Data processing for BEER

Updates

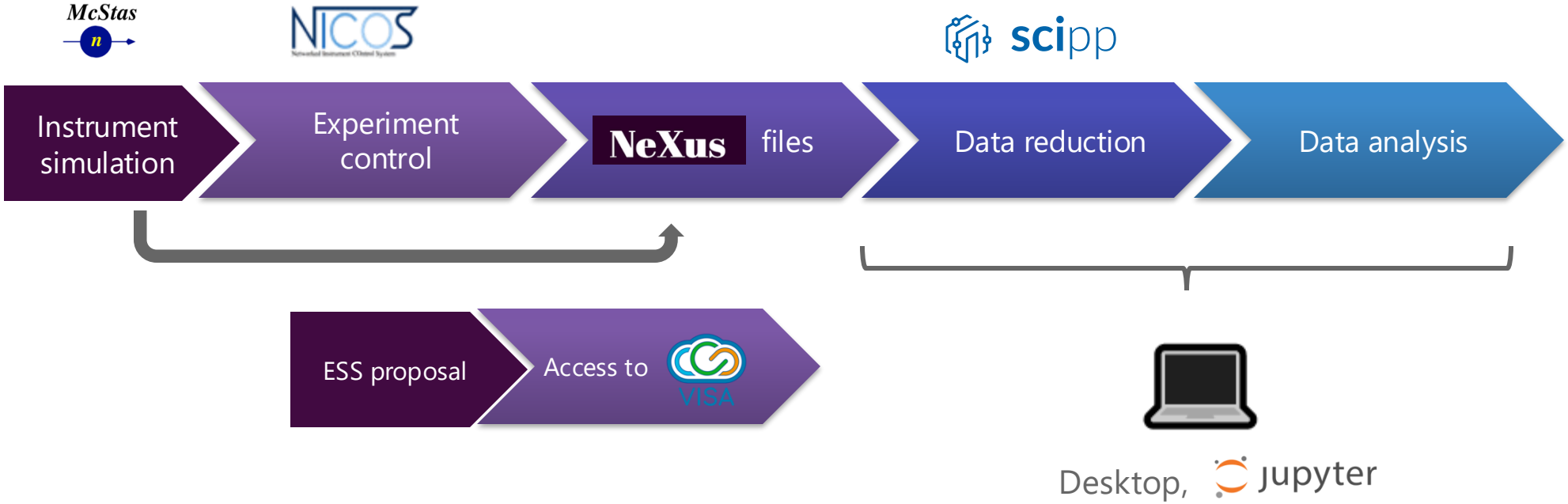
Céline Durniak

IDS for Diffraction (DREAM and BEER)

2025-09-26

Data workflow @ ESS

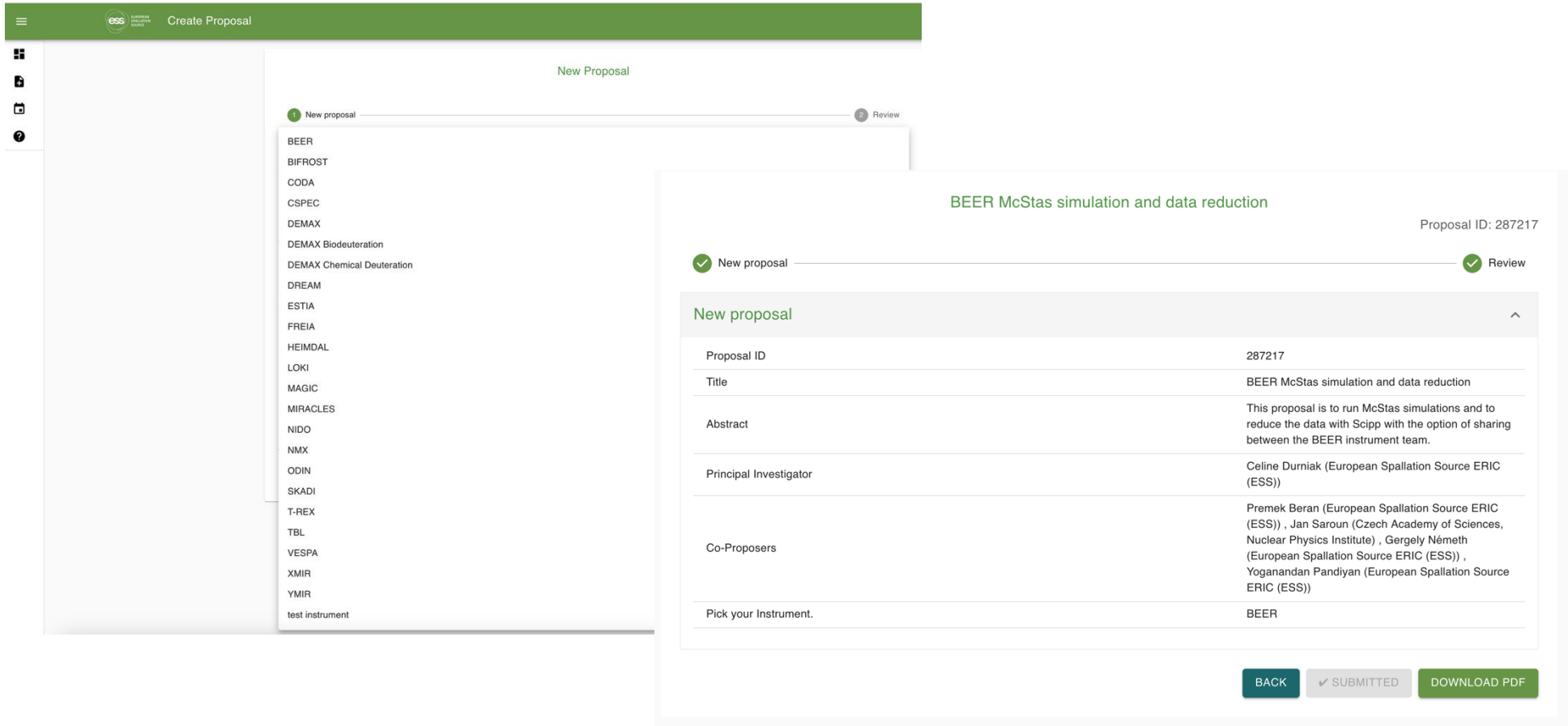
Software & frameworks



scipp.github.io nexusformat.org mcstas.org

ESS User Proposal

Request to access VISA

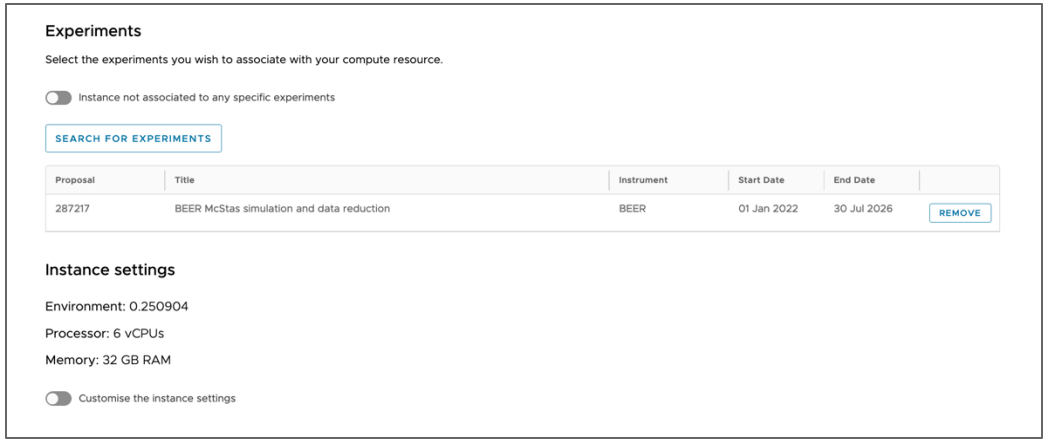


→ Proposal number and access to VISA

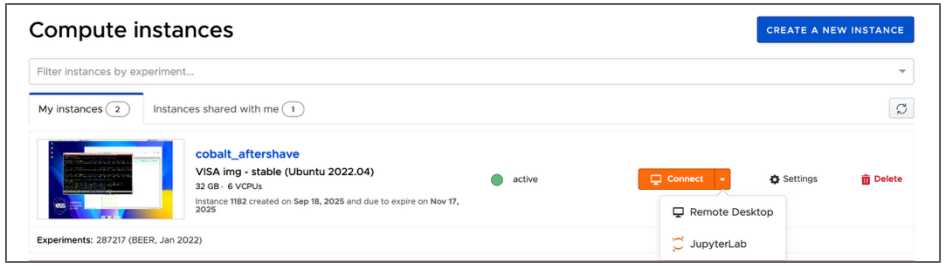
VISA

Access to computing resources

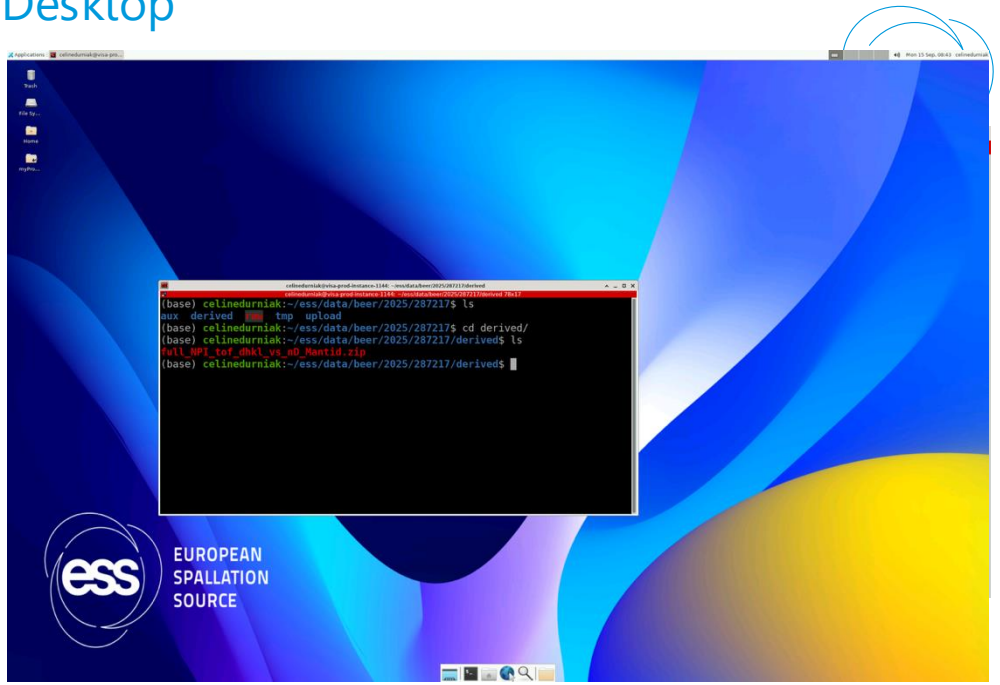
- Creating instances



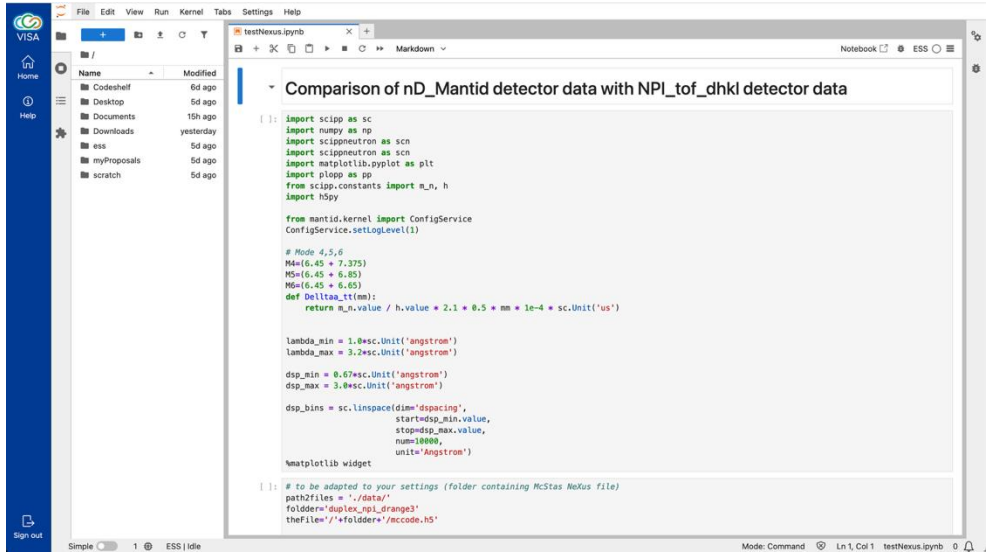
- Access to desktop or Jupyter lab



Desktop



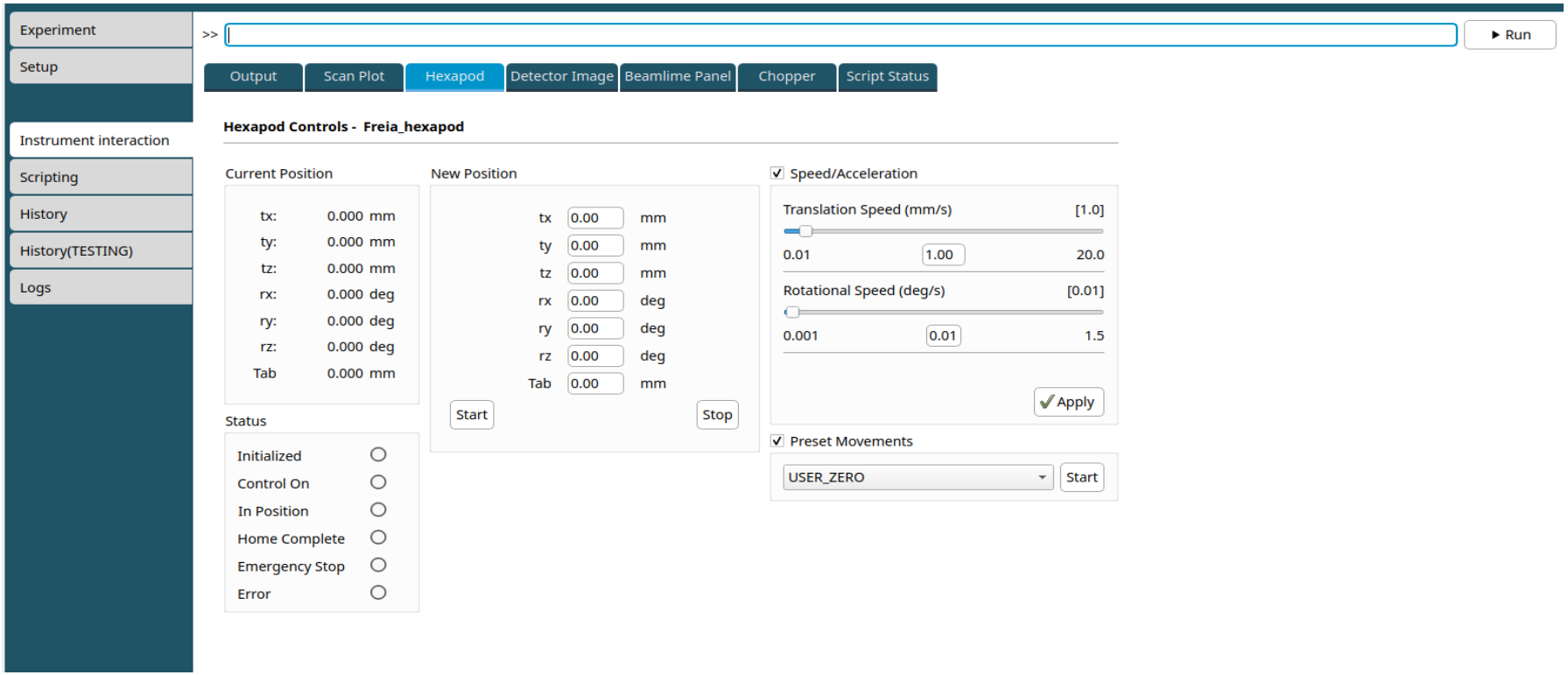
Jupyter Lab



Instrument control

NICOS

- Symétrie Hexapod Control Panel panel UI – joint work for BEER and FREIA



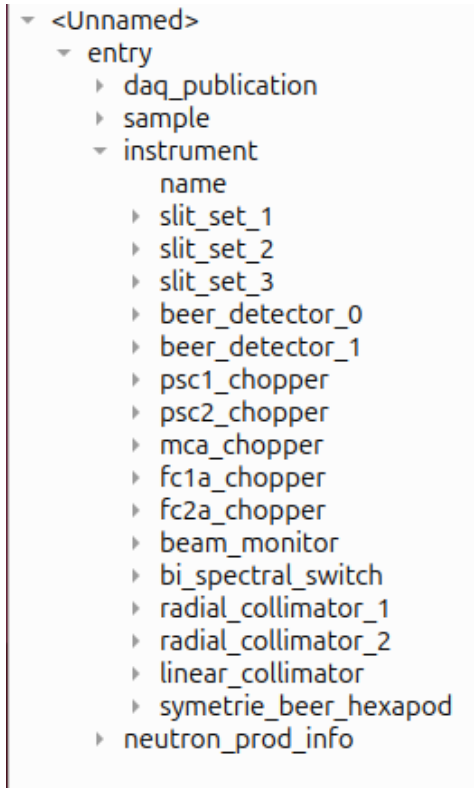
- Currently waiting for BEER NICOS server to be provisioned

ESS NeXus file

Neutron events & instrument settings

- Work in Progress
- Stores
  - time and positions on detectors
  - settings about
    - slits
    - choppers
    - sample environment
    - monitors…

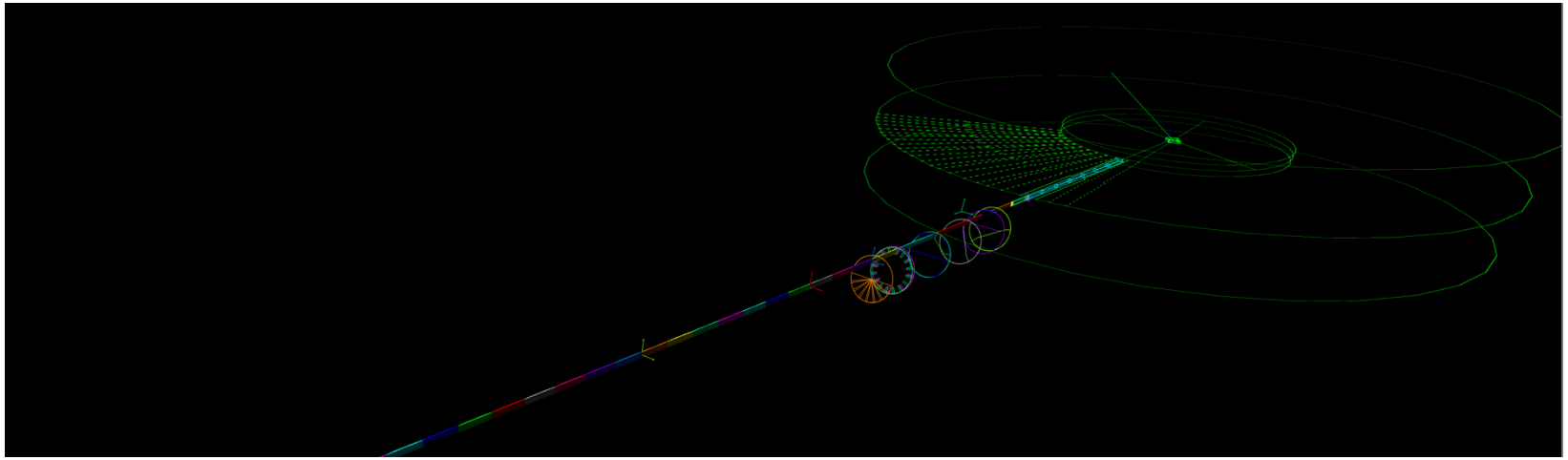
Draft of ESS NeXus tree structure for BEER



Instrument simulation

McStas

- 2 ±90° detector banks
  - 2D flat panels ✅
  - 3D layered structures ◕
- “Mantid” NeXus output files ✅
- Modulation and pulse-shaping chopper modes of operation ✅



Data reduction

scipp

Multi-dimensional data arrays with labelled dimensions

Scipp

Scippneutron

Neutron-scattering specific

Utility for NeXus files with seamless Scipp integration

Scippnexus

tof

Simple tool to create time-of-flight chopper cascade diagrams

Plotting library

Plopp

Sciline

Tool to build scientific pipelines

esssans

essdiffraction

esspolarization

...

ESS-specific technique submodules

Scipp

Data reduction

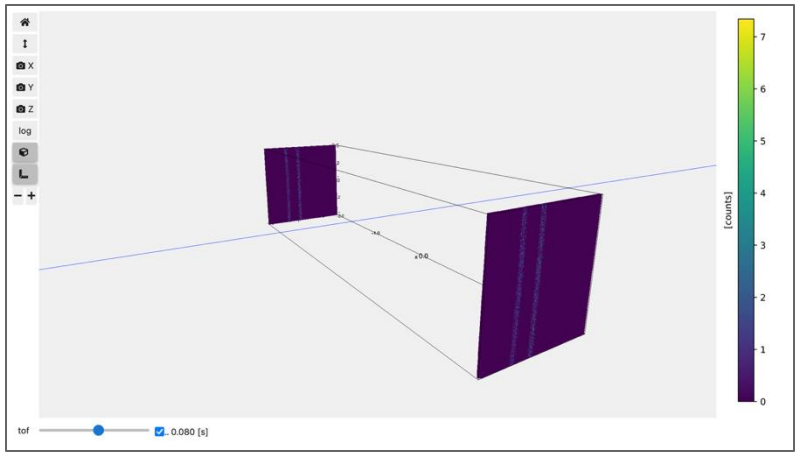
Existing algorithms

- loading McStas NeXus files (Mantid)
- selecting banks
- adding coordinates
- converting to d-spacing, λ…
- binning, histogramming
- 1, 2, 3D plotting

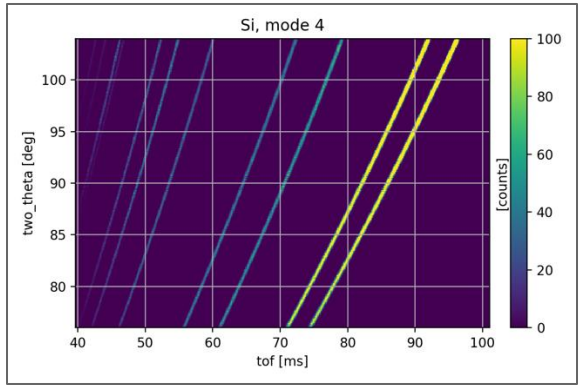
Specific algorithms for BEER

- 1D peak finding (WIP)
- modulation correction
- BEER NeXus file loader (WIP)

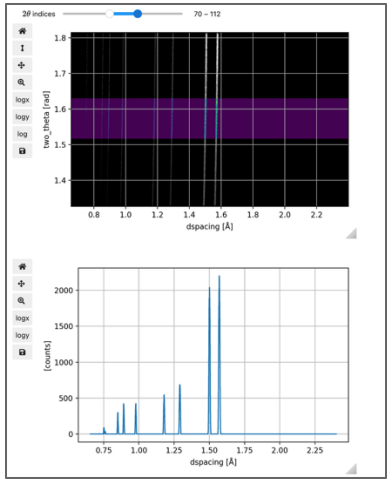
Instrument view with widget



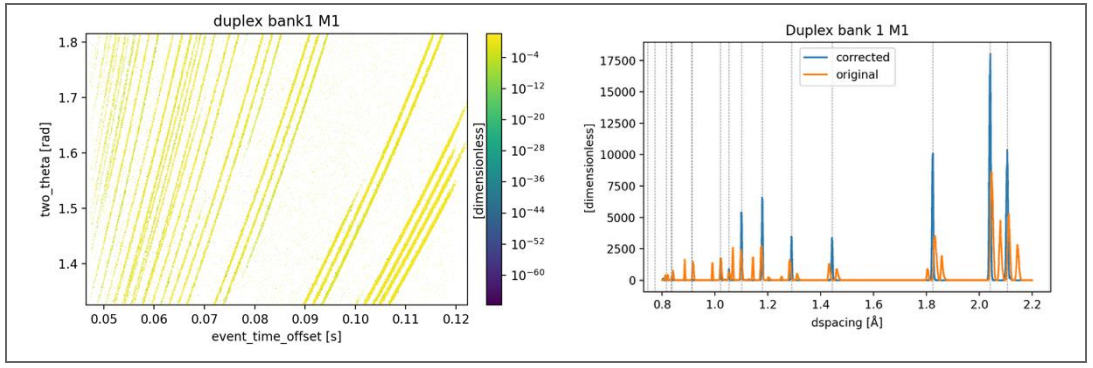
Pulse shaping mode

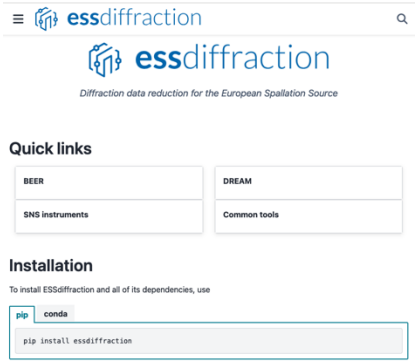


1, 2D plots with widgets



Modulation correction



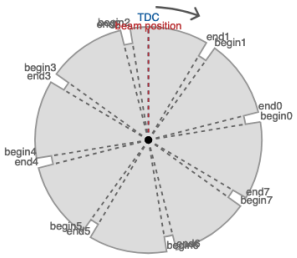


Data reduction

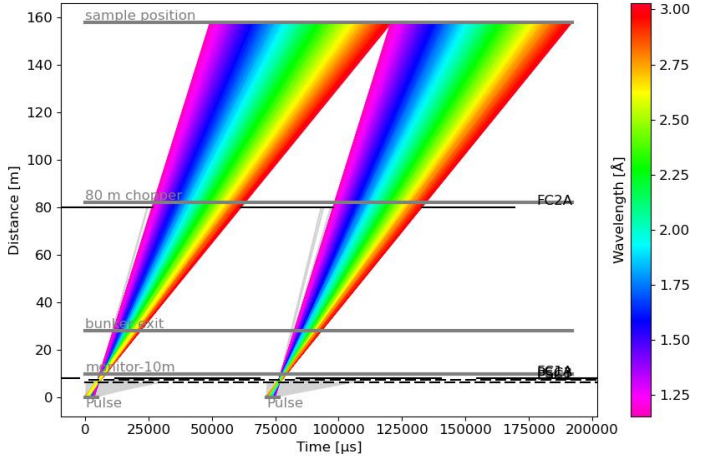
Choppers / Commissioning tools

▾ DiskChopper (slit: 8)

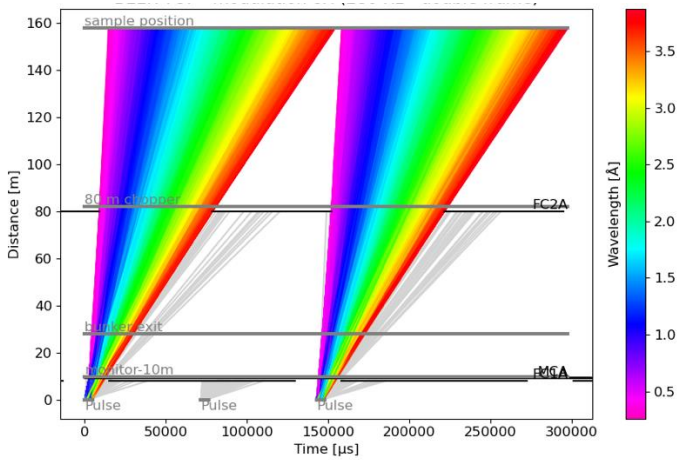
axle_position	scipp	Variable	()	vector3	m	[0. 0. 9.3]
frequency	scipp	Variable	()	float64	Hz	-280.0
beam_position	scipp	Variable	()	float64	deg	0.0
phase	scipp	Variable	()	float64	deg	639.2696515881335
slit_begin	scipp	Variable	(slit: 8)	float64	deg	639.270, 684.270, ..., 909.270, 954.270
slit_end	scipp	Variable	(slit: 8)	float64	deg	644.270, 689.270, ..., 914.270, 959.270
slit_height	scipp	Variable	(slit: 8)	float64	m	0.05, 0.05, ..., 0.05, 0.05
radius	scipp	Variable	()	float64	m	0.375



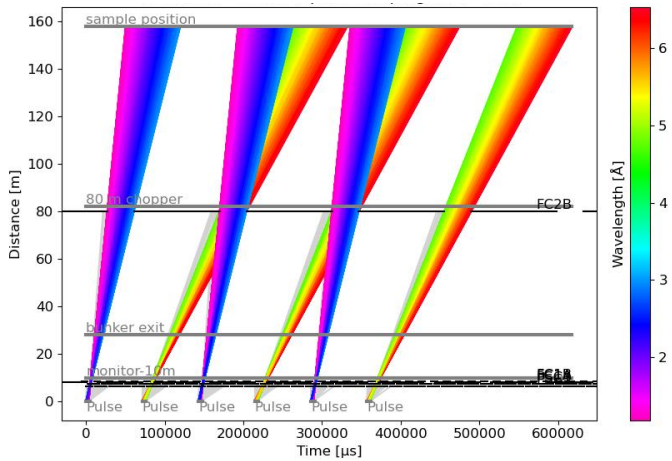
Pulse shaping



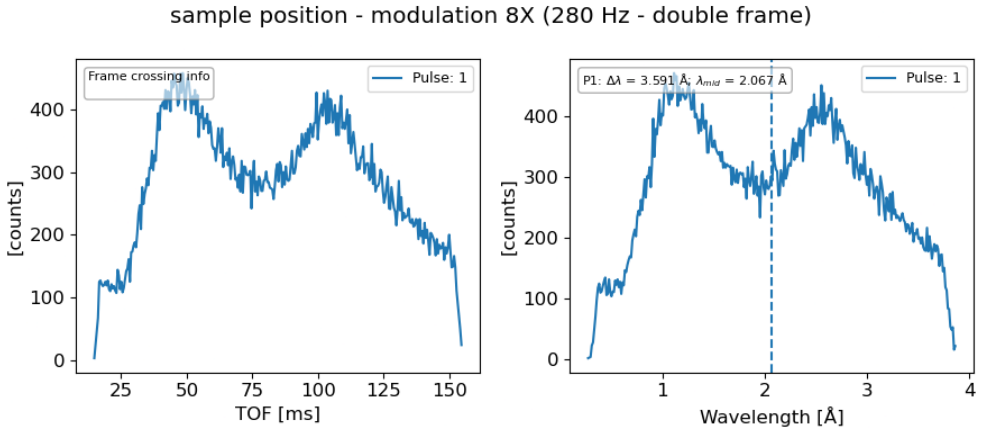
Modulation double frame

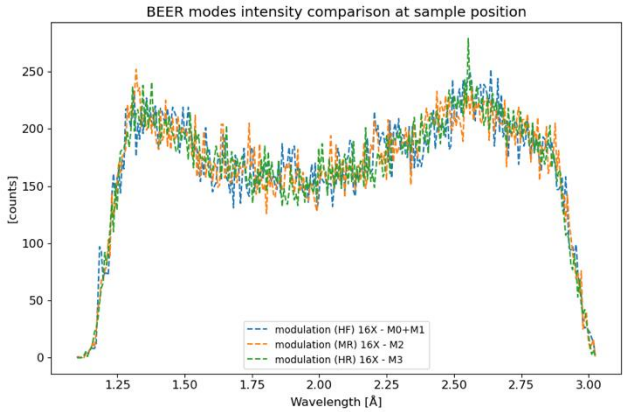


Pulse shaping+SANS



Spectra at different positions in TOF and λ & comparison between different settings



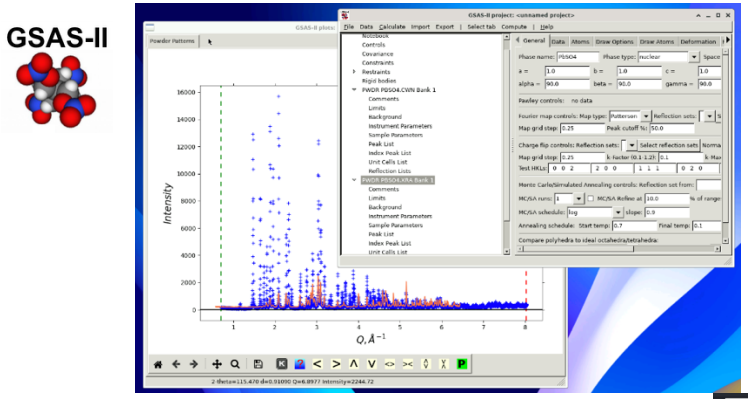


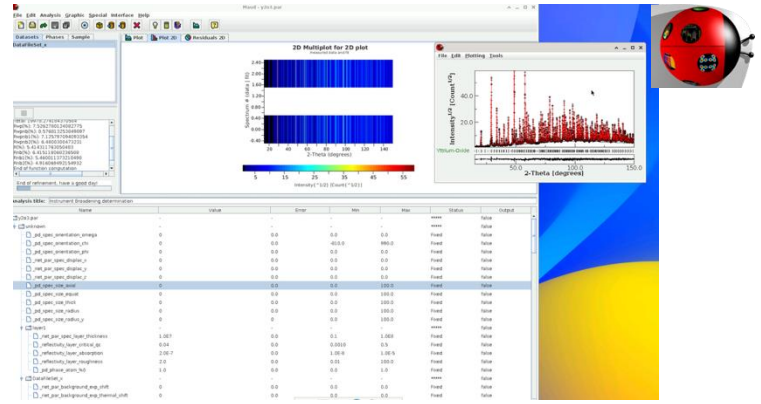
→ Notebook to be stored on Code Shelf (WIP)

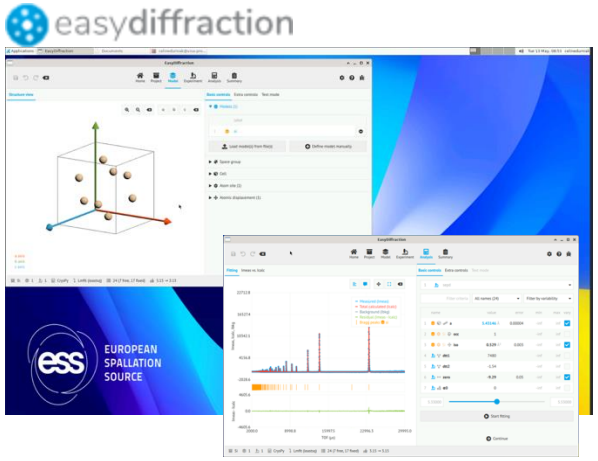
Data analysis

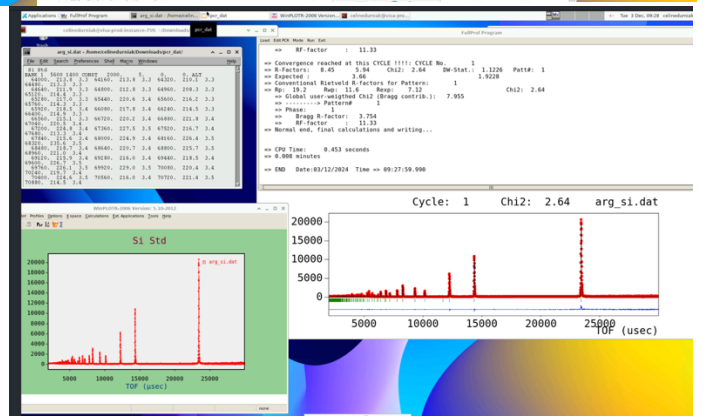
Diffraction software available on VISA

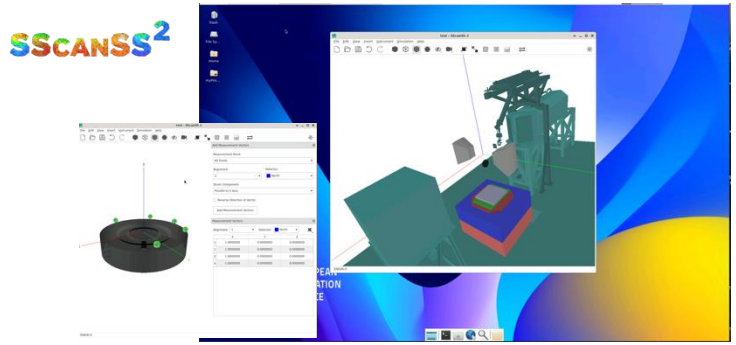
- GSAS-II
- FullProf
- MAUD
- EasyDiffraction
- SScanSS











Project planning

JIRA board

Milestones for hot and cold commissionings

ICON	KEY	SUMMARY	STATUS [CHILDREN STATUS CA...	PRIORITY	ASSIGNEE
	DMSCBEER-1	User Office Software for Cold Commissioning	0% 0% 100%		Celine Durniak
	DMSCBEER-10	Instrument team can create and access fake proposal	DONE		Celine Durniak
	DMSCBEER-3	Scicat for Cold Commissioning	100% 0% 0%		Unassigned
	DMSCBEER-16	Store test raw data	TO DO		Unassigned
	DMSCBEER-17	Store derived data	TO DO		Unassigned
	DMSCBEER-18	Test access to "BEER" data stored on Scicat	TO DO		Unassigned
	DMSCBEER-9	Analysis for Cold Commissioning	100% 0% 0%		Celine Durniak
	DMSCBEER-41	Analysis of BEER diffraction data	TO DO		Unassigned
	DMSCBEER-42	Test whole DMSC data processing pipeline for Engineering Diffraction	TO DO		Unassigned
	DMSCBEER-6	NeXus for Cold Commissioning	50% 50% 0%		Celine Durniak
	DMSCBEER-27	Create skeleton of ESS NeXus file	IN PROGRESS		Celine Durniak
	DMSCBEER-28	Add simulated counts to ESS NeXus file	TO DO		Unassigned
	DMSCBEER-8	Scipp for Cold Commissioning	62.5% 37.5% 0%		Unassigned
	DMSCBEER-33	Load McStas NeXus file	IN PROGRESS		Celine Durniak
	DMSCBEER-34	Load ESS NeXus files	TO DO		Unassigned
	DMSCBEER-35	Adapt DREAM powder diffraction reduction workflow to BEER	IN PROGRESS		Celine Durniak
	DMSCBEER-36	Implement tools for detectors' diagnostics	TO DO		Unassigned
	DMSCBEER-37	Test link with Scicat	TO DO		Unassigned
	DMSCBEER-38	Create template for calibration file	TO DO		Unassigned
	DMSCBEER-39	Test live data reduction with simulated data	TO DO		Unassigned
	DMSCBEER-40	Implement multiplexing correction	IN PROGRESS		Celine Durniak
	DMSCBEER-7	McStas for Cold Commissioning	50% 50% 0%		Celine Durniak
	DMSCBEER-29	Update BEER model with 3D detectors	IN PROGRESS		Celine Durniak
	DMSCBEER-30	Link with EFU to simulate live experiment	TO DO		Unassigned
	DMSCBEER-31	Make library of SEs	TO DO		Unassigned
	DMSCBEER-32	Benchmark different configurations of the instrument	IN PROGRESS		Celine Durniak
	DMSCBEER-5	Instrument Control for Cold Commissioning	100% 0% 0%		Celine Durniak
	DMSCBEER-24	Live customizable display of detectors	TO DO		Unassigned
	DMSCBEER-25	Access to settings of choppers, slits, SE...	TO DO		Unassigned
	DMSCBEER-26	Write metadata to ESS NeXus files	TO DO		Unassigned
	DMSCBEER-4	VISA for Cold Commissioning	60% 40% 0%		Celine Durniak
	DMSCBEER-19	Instrument team can access VISA	IN PROGRESS		Celine Durniak
	DMSCBEER-20	Instrument team can create BEER instance	TO DO		Unassigned

DMSC-BEER / DMSCBEER-10

Instrument team can create and access fake proposal

Edit | Add comment | Assign | More | Done

Details

Type: Task
Priority: Major
Component/s: DM, SIMS
Labels: None
Epic Link: User Office Software for Cold Commissioning
Resolution: Done

Description

The proposal related to BEER should contain relevant information to prepare an experiment (request access to lab, SE, safety training and programming tutorials)

Attachments

Drop files to attach, or browse.

Activity

All | Comments | Work Log | History | Activity | Newest first

Celine Durniak added a comment - 2025-Jun-20 04:32 +0200 - edited

Users can submit a BEER proposal -> create a VISA instance and a dedicated folder whose name is the proposal number) can be found at ess/data/beer/2025.

There are already analysis software available on VISA: FullProf, MAUD, SScanSS...

Edit · Delete · Pin ·

Future plans

Short-term plans

- Instrument simulation
  - 3D detector models (WIP)
  - textured sample (WIP)

- ESS NeXus files for raw data (WIP) → integration in CODA pipeline

- Data reduction
  - support for NXStress output format
  - fitting routines

- Data curation
  - definition of metadata for BEER and its science cases

- Update old requirements for BEER science cases

Acknowledgements

Contributors

- BEER instrument team
- McStas developers
- scipp developers
- Experiment Control and Data Curation (ECDC) team
- Scientific Information Management Systems (SIMS) team