



# Data processing for BEER

## Updates

Céline Durniak

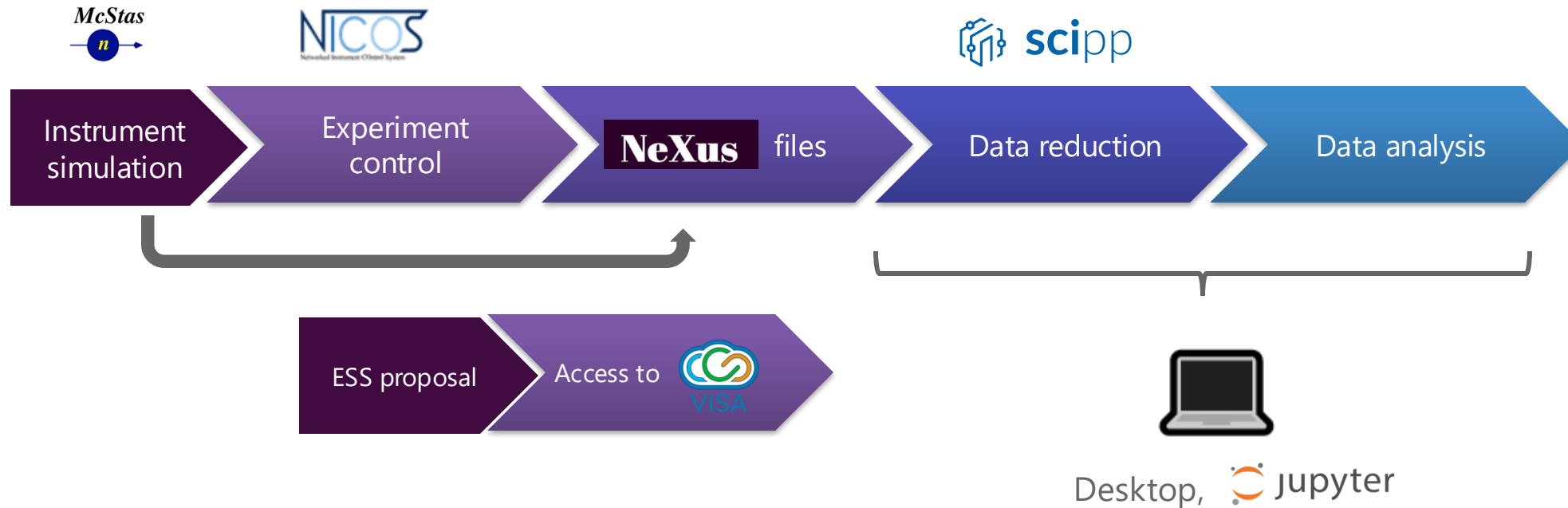
IDS for Diffraction (DREAM and BEER)

2025-09-26



# Data workflow @ ESS

## Software & frameworks





# ESS User Proposal

## Request to access VISA

Create Proposal

New Proposal

1 New proposal

2 Review

BEER

BIFROST

CODA

CSPEC

DEMAX

DEMAX Biodeuteration

DEMAX Chemical Deuteration

DREAM

ESTIA

FREIA

HEIMDAL

LOKI

MAGIC

MIRACLES

NIDO

NMX

ODIN

SKADI

T-REX

TBL

VESPA

XMIR

YMIR

test instrument

BEER McStas simulation and data reduction

Proposal ID: 287217

✓ New proposal

✓ Review


New proposal

Proposal ID	287217
Title	BEER McStas simulation and data reduction
Abstract	This proposal is to run McStas simulations and to reduce the data with Scipp with the option of sharing between the BEER instrument team.
Principal Investigator	Celine Durniak (European Spallation Source ERIC (ESS))
Co-Proposers	Premek Beran (European Spallation Source ERIC (ESS)) , Jan Saroun (Czech Academy of Sciences, Nuclear Physics Institute) , Gergely Németh (European Spallation Source ERIC (ESS)) , Yoganandan Pandiyan (European Spallation Source ERIC (ESS))
Pick your Instrument.	BEER

BACK

✓ SUBMITTED

DOWNLOAD PDF

→ Proposal number and access to 

# VISA

## Access to computing resources

### ■ Creating instances

#### Experiments

Select the experiments you wish to associate with your compute resource.

☐ Instance not associated to any specific experiments

[SEARCH FOR EXPERIMENTS](#)

Proposal	Title	Instrument	Start Date	End Date	
287217	BEER McStas simulation and data reduction	BEER	01 Jan 2022	30 Jul 2026	<a href="#">REMOVE</a>

#### Instance settings

Environment: 0.250904

Processor: 6 vCPUs

Memory: 32 GB RAM

☐ Customise the instance settings


### ■ Access to desktop or Jupyter lab

#### Compute instances

[CREATE A NEW INSTANCE](#)

Filter instances by experiment...

My instances (2) Instances shared with me (1)



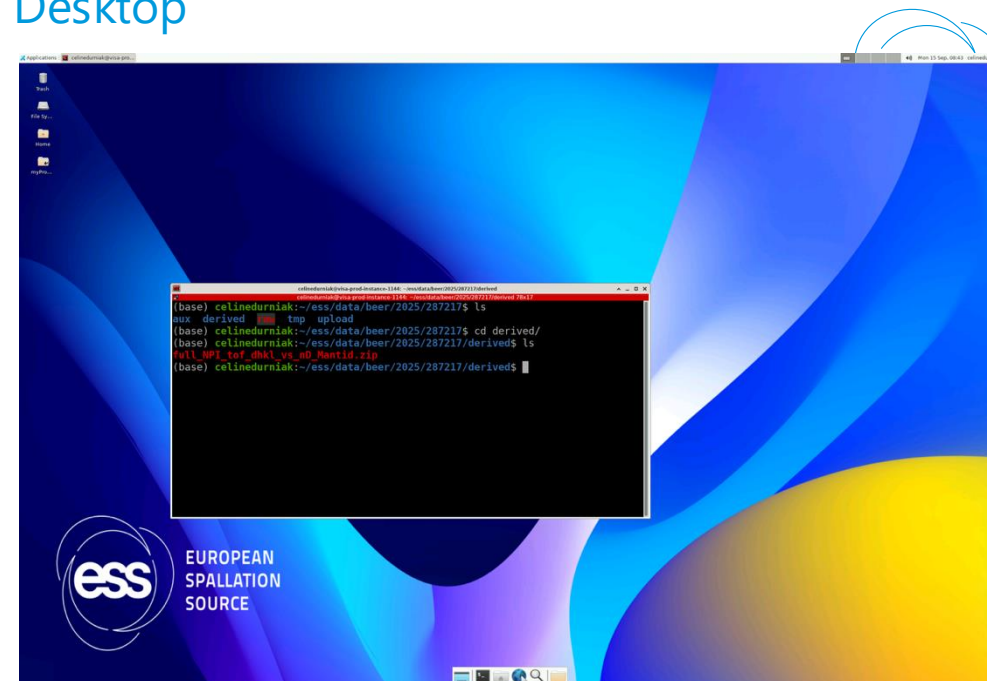
**cobalt\_aftershave**  
VISA img - stable (Ubuntu 2022.04)  
32 GB - 6 vCPUs  
Instance 1182 created on Sep 18, 2025 and due to expire on Nov 17, 2025  
active

[Connect](#) [Settings](#) [Delete](#)

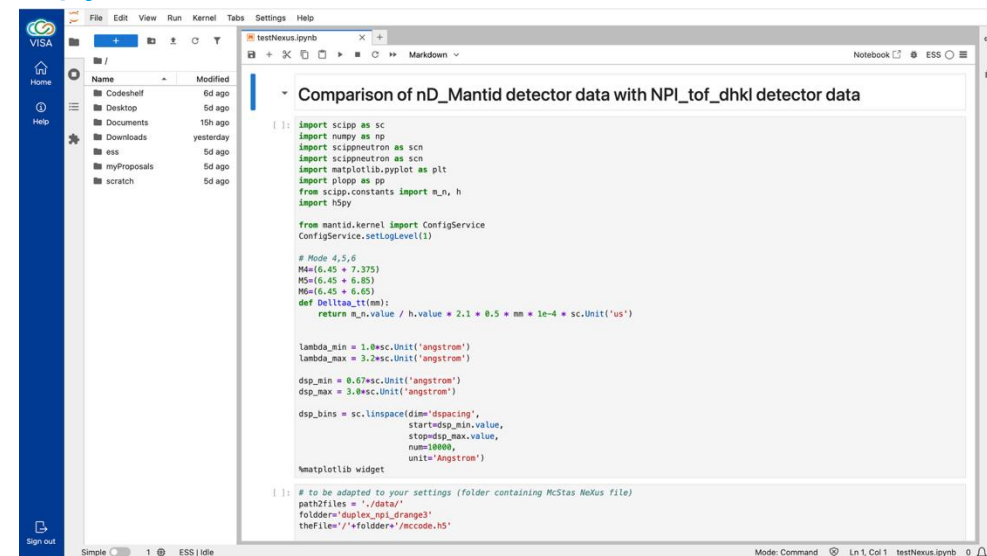
Experiments: 287217 (BEER, Jan 2022)

[Remote Desktop](#)  
[JupyterLab](#)

## Desktop



## Jupyter Lab



# Instrument control

## NICOS



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

The screenshot displays the Symétrie Hexapod Control Panel interface. On the left is a vertical sidebar with buttons for 'Experiment', 'Setup', 'Instrument interaction', 'Scripting', 'History', 'History(TESTING)', and 'Logs'. The main area features a top bar with a command input field and a 'Run' button. Below this is a tabbed interface with 'Output', 'Scan Plot', 'Hexapod' (selected), 'Detector Image', 'Beamline Panel', 'Chopper', and 'Script Status'. The 'Hexapod Controls - Freia\_hexapod' section contains three main panels: 'Current Position' showing coordinates (tx, ty, tz, rx, ry, rz, Tab) all at 0.000; 'New Position' with input fields for the same coordinates, currently set to 0.00, and 'Start'/'Stop' buttons; and 'Speed/Acceleration' with sliders for 'Translation Speed (mm/s)' (range 0.01 to 20.0, set at 1.00) and 'Rotational Speed (deg/s)' (range 0.001 to 1.5, set at 0.01), plus an 'Apply' button. A 'Preset Movements' section at the bottom shows a dropdown set to 'USER\_ZERO' and a 'Start' button. A 'Status' panel on the left lists 'Initialized', 'Control On', 'In Position', 'Home Complete', 'Emergency Stop', and 'Error', each with an unchecked radio button.

- 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...

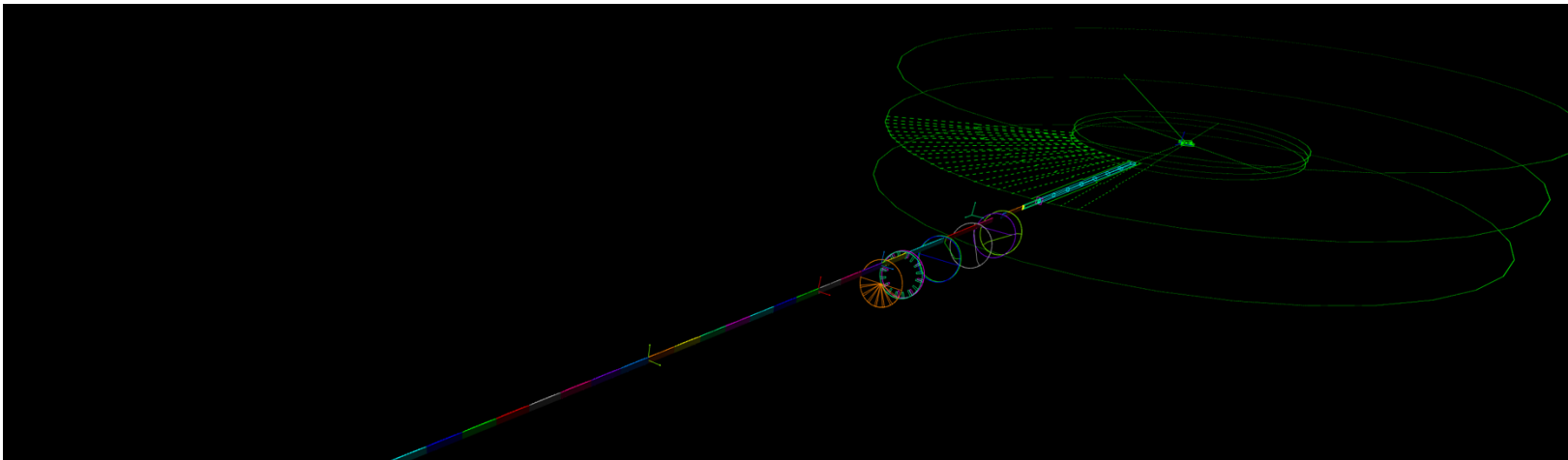
*Draft of ESS NeXus tree structure for BEER*

```
<Unnamed>
└─ entry
   └─ daq_publication
      └─ sample
         └─ instrument
            └─ name
               └─ slit_set_1
                  └─ slit_set_2
                     └─ slit_set_3
                        └─ beer_detector_0
                           └─ beer_detector_1
                              └─ psc1_chopper
                                 └─ psc2_chopper
                                    └─ mca_chopper
                                       └─ fc1a_chopper
                                          └─ fc2a_chopper
                                             └─ beam_monitor
                                                └─ bi_spectral_switch
                                                   └─ radial_collimator_1
                                                      └─ radial_collimator_2
                                                         └─ linear_collimator
                                                            └─ symetrie_beer_hexapod
                                                               └─ neutron_prod_info
```

# Instrument simulation

## McStas

- $2 \pm 90^\circ$  detector banks
  - 2D flat panels 
  - 3D layered structures 
- "Mantid" NeXus output files 
- Modulation and pulse-shaping chopper modes of operation 



# Data reduction



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

essans

essdiffraction

esspolarization

...

ESS-specific technique submodules



# Scipp

## Data reduction

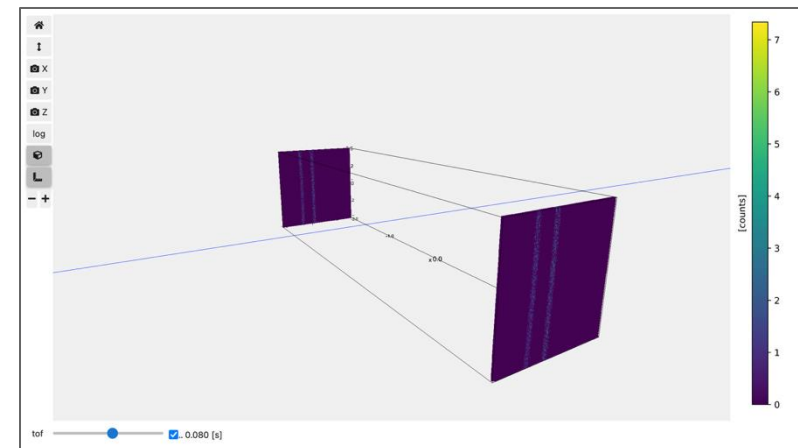
### Existing algorithms

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

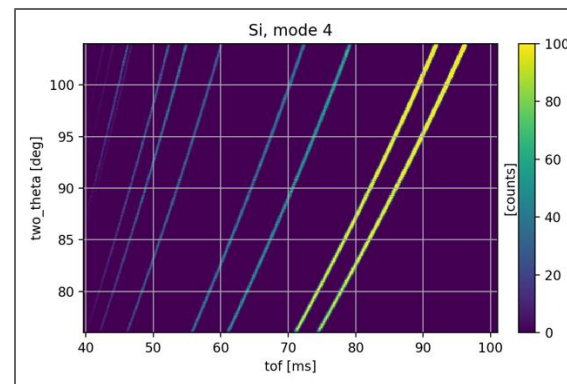
### Specific algorithms for BEER

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

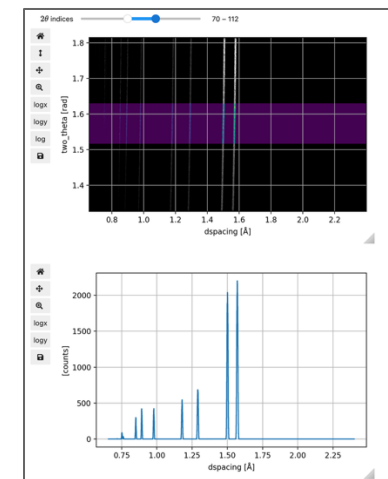
### Instrument view with widget



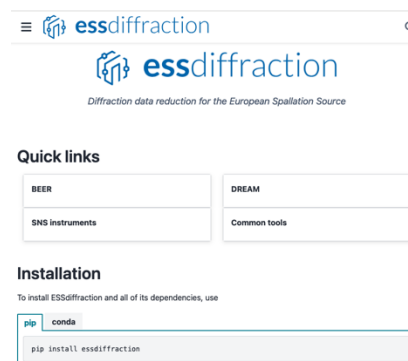
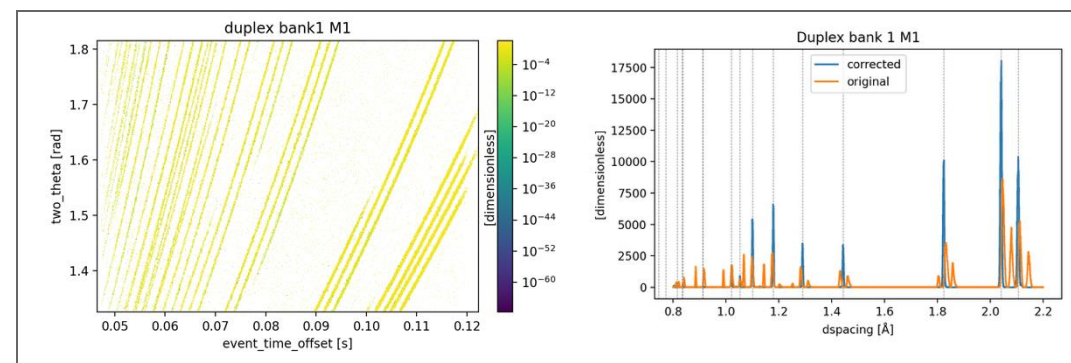
### Pulse shaping mode



### 1, 2D plots with widgets



### Modulation correction

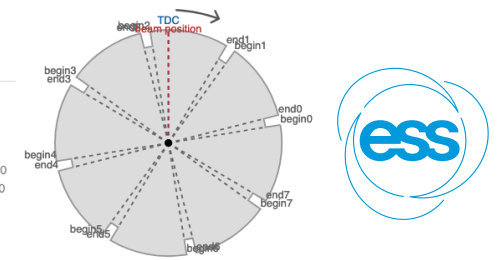


# Data reduction

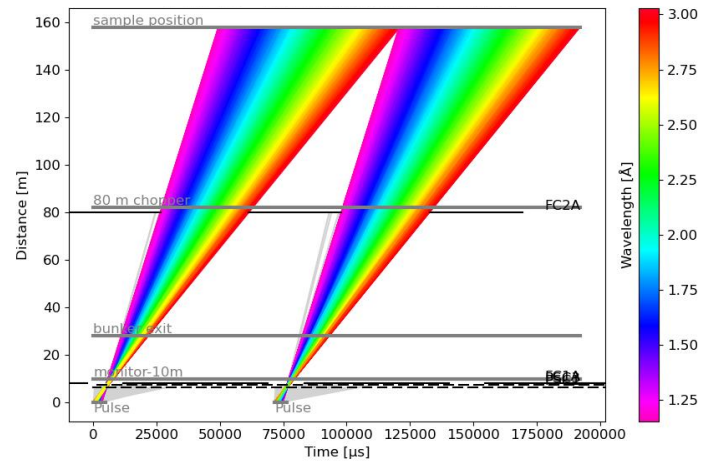
## Choppers / Commissioning tools

▼ DiskChopper (slit: 8)

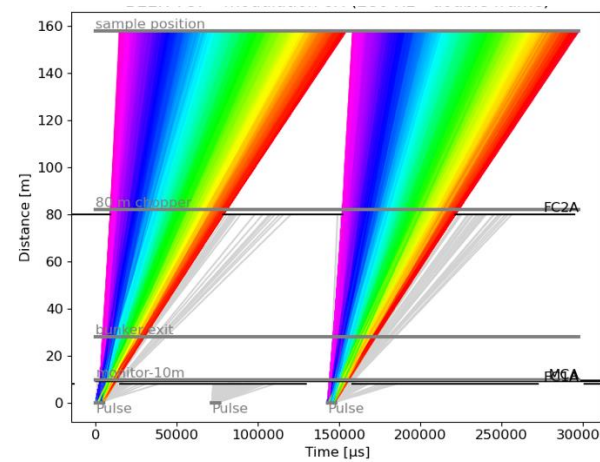
axle_position	scipp	Variable ()	vector3	m	[0. 0. 9.3]
frequency	scipp	Variable ()	float64	Hz	-280.0
beam_position	scipp	Variable ()	float64	deg	0.0
phase	scipp	Variable ()	float64	deg	639.2696515881335
slit_begin	scipp	Variable (slit: 8)	float64	deg	639.270, 684.270, ..., 909.270, 954.270
slit_end	scipp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



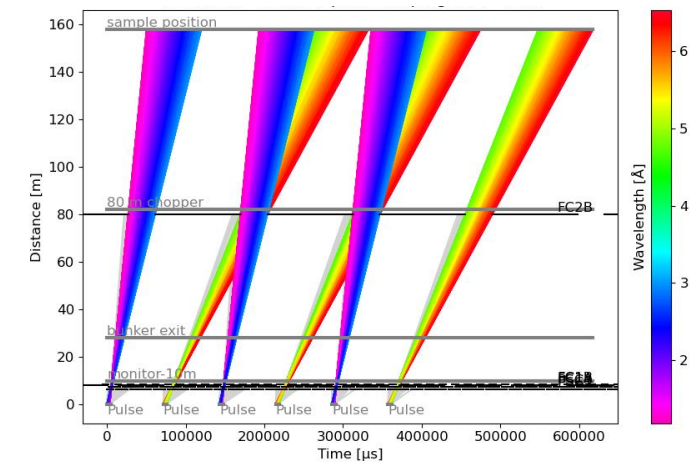
### Pulse shaping



### Modulation double frame

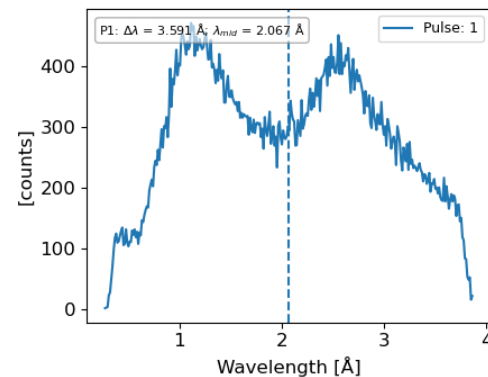
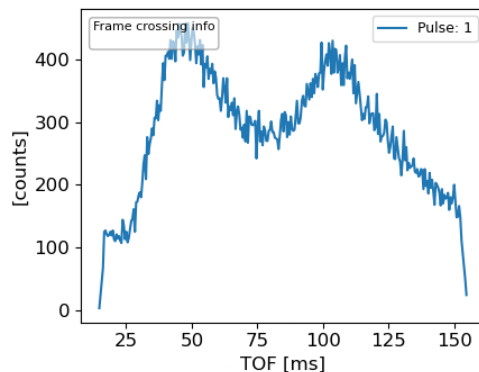


### Pulse shaping+SANS

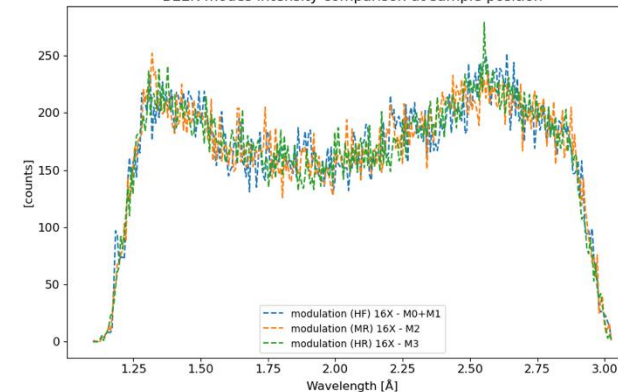



## Spectra at different positions in TOF and $\lambda$ & comparison between different settings

sample position - modulation 8X (280 Hz - double frame)



BEER modes intensity comparison at sample position

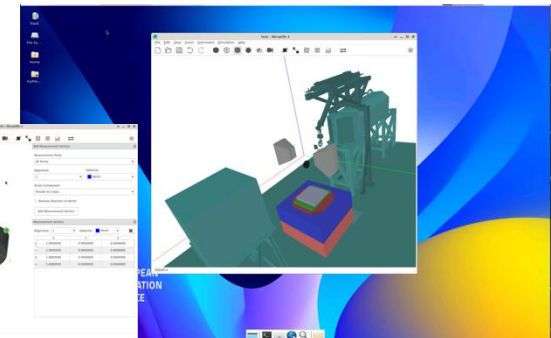
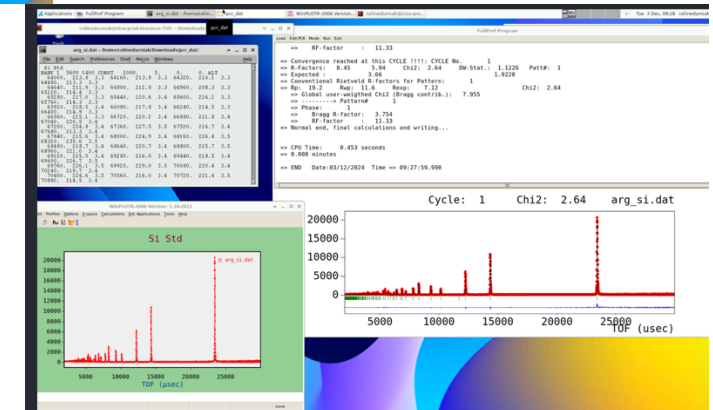
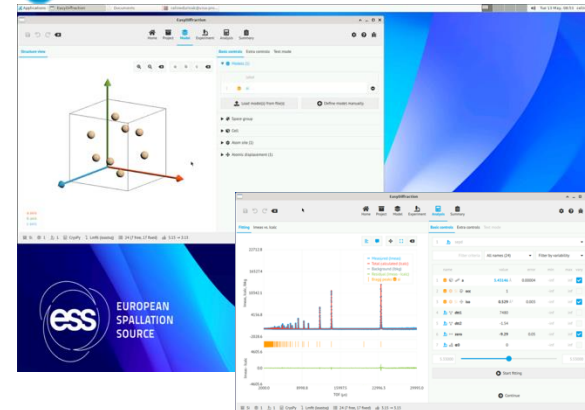
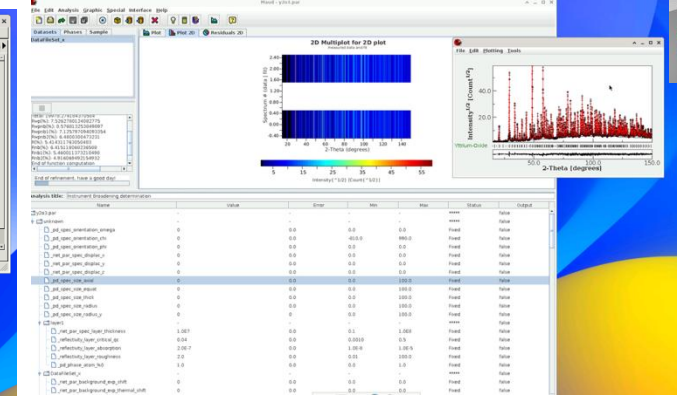
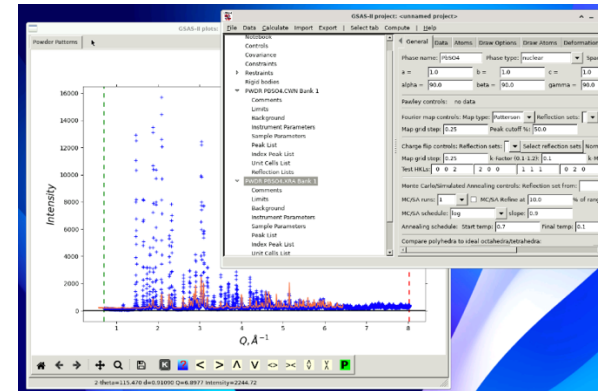


→ Notebook to be stored on  
 Code Shelf (WIP)

# 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

EditAdd commentAssignMoreDone

Details

Type:TaskResolution:Done

Priority:Major

Component/s:DM, SIMS

Labels:None

Epic Link:User Office Software for Cold Commissioning

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

AllCommentsWork LogHistoryActivityNewest 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...

EditDeletePin



# 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
-  **sci**pp developers
- Experiment Control and Data Curation (ECDC) team
- Scientific Information Management Systems (SIMS) team