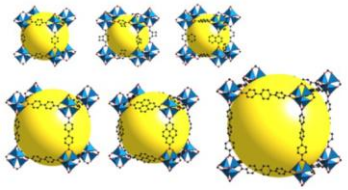
Energy Materials

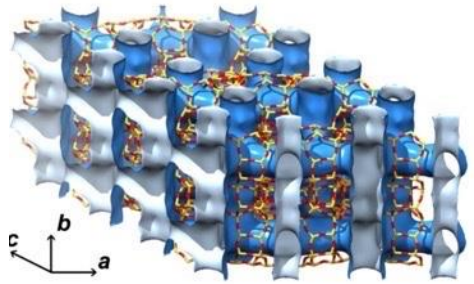


multiphase
catalysts
in-operandi
batteries

Large Unit Cells

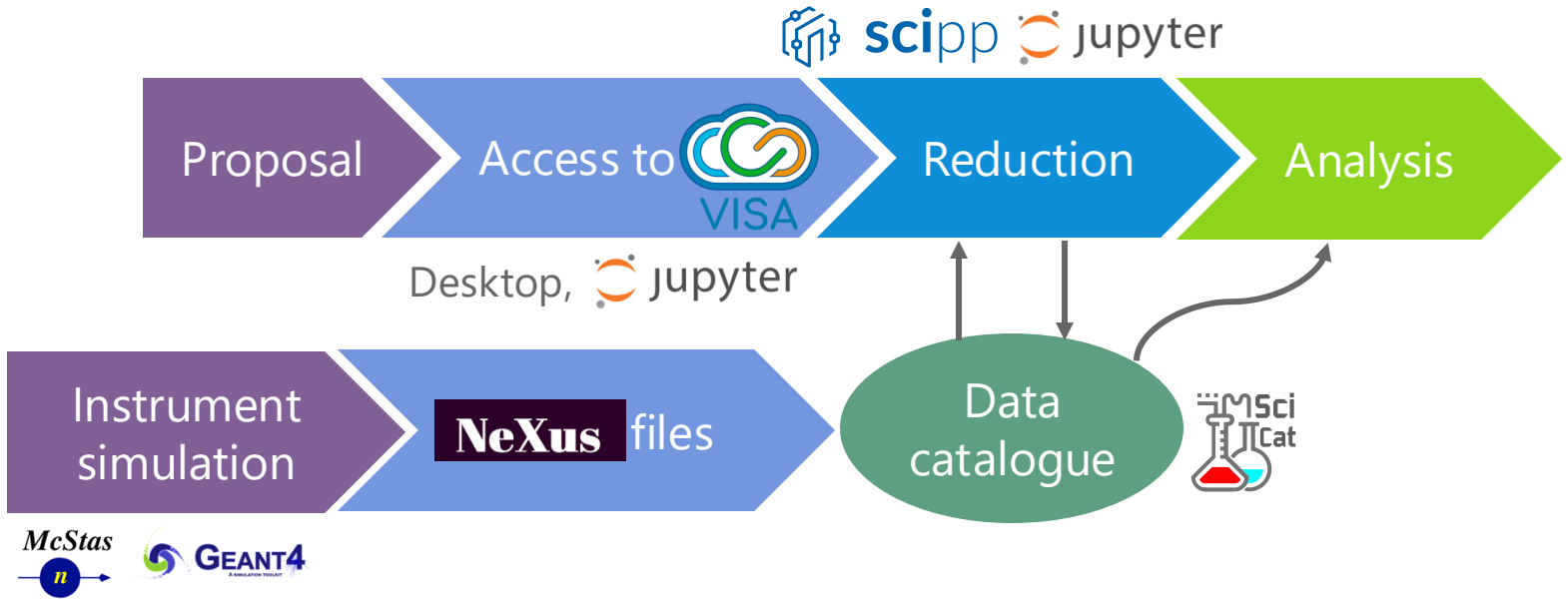
MOFs
Thermo-electrics
molecular sieves
H_2 - storage





Data workflow @ ESS

Software & frameworks for Powder Diffraction



Derived data

- different science cases to support
- no standard format in Diffraction

→ importance of metadata

scipp.github.io scicat.ess.eu nexusformat.org mcstas.org geant4.web.cern.ch

“Raw” and derived data on Scicat

Raw data

General Information

Dataset Name	Simulated Silicon powder at DREAM
Description	McStas/GEANT4 Si powder at DREAM (High Flux configuration)
Pid	20.500.12269/76f5ff02-2dc2-4bfb-a903-2ff28da91999
Type	raw
Creation time	2024-10-04 00:00
Keywords	POWDER_DIFFRACTION, DIFFRACTION, POWDER, ESS, DREAM, SI, SILICON, HIGH FLUX, DMSC_STAP, MCSTAS

Edit

Creator Information

Owner	Celine Durniak
Principal Investigator	Celine Durniak
Contact Email	celine.durniak@ess.eu
Owner Group	339400
Access Groups	ecdc,sims,dram,ess,scientific information management systems group,ess employees

File Information

Source Folder	/ess/data/dream/2024/339400/derived/ac716bda-81bf-11ef-8e41-5f58ffa4375a

Related Documents

Proposal	DREAM for DMSC STAP
Sample	Simulated Silicon Powder
Instrument	dream

Derived data

General Information

Name	DREAM demo reduced data for Raw sample id 20.500.12269/76f5ff02-2dc2-4bfb-a903-2ff28da91999, reduction id 0d7692ec-ca2d-46b8-bf9d-60d73254de28
Description	DREAM derived dataset created for DMSC STAP demo with raw sample id 20.500.12269/76f5ff02-2dc2-4bfb-a903-2ff28da91999, vanadium id 20.500.12269/084d8676-ca50-4a07-a16f-81ceffd064cf, Proposal 339400, Reduction id 0d7692ec-ca2d-46b8-bf9d-60d73254de28
PID	20.500.12269/e6edbebf-5e4b-46c4-a693-316699d4ccfa
Type	derived
Creation Time	2024-10-22 14:57
Keywords	DREAM, DMSC_STAP

Edit

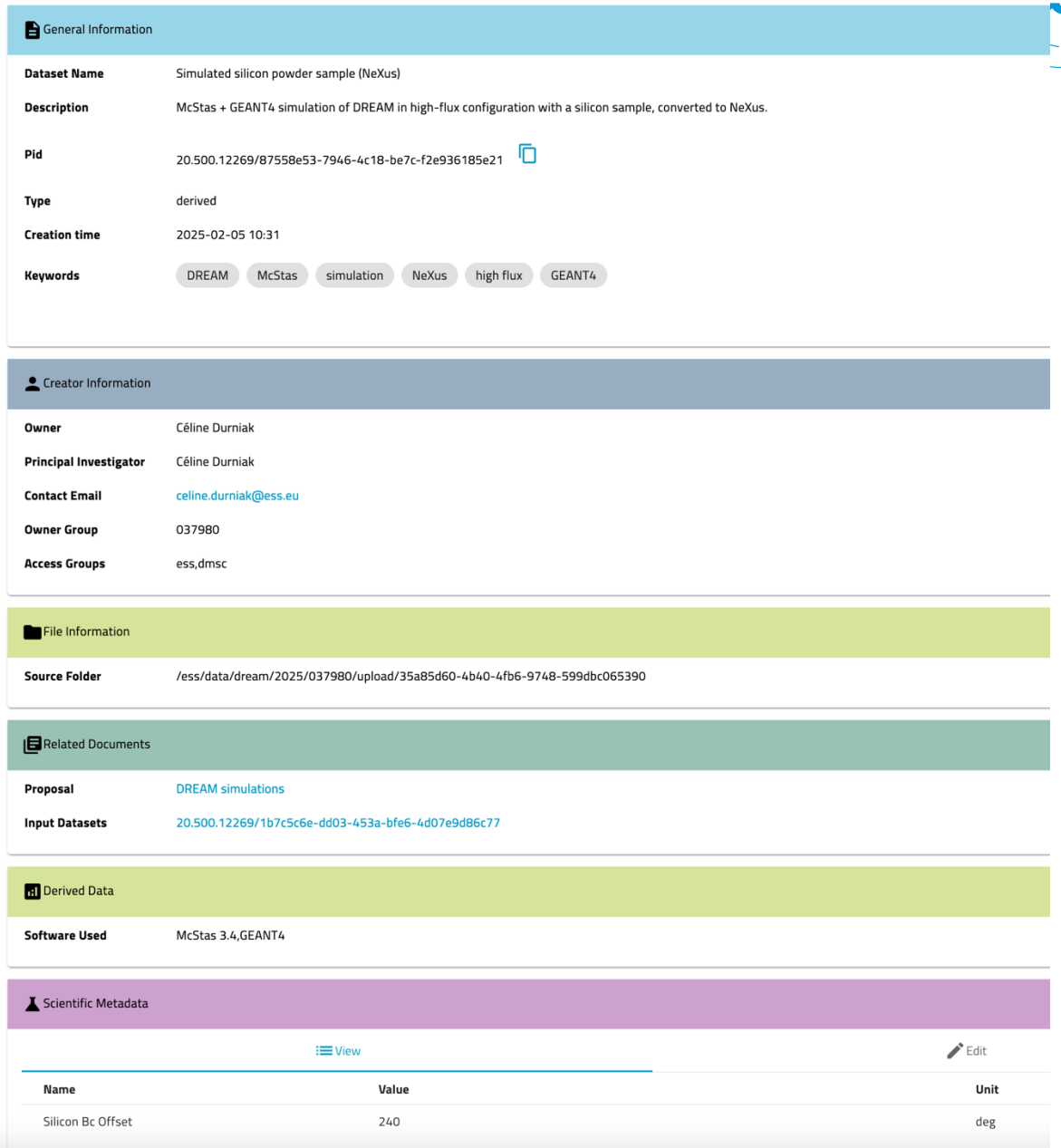
Creator Information

Owner	Celine Durniak
Principal Investigator	Celine Durniak
Contact Email	celine.durniak@ess.eu
Owner Group	339400
Access Groups	ecdc,sims,dram,ess,scientific information management systems group,ess employees

Simulated data on Scicat

McStas/GEANT 4 simulations (csv and NeXus files)

Name	Run No.	Source Folder
Simulated silicon powder sample (NeXus)		...9dbc06539(
Simulated vanadium sample (NeXus)		...6d20a9a0df
Simulated silicon powder sample		...cd314f9e24
Simulated MOF (MIL-53) sample, high flux		...63fd23ca3a
Simulation Si powder sample, high flux, new hkl		...a3f4fed1e6
Simulated vanadium sample, incoherent + coherent scattering, high flux		...70653d744
Simulated vanadium sample, incoherent scattering, high flux		...aef943309c
Simulated vanadium can, high flux		...0db4e77b0c
Simulation diamond powder sample in vanadium can, run 2		...138c17b23e
Simulation diamond powder sample in vanadium can, run 1		...8a3f8fcf3f



General Information

Dataset Name	Simulated silicon powder sample (NeXus)
Description	McStas + GEANT4 simulation of DREAM in high-flux configuration with a silicon sample, converted to NeXus.
Pid	20.500.12269/87558e53-7946-4c18-be7c-f2e936185e21
Type	derived
Creation time	2025-02-05 10:31
Keywords	DREAM, McStas, simulation, NeXus, high flux, GEANT4

Creator Information

Owner	Céline Durniak
Principal Investigator	Céline Durniak
Contact Email	celine.durniak@ess.eu
Owner Group	037980
Access Groups	ess,dmsc

File Information

Source Folder	/ess/data/dream/2025/037980/upload/35a85d60-4b40-4fb6-9748-599dbc065390

Related Documents

Proposal	DREAM simulations
Input Datasets	20.500.12269/1b7c5c6e-dd03-453a-bfe6-4d07e9d86c77

Derived Data

Software Used	McStas 3.4,GEANT4

Scientific Metadata

View | Edit

Name	Value	Unit
Silicon Bc Offset	240	deg

Experimental data

From other institute(s) SNS ORNL

POWGEN

Datasets / 20.500.12269/2b0d9e7f-a98f-462e-be0c-4ecf5a89840b /

Details | Datafiles | Related Datasets | Logbook | Lifecycle

General Information

Dataset Name	2020B Calibration Empty PAC instrument HR July13rd
Description	Empty instrument run at POWGEN.
Pid	20.500.12269/2b0d9e7f-a98f-462e-be0c-4ecf5a89840b
Type	raw
Creation time	2023-02-21 14:07
Keywords	powder diffraction, diffraction, powder, external, legacy, empty instrument

Creator Information

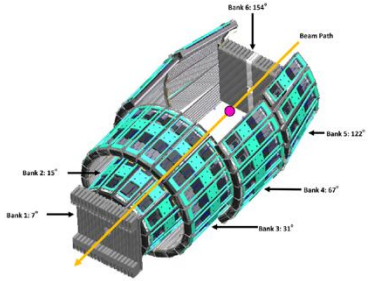
Owner	Qiang Zhang
Principal Investigator	Celine Durniak;Qiang Zhang
Orcid	orcid.org/0000-0003-0389-7039
Contact Email	celine.durniak@ess.eu
Owner Group	276591
Access Groups	ess,swap,dram,dream

File Information

Source Folder	/ess/data/dream/2023/276591/legacy/2b0d9e7f-a98f-462e-be0c-4ecf5a89840b
Size	672 MiB
Data Format	NeXus

SNS website doi.org/10.1016/j.nima.2021.165851

NOMAD



SciCat | ESS STAGING

Details | Datafiles | Related Datasets | Logbook | Attachments | Lifecycle

Public

General Information

Dataset Name	NOMAD Calibration file
Description	Calibration file for NOMAD instrument
Pid	20.500.12269/74988253-ca91-4305-a7a8-1b8251db8ab8
Type	raw
Creation time	2023-06-28 15:35
Keywords	diffraction, external, legacy, pair distribution function, NOMAD, calibration

Edit

Creator Information

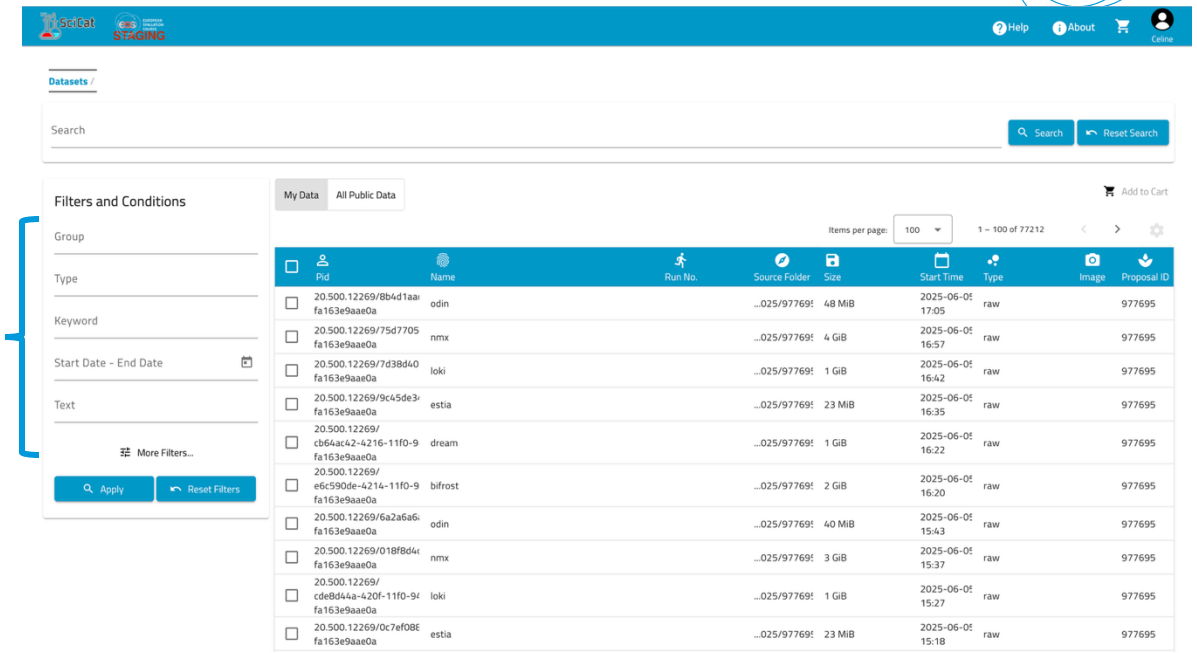
Owner	Yuanpeng Zhang
Principal Investigator	Celine Durniak; Qiang Zhang
Orcid	orcid.org/0000-0003-4224-3361
Contact Email	celine.durniak@ess.eu
Owner Group	662861
Access Groups	swap,dram,dream

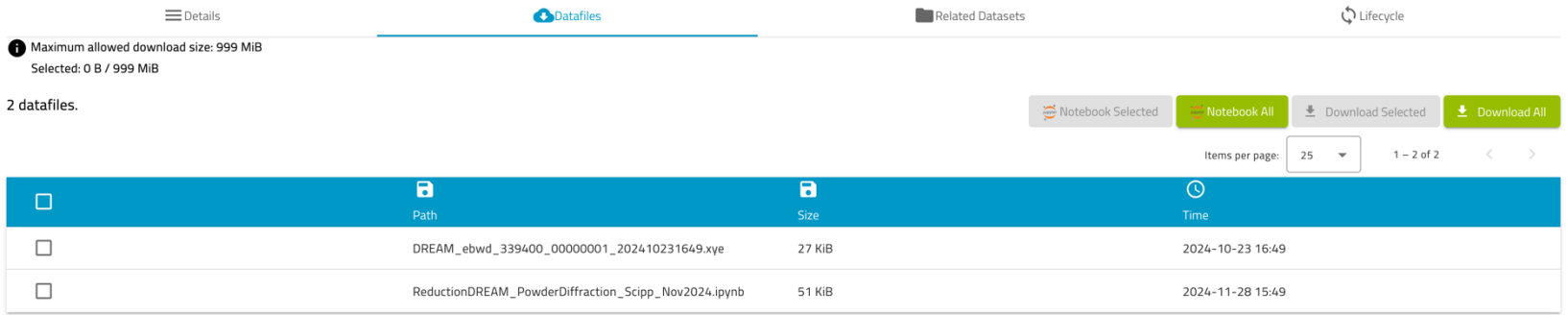
User feedback

Scicat

Webpage

- Unclear terminology
- No distinction between datafiles and scripts
- Cannot compare files from different datasets





Scicat

Accessing stored data

- `scp` from terminal
- `scitacean` in Python script or Jupyter notebooks
- direct download from Scicat webpage for small files

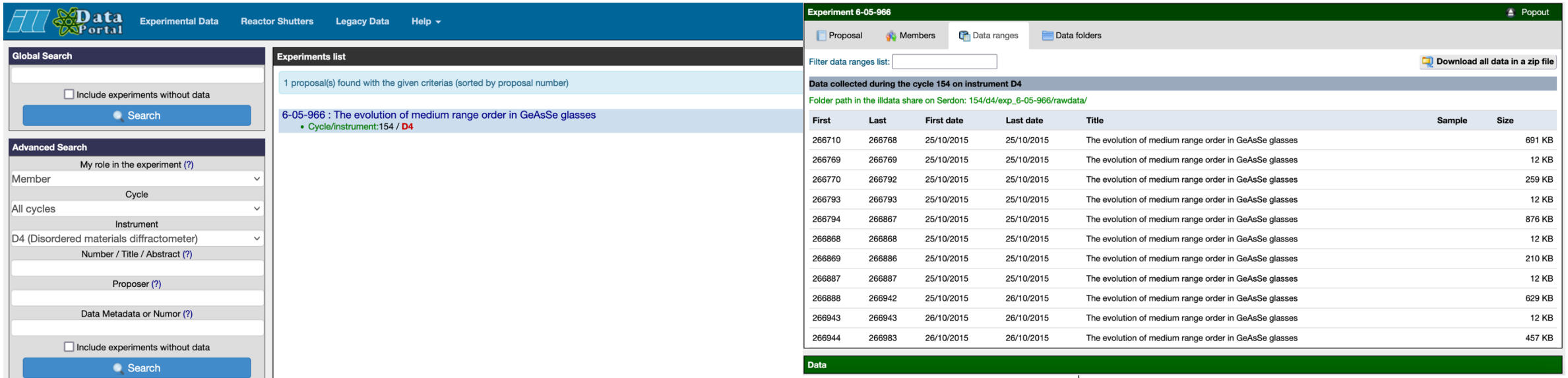
Unknowns at this stage of the project

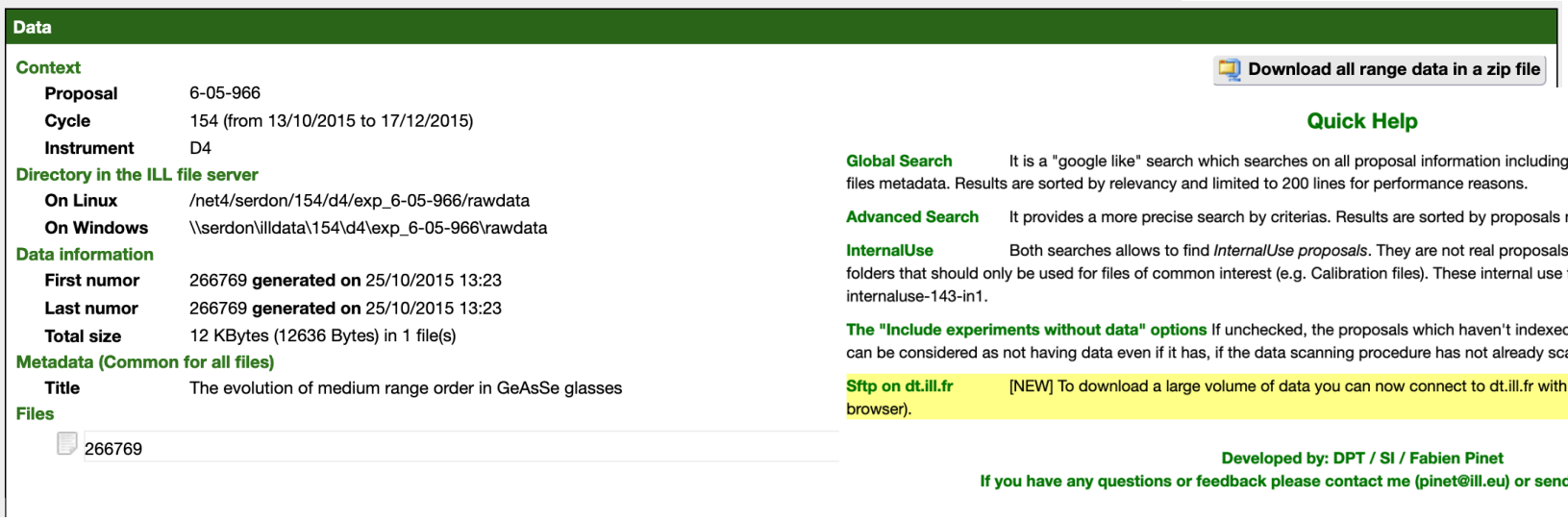
- storing electronic logbooks
- interface with Scichat: any filters?

Examples from other facilities

Examples from other facilities

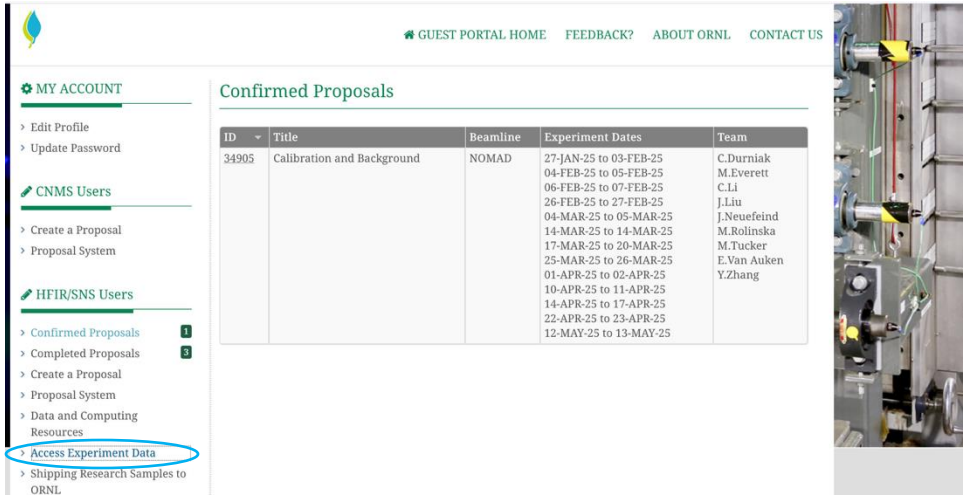
ILL data.ill.eu

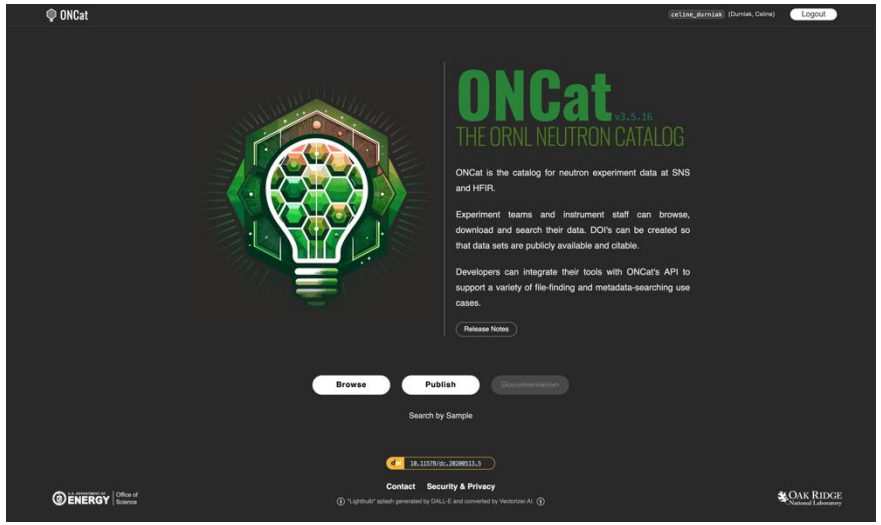


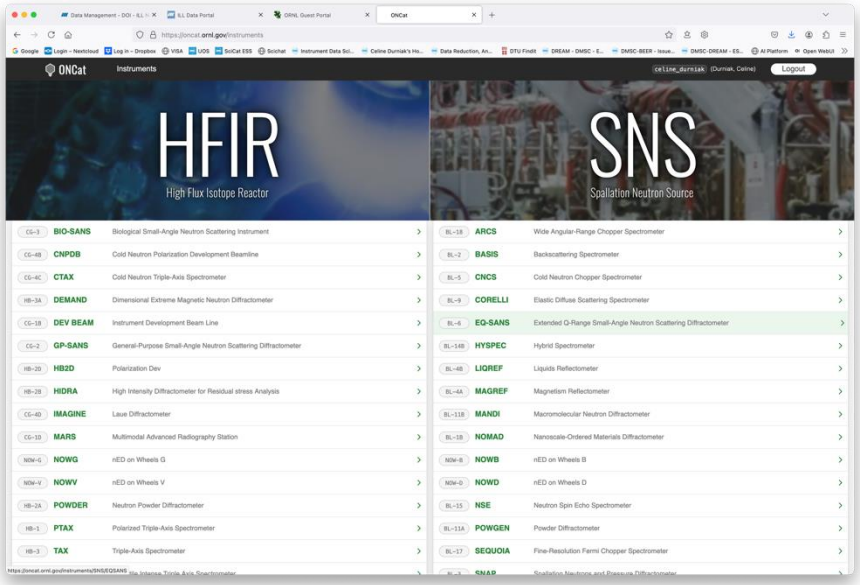


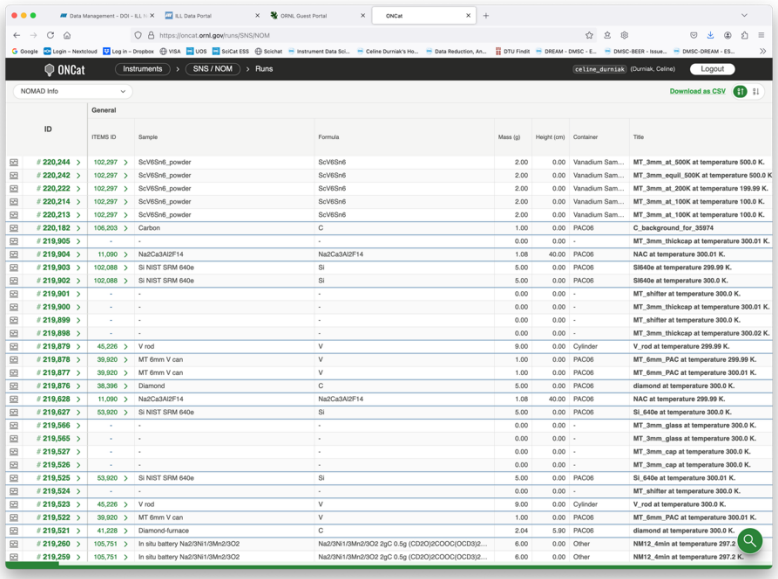
Examples from other facilities

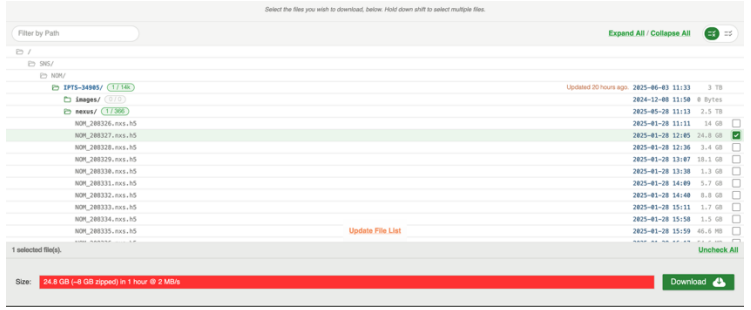
SNS ORNL











Examples from other facilities

SNS ORNL

List of methods and commands to download data

Terminal (SSH)

scp

bash

```
> scp -r <your-username>@analysis.sns.gov:/SNS/NOM/IPTS-34905 .
```

rsync

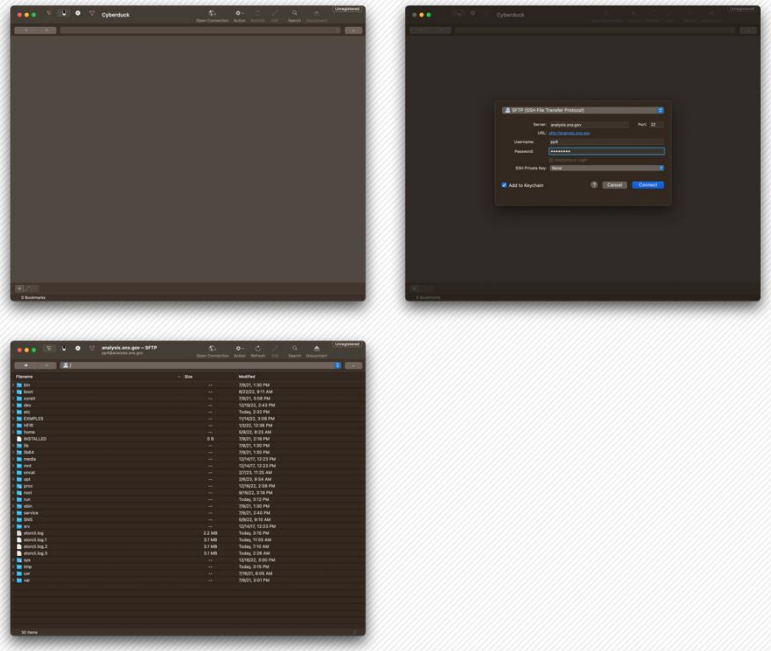
bash

```
> rsync -rP --rsh=ssh <your-username>@analysis.sns.gov:/SNS/NOM/IPTS-34905 .
```

CyberDuck

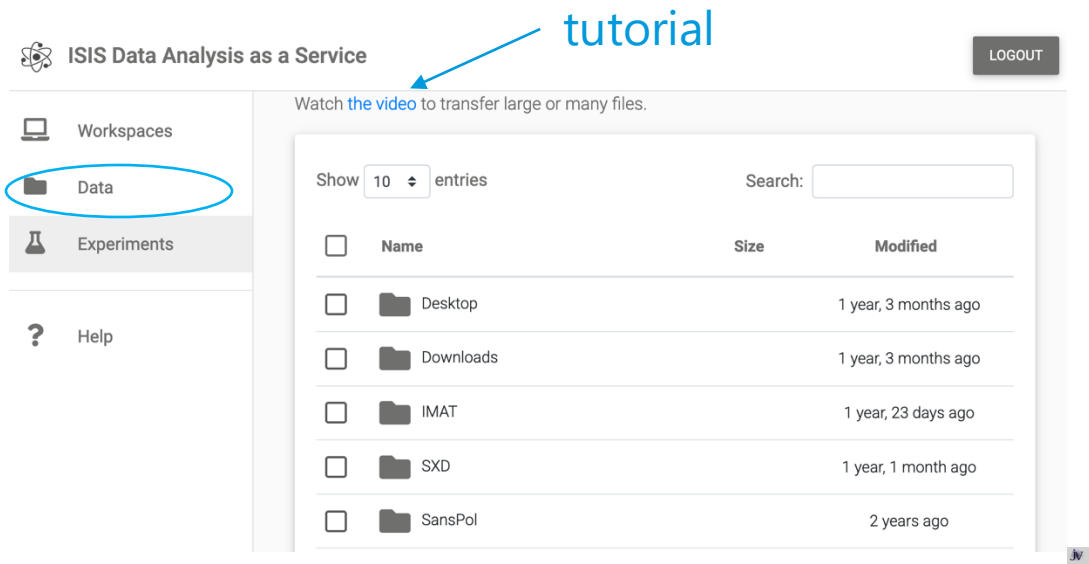
Download CyberDuck Client

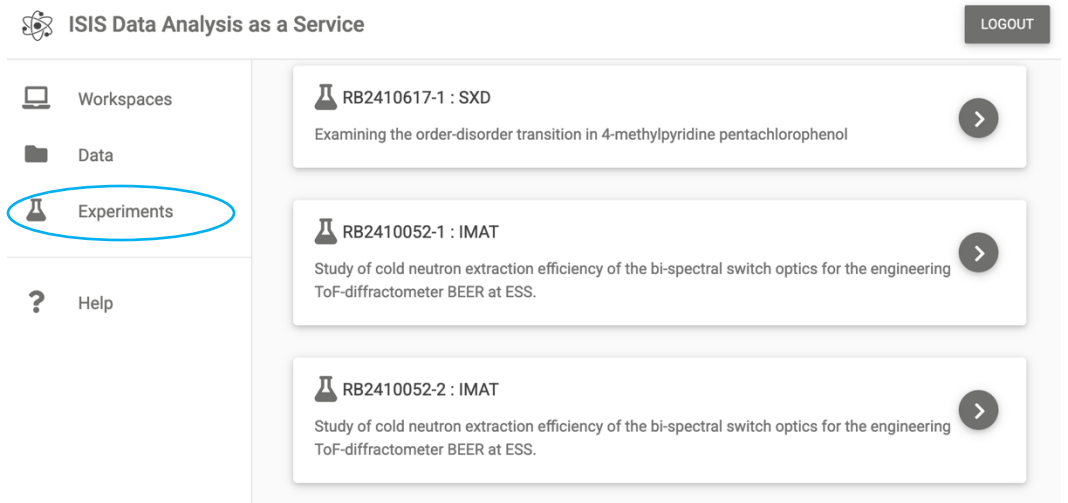
Protocol	SFTP (SSH File Transfer Protocol)
Server	analysis.sns.gov
Port	22
Username	celine_durniak
Password	********
Directory	/SNS/NOM/IPTS-34905



Examples from other facilities

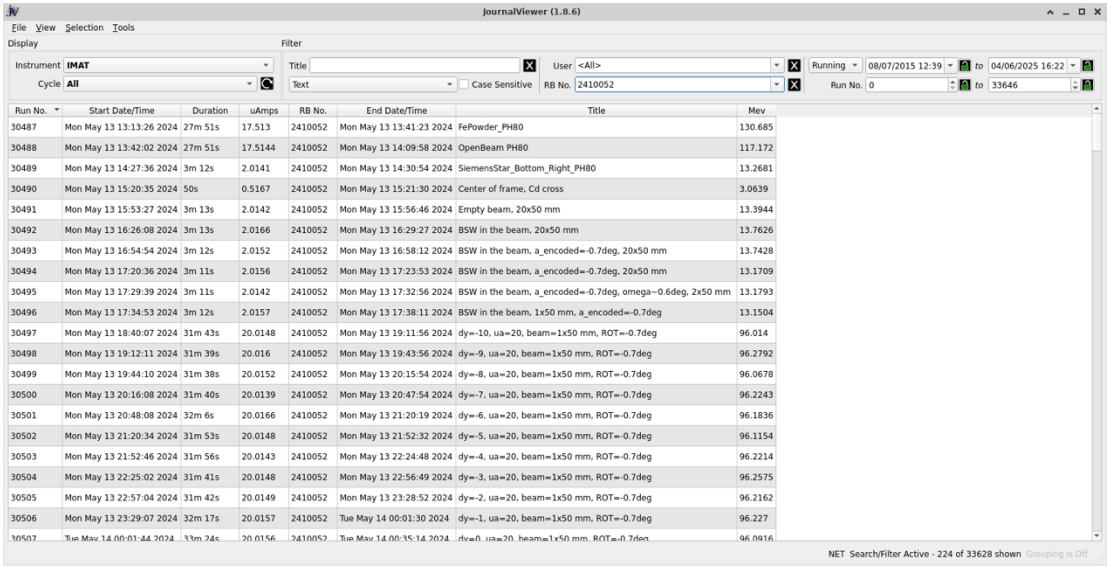
ISIS Data Analysis as a Service (IDAaaS)





Journal viewer

Summary of data and metadata
Different filters
Customizable display
Saving to file



Conclusion

Usage of Scicat

Storage

- simulated data (proposal)
- experimental data from other facilities (testing ESS data processing workflow)

Usage

Download / upload ”raw” and derived data