



**EUROPEAN  
SPALLATION  
SOURCE**

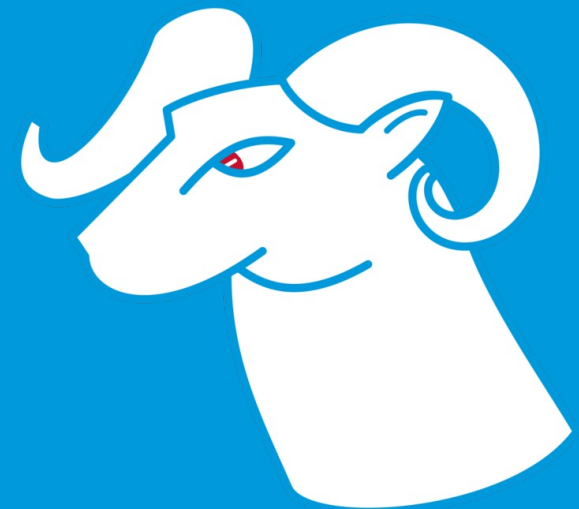


# DMSC STAP

Updates from DRAM

TORBEN NIELSEN

April 2024



# Agenda



1. DRAM
2. Staff
3. Scipp
4. Data Analysis
5. Modelling
6. Summary

# DRAM

## Data Reduction, Analysis and Modelling



### Data reduction

- **scipp** will be used for all instruments
- Possibly in combination with other software for NMX & Imaging
- Are looking for partners

### Data analysis

- **easyScience** for powder, sxtal & reflectometry
  - Planning for QENS and TOF imaging
  - But always in combination with other libraries (cal. engines)
- **SasView** for SANS
- **PACE** for spectroscopy
- **(Py)MuhRec** for Tomography.

### Data modelling

- **McStas** for instrument simulations
- Now also with Python API **McStasScript**
- and optimized for GPU
- **NCrystal**

# DRAM

## Data Reduction, Analysis and Modelling - Staff



Simon Heybrock



Neil Vaytet



Jan-Lukas Wynen



Sunyoung Yoo\*



Johannes Kasimir\*



Mridul Seth\*



Piotr Rozyczko



Andrew Sazonov



Andreas Pedersen \*



Henrik Jacobsen\*



Christian Vedel\*



Peter Willendrup\*\*



Mads Bertelsen\*



Thomas Kittlemann\*\*

- 3 teams (14+ persons)
- 1. Data Reduction (scipp)
- 2. Data Analysis (SasView, SpinW, EasyScience, external collaborations )
- 3. Modelling (McStas++, pan-learning.org, Detector Group)

\*/\*\* "new" contract

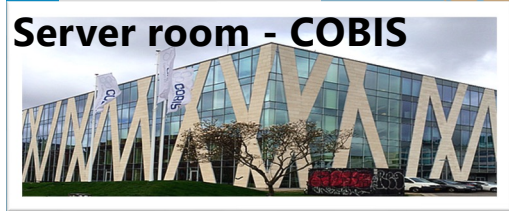
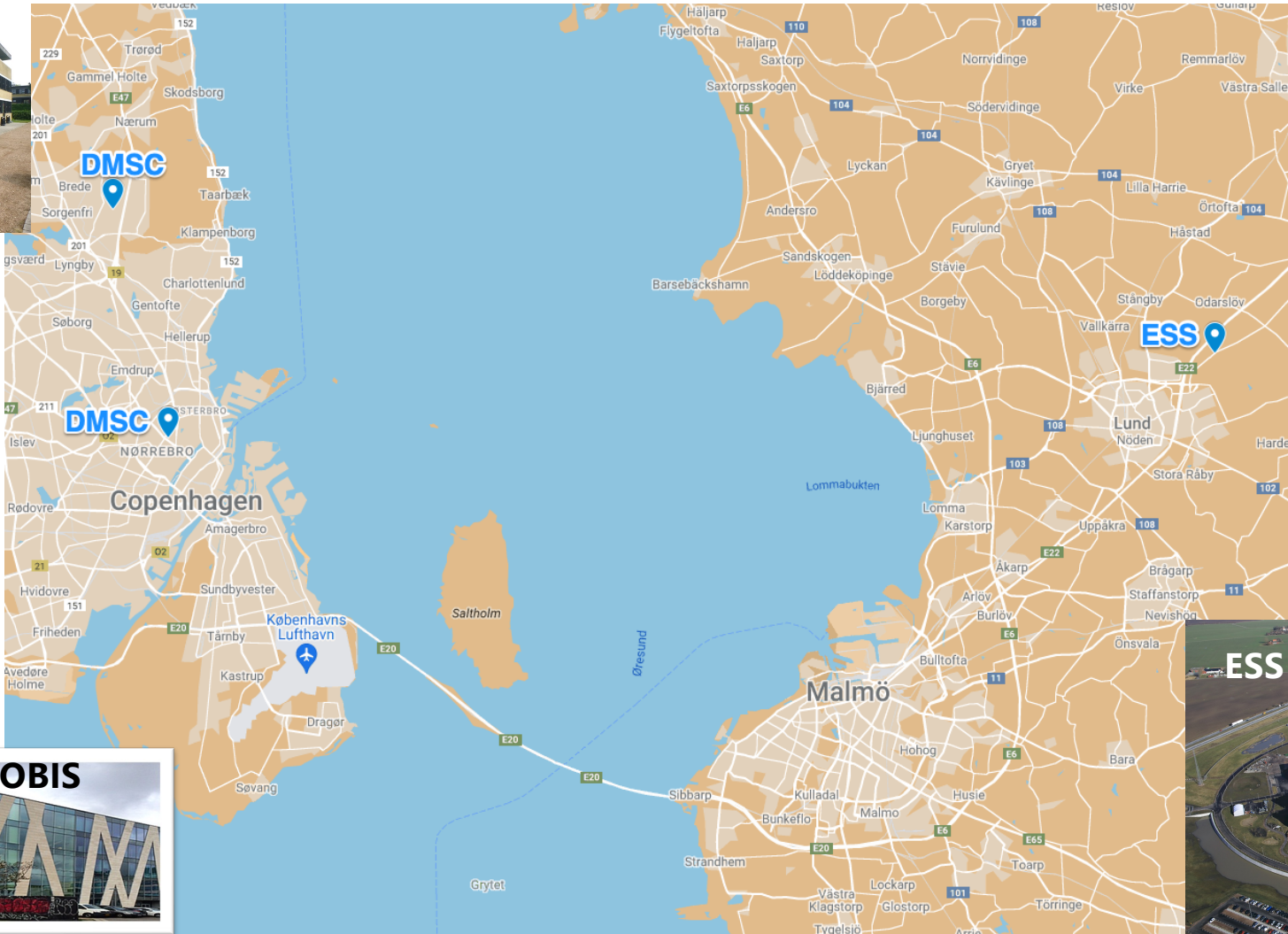
### Scope

The DRAM group is responsible for providing the data reduction, analysis and modelling soft-ware for all instruments at ESS.

# DMSC –Lyngby/Copenhagen – ESS/LUND



Office - Lyngby



Server room - COBIS



ESS - Lund

# Scipp – Updates 1

## General activities

1. New team member joined
2. Sciline – a workflow manager
3. **A lot of new instrument specific packages**
4. Beamline – for live data
5. Copier Template
6. Chexus – for checking NeXus files
7. CI – with ECDC data
8. IDS requirements & GitHub template
9. A lot of releases > 40 packages



Related projects ▾ 24.1.1.dev5+g8409fb3 (latest) 🗄️ 🔍 📄

# ESS

Data reduction for ESS instrumentation

**Attention**

The `ess` python package is being split-up into technique and instrument specific packages, and should be considered deprecated. The documentation here is kept for historical reasons. **Below, you will find links to the new packages.**


|   |   |
|---|---|
| <b>ESSdiffraction</b><br>Diffraction data reduction     | <b>ESSnmx</b><br>Data reduction for the NMX instrument  |
| <b>ESSpolarization</b><br>Polarization data reduction   | <b>ESSreflectometry</b><br>Reflectometry data reduction |
| <b>ESSsans</b><br>SANS data reduction                   | <b>ESSspectroscopy</b><br>Spectroscopy data reduction   |
| <b>ESSreduce</b><br>Common tools for ESS data reduction |   |

# Scipp – Updates 2

New instrument specific packages (breaking ess pacakge apart)




- Sciline
- ESSreduce
  
- ESSsans
- ESSnmx
- ESSdiffraction
- ESSreflectometry
- ESSpolarization
- ESSspectroscopy\*
- ESSimaging\*

 **essnmx**

---

**Section Navigation**


- Workflow**
- ☰ On this page
  - Build Pipeline (Collect Parameters and Providers)
  - Build Workflow
  - Compute Desired Types
  - [Export Results](#)
  - Instrument View

 **esssans**

---

**Section Navigation**


- Installation
- LoKI**
  - Direct beam iterations for LoKI**
  - ISIS instruments
  - Common tools
- ☰ On this page
  - Introduction**
    - Define reduction parameters
    - Create pipeline using Sciline
    - Finding the beam center
    - Expected intensity at zero Q
    - A single direct beam function for all layers
    - Direct beam function per layer
    - Combining multiple runs to boost signal

 **essdiffraction**

---

**Section Navigation**


- POWGEN data reduction**
- ☰ On this page
  - Introduction**
    - Define reduction parameters
    - Create pipeline using Sciline
    - Use the pipeline
      - Compute final result
      - Save reduced data to file
      - Compute intermediate results
    - Group by scattering angle











 **essreflectometry**

---

**Section Navigation**

- Divergent data reduction for Amor**
- ☰ On this page
  - Make a  $(\lambda, \theta)$  map
  - [Save data](#)

 **Packages** View all (20)

-  **esssans** 10 days and 17 hours ago
-  **chexus** 10 days and 19 hours ago
-  **sciline** 11 days and 2 hours ago
-  **scippneutron** 21 days and 17 hours ago
-  **essreduce** 1 month and 4 days ago
-  **scippnexUS** 1 month and 10 days ago
-  **essreflectometry** 1 month and 11 days ago
-  **essnmx** 1 month and 14 days ago
-  **plopp** 1 month and 27 days ago
-  **scipp** 1 month and 27 days ago



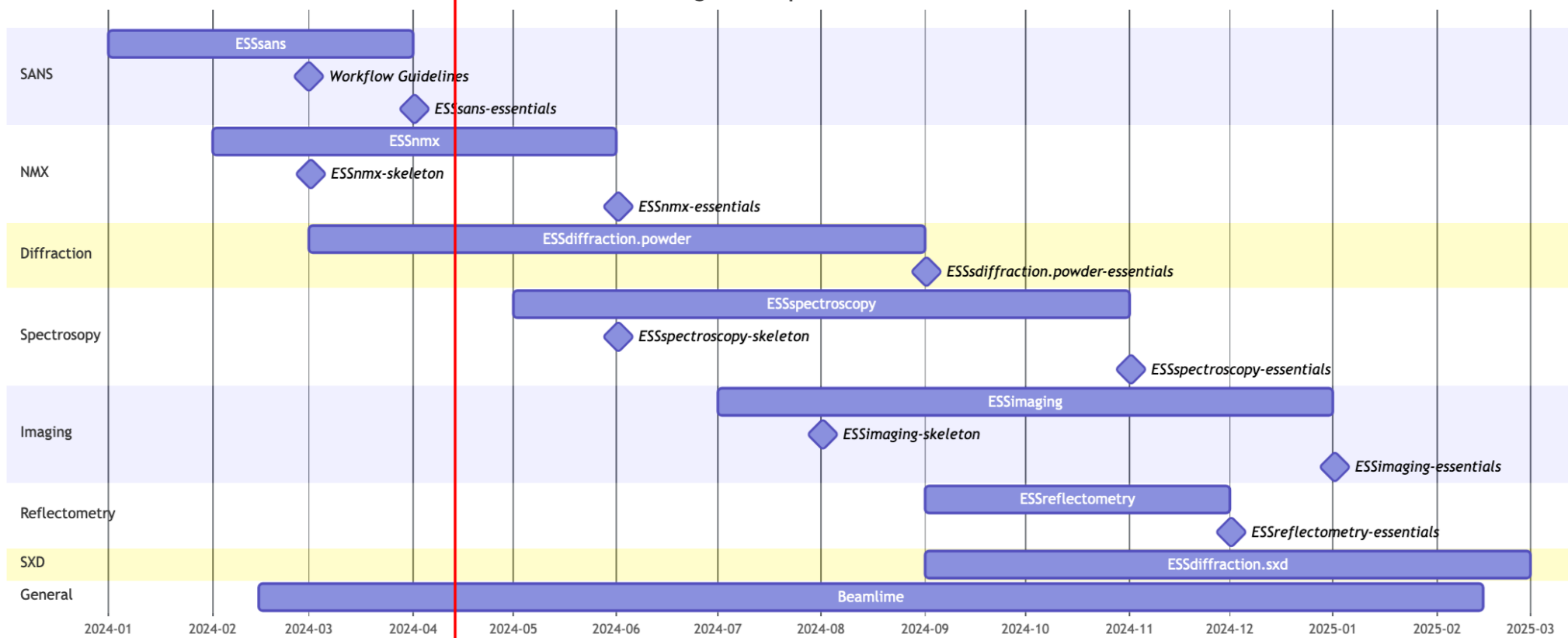


# Scipp – Updates 3

Preliminary – Live – Plan – Scipp (April 12 2024)



High-level plan 2024 - 2025



# Scipp – Updates 4

General (follow up on Requirements from the IDS from last STAP)



- Different techniques are scheduled to be worked on in a staggered manner
- We created two milestones for each technique:
  - The first **requires that a package exists and is installable**, and contains a basic skeleton for a workflow as well as rudimentary documentation
  - The second **requires that the package contains all the essentials** for performing fundamental data reduction during hot-commissioning.
- The motivation is to **ensure the team does not spread out in too many directions** at the same time, as well as provide the **satisfaction that a package is considered ‘done’** (for the time being) and can be ticked off the long list of tasks that remain before experiments begin at ESS. **The criterion for being ‘done’ is usually determined by the IDS.**
- **Disclaimer:** A software project is of course **never fully ‘done’**, and we will pursue maintenance on these packages, but no new features will be added unless identified as absolutely critical by the instrument scientists.

# Scipp – Updates 5



NeXus channel on Slack: -> Chexus (first release Nov 13)

- ❑ We have encountered broken data structures in some NeXus files written by the file-writer.
- ❑ Therefore, we have developed a minimal NeXus structure analyzing tool, [chexus](#), for earlier and easier detection of potential errors of loading NeXus files.
- ❑ Using chexus, we could give more detailed and consistent form of feedback to ECDC and address the problems in the files efficiently.
- ❑ CI set-up for fetching NeXus files and running chexus has been done in **collaboration with ECDC, SIMS, & DST**

- ❑ A bit of background information:
- ❑ Monthly meeting with ECDC related to NeXus files
- ❑ Discussions on Confluence and Slack
- ❑ **“Breakthrough”** over the last 2 months


The screenshot shows a GitHub Actions workflow run for the repository 'ecdcfiles-scipp'. The workflow name is 'odin-fileloading'. It shows a 'Passed' status with a green checkmark. The run was started 35 minutes ago by user 'Neil Vaytet'. The interface includes navigation icons for repository, workflow, and jobs, along with a search bar.

| Name       | Last commit                                 | Last update |
|------------|---|-------------|
| ..         |   |             |
| bifrost    | formatting                                  | 9 hours ago |
| nmx        | formatting                                  | 9 hours ago |
| odin       | add odin tests                              | 9 hours ago |
| common.py  | make local copies again before inspecting   | 9 hours ago |
| confest.py | add a test to load the file with scippnexus | 1 day ago   |

# Scipp – Updates 6

NeXus channel on slack: ---> Chexus (first release Nov 13)



 **Celine Durniak** 4:12 PM  
replied to a thread:

I ran `chexus` on the NeXus file for DREAM and got the following output

## Violations

```
-----  
depends_on_missing @ /entry/instrument/polarizer  
depends_on_missing @ /entry/sample
```

•  
•  
•

## Summary

```
-----  
depends_on_missing: 2/19  
depends_on_target_missing: 0/35  
float_dataset_units_missing: 33/93  
group_has_units: 0/63  
index_has_units: 0/35  
mask_has_units: 0/0  
non_numeric_dataset_has_units: 0/56  
NX_class_attr_missing: 0/63  
NX_class_is_legacy: 0/63  
transformation_depends_on_missing: 0/18  
transformation_offset_units_missing: 0/0  
units_invalid: 0/68
```

```
Total: 35/513  
File: DREAM_nexus_sorted.nxs  
Created: 2023-11-17 14:47:39.173679  
Modified: 2023-11-13 13:59:44  
Size: 530.67 MByte
```

## Fetching data on DMSC storage

```
common.py 1.06 KiB  
1 # SPDX-License-Identifier: BSD-3-Clause  
2 # Copyright (c) 2024 Scipp contributors (https://github.com/scipp)  
3 import glob  
4 import os  
5 import shutil  
6  
7 import scippnexus as sx  
8  
9  
10 def find_latest_file(  
11     instrument: str, path: str = "/ess/data/coda/2024/616254/raw"  
12 ) -> str:  
13     recent_files = sorted(glob.glob(os.path.join(path, "*.hdf")))[-10::][::-1]  
14     print(recent_files)  
15     for file in recent_files:  
16         print(f"Copying file {file} to local folder.")  
17         local_copy = file.split("/")[-1]  
18         shutil.copy(file, local_copy)  
19         try:  
20             with sx.File(local_copy, "r") as f:  
21                 instrument_in_file = f["/entry/instrument/name"][(0)]  
22                 if instrument_in_file == instrument:  
23                     print(f"Found {instrument} file: {local_copy}")  
24                     return local_copy  
25                 print(  
26                     f"File instrument is {instrument_in_file}, but {instrument} was "  
27                     f"requested. Skipping file."  
28                 )  
29         except OSError:  
30             print(f"File {file} could not be opened.")  
31             continue
```

# Data Analysis – Updates 1

## In-house projects

- ❑ [EasyScience](#)
- ❑ [EasyDiffractionApp](#) – EasyDiffractionLib
- ❑ [EasyReflectometryApp](#) – EasyReflectometryLib
- ❑ EasyCore
- ❑ EasyCrystallography

The screenshot shows the top navigation bar of the EasyScience website with links for Home, Projects, Features, and Contact. The main heading reads "Making scientific data analysis and modelling easy". Below this, a paragraph describes EasyScience as a Python/SQL framework for data analysis. A section titled "Projects" features a sub-heading "easydiffraction" and a small image of the application interface.

The screenshot displays the header of the easydiffraction website, including navigation links for Home, Features, Docs, and Contact. The main heading is "Making diffraction data analysis and modelling easy". The text below describes it as an intuitive application for simulating diffraction patterns. It lists download options for Windows, macOS, and Ubuntu, and includes a "Get it from the Snap Store" button. A section titled "You can also build it from source." is followed by a screenshot of the application's diffraction pattern simulation interface.

The screenshot shows the header of the easyreflectometry website with navigation links for Home, Features, Docs, and Contact. The main heading is "Making reflectometry data analysis and modelling easy". The text describes it as an application for simulating reflectometry profiles. It provides download options for Windows, macOS, and the Snap Store, along with a "You can also build it from source." link. A screenshot of the application interface shows a reflectometry profile plot and a parameter table.

| No. | Label                     | Value    | Error   | Fit |
|-----|---------------------------|----------|---------|-----|
| 1   | Vacuum SLD                | 0.0000   | 1.0E-10 |     |
| 2   | Vacuum SLD                | 0.0000   | 1.0E-10 |     |
| 4   | DDO SLD                   | 6.3150   | 1.0E-10 |     |
| 7   | DDO SLD                   | 0.0000   | 1.0E-10 |     |
| 8   | DDO Layer Thickness       | 100.0000 | 1       |     |
| 9   | DDO Layer Upper Roughness | 3.0000   | 1       |     |
| 11  | Si SLD                    | 2.6740   | 1.0E-10 |     |
| 12  | Si SLD                    | 0.0000   | 1.0E-10 |     |

The screenshot shows the GitHub repository page for EasyScience. The repository name is "EasyScience" and it is described as "A framework for building applications and libraries for data analysis and modelling". It has 8 followers and is located in Copenhagen, DK. The "Pinned" section lists several related repositories: EasyDiffraction, EasyReflectometry, EasyQENS, EasyBragg, EasyCore, and EasyCrystallography. Each repository has a brief description and a star count.

# Data Analysis – Updates 2



Other projects with active collaboration on our side

| Project      | Collaboration with | Used for     | Person involved |
|--------------|--------------------|--------------|-----------------|
| CrysFML      | ILL                | Diffraction  | Andrew, Piotr   |
| CrysPy       | ILL, LLB           | Diffraction  | Andrew, Piotr   |
| ImagingSuite | PSI                | Imaging      | Christian       |
| PySpinW      | ISIS               | Spectroscopy | Henrik          |
| PACE         | ISIS               | Spectroscopy | Henrik          |
| SasView      | NIST, ISIS, ILL    | Small Angle  | Piotr           |

# Data Analysis – Updates 3

## General activities



### ❑ **Recruiting**

- ❑ 3 new team members (Took 6 mths. + addition time for being able to start )
- ❑ Andreas starting Dec., Henrik and Christian starting Feb.

### ❑ **Travel to facilities**

- ❑ Piotr visit JPARC for 3 weeks
- ❑ Henrik and Christian at ILL for beam time

### ❑ **ILL collaboration**

- ❑ Continue collaboration with ILL related EasyDiffraction and using CrysFML as backend calculation engine.
- ❑ Piotr, Andrew and Celine at ILL for a mini codecamp with Elisa and Nebil (March 2024)
- ❑ July 8-12 2024 Elisa, Nebil and Stephane Rols coming to Lyngby
- ❑ Planning joint ILL-ESS/DMSC PhD. project. 1 year at DMSC 2 years at ILL.

# Data Analysis – Updates 4

## Project activities



### **Imaging**

- CI updates for MuhRec
- Looking ahead to PyMuhRec (for VISA)

### **Diffraction**

- Work has started to bring the EasyDiffraction application (version 0.9.0-beta) back into the EasyScience framework.
- Related work is also underway **to restructure the entire EasyScience framework** to make it **easier** to use for developing other technique-specific applications and libraries, such as **EasyQens** and **EasyBragg**.
- Discussions have started on an **improved user interface** for the EasyDiffraction library.

### **Reflectometry**

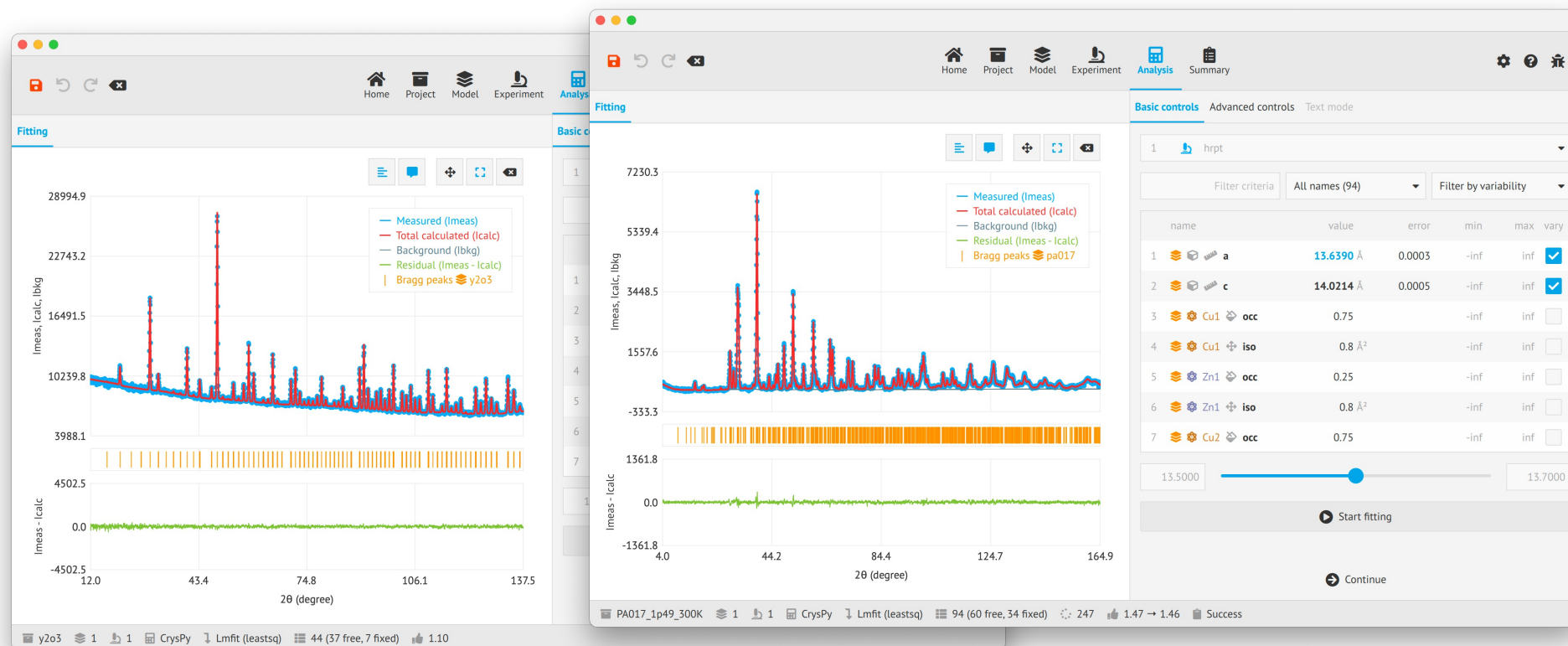
- Regular meetings with IS Jos Copper from ESS/Lund
- A few releases of App and Lib



# Data Analysis – Updates 5

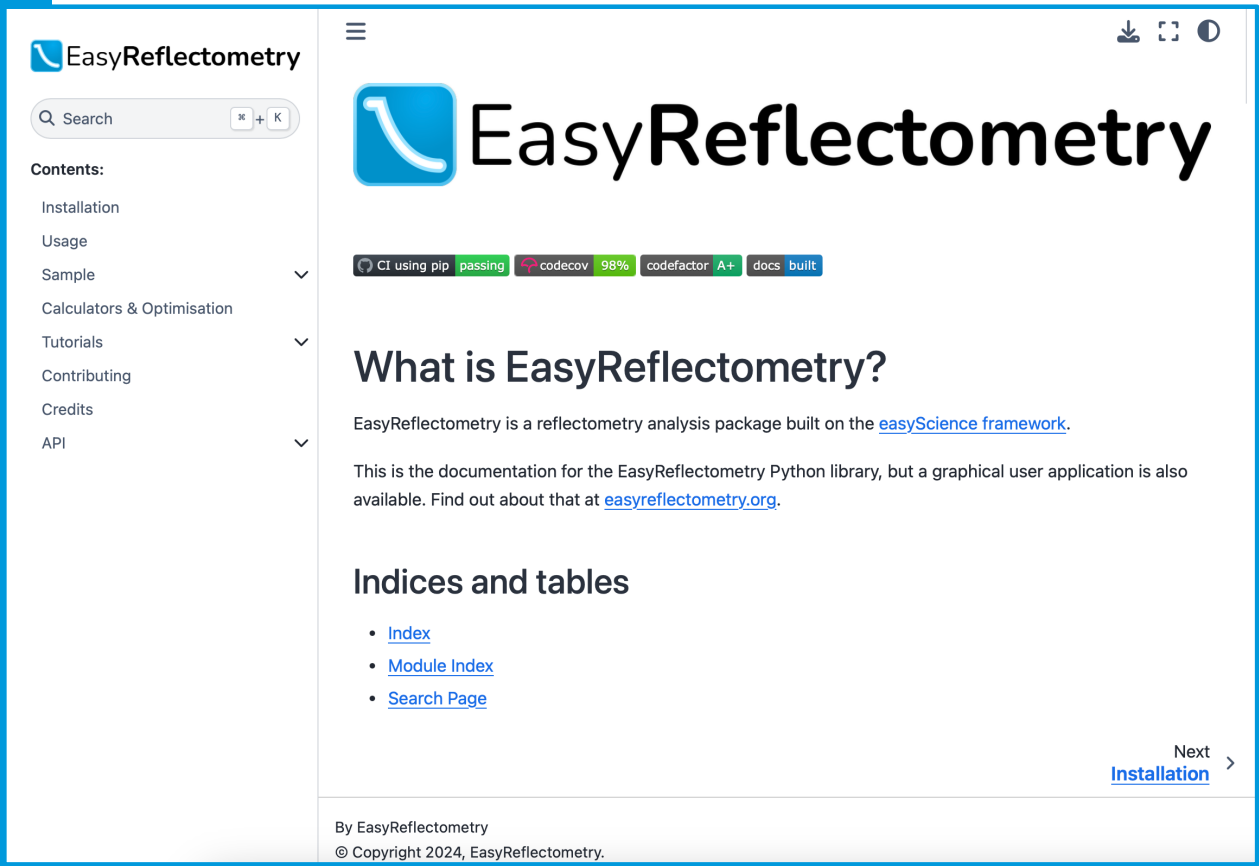


EasyDiffraction: More testing on data from HRPT@PSI and SPODI@MLZ



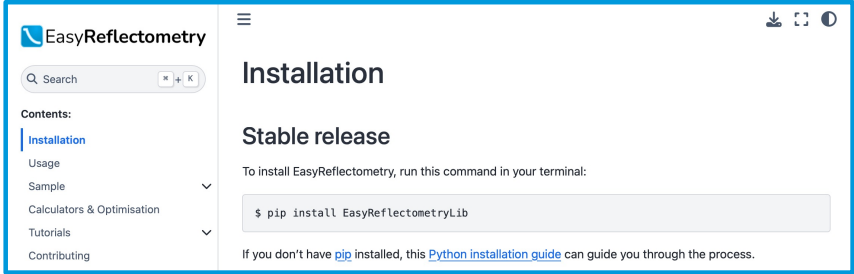
# Data Analysis – Updates 6

## EasyReflectometryLib - Documentation



The screenshot shows the homepage of the EasyReflectometry documentation. At the top left is the 'EasyReflectometry' logo and a search bar. A 'Contents' sidebar on the left lists sections like Installation, Usage, Sample, Calculators & Optimisation, Tutorials, Contributing, Credits, and API. The main content area features the 'EasyReflectometry' logo, a status bar with 'CI using pip passing', 'codecov 98%', 'codefactor A+', and 'docs built'. The main heading is 'What is EasyReflectometry?' followed by a paragraph explaining it's a reflectometry analysis package built on the 'easyScience framework'. Below this is a section for 'Indices and tables' with links to 'Index', 'Module Index', and 'Search Page'. A 'Next Installation >' button is at the bottom right. The footer contains 'By EasyReflectometry' and '© Copyright 2024, EasyReflectometry.'

- Now installable with pip
- New slightly redesigned doc pages
- For better usability
- E.g. new search function included



The screenshot shows the 'Installation' page of the EasyReflectometry documentation. The 'Contents' sidebar on the left has 'Installation' selected. The main content area is titled 'Installation' and 'Stable release'. It contains the text 'To install EasyReflectometry, run this command in your terminal:' followed by a terminal code block: `$ pip install EasyReflectometryLib`. Below the code block, it says 'If you don't have pip installed, this Python installation guide can guide you through the process.'

# Instrument modelling – Update 1

## McStas etc. updates



← mcstas-autobuild

✓ **mcstas-autobuild #132**

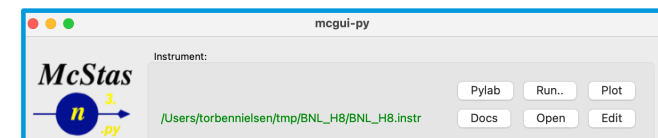
- ❑ Focus on CI & conda-forge
  - ❑ McStas on conda-forge (with NeXus)
- ❑ McStas-McStasScript
  - ❑ Tighter integration with McStasScript
  - ❑ mcgui has(button to launch jupyter-version of instrument)
- ❑ EU proposal NEMO (on "nested mirror optics"/Wolter, lead by Valentina Santoro)
- ❑ Work on polarization (with input from Hal Lee)

## Installers

- linux-64 v3.4.29
- osx-arm64 v3.4.29
- osx-64 v3.4.29
- win-64 v3.4.29

## Schools and E-learning

- ❑ McStas training for ESS staff in January
- ❑ Preparations for 2024 courses that utilize e-learning.pan-training.eu and McStas
- ❑ Prospect IAEA-sponsored McStas/McXtrace training in South Africa fall 2024



# Instrument modelling – Update 2

## McStas etc. updates



- ❑ Initiated several new student projects
- ❑ Related to **HighNESS workpackage 7** a paper was published **documenting the final instrument designs** and comparison to ESS instruments in the same class. (“Neutron Instrument Concepts for a High Intensity Moderator at the European Spallation Source” – See [link](#))
- ❑ Petroula Karakosta submitted and successfully defended her **master thesis on simulation of a cryomagnet purchased for the BIFROST instrument including training of a machine learning model to distinguish between background and signal.**
- ❑ A publication (MB) with the aim of **verifying accuracy of McStas by simulation of two diffractometers at the IRR-1 and IRR-2 reactors** was accepted for publication, this thorough work by Daniel Potashnikov showed both comparison of data on the final detector, but also analysis of intensity throughout the instrument using activation measurements.

# Instrument modelling – Update 3

Verifying accuracy of McStas by simulation of two diffractometers



## KANDI-II at IRR-2

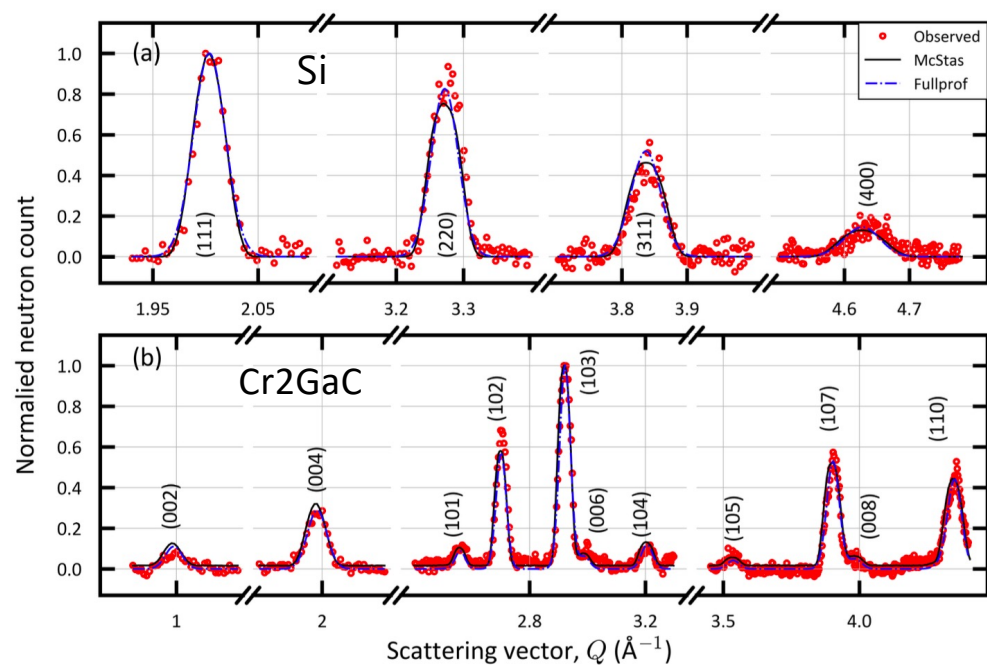


Figure 3: Observed (symbols) and calculated (lines) neutron powder diffraction pattern of (a) Si and (b) Cr<sub>2</sub>GaC using the KANDI-II diffractometer (2.47 Å). Solid line indicates a calculation performed using McStas, while dash-dotted line represents a Rietveld refined profile calculated using FULLPROF. Uncertainties on data points are represented by the spread of the data. Excess neutron count at the (102) reflection originates from an impurity phase.

See [link](#)

## KARL at IRR-1

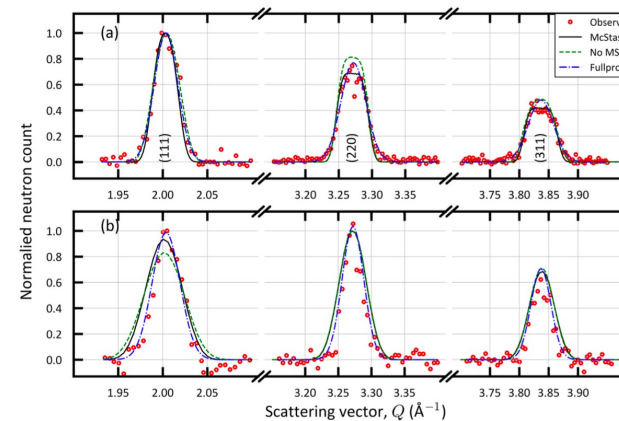


Figure 4: Observed (symbols) and calculated (lines) neutron diffraction patterns of Si powder using the KARL diffractometer with (a) PG monochromator (2.421 Å) and (b) Cu monochromator (0.98 Å). Solid line indicates a calculation performed using McStas, while dash-dotted line represents a Rietveld refined profile calculated using FULLPROF. Dashed line is a McStas calculation, where Soller slits were removed from the MSC (see text). Uncertainties on data points are represented by the spread of the data.

# Instrument modelling – Update 4

## McStas etc. updates

- ❑ Celebrating the **25<sup>th</sup> anniversary of the McStas** package
- ❑ An event at **DMSC** where all previous developers were invited
- ❑ It was decided to host another **DMSC summer school** in September **2024**.
- ❑ Due to the success of last year's school, it was chosen to keep changes to the format minimal, though with the ambition of **expanding the number of students from 14 to 20**.



DMSC Summer School 2023



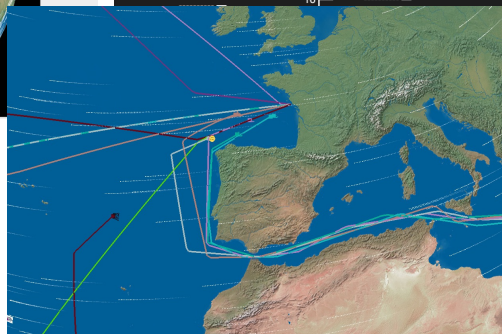
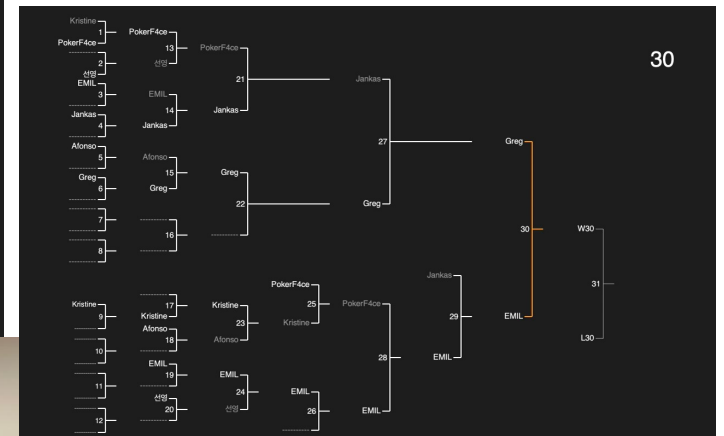
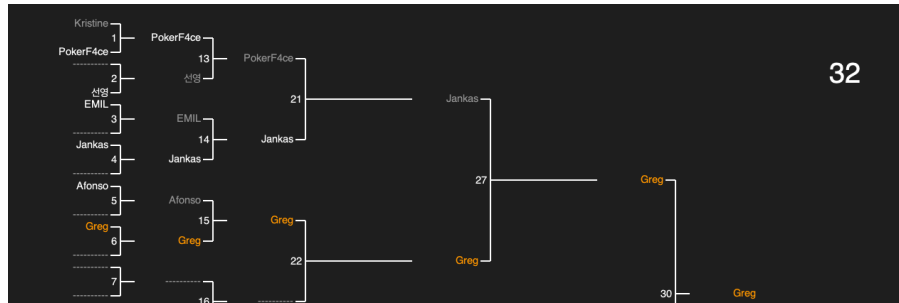
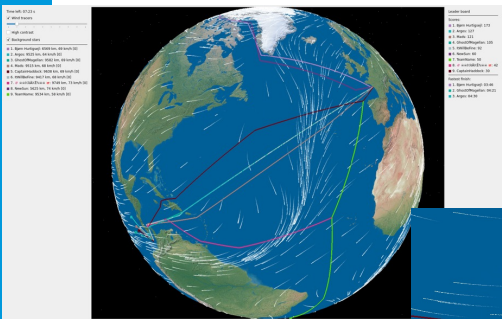
# DMSC - python AI tournaments



Open for all

- ❑ December 2023
- ❑ VendéeGlobe results:
  - ❑ 1st: Jan-Lukas
  - ❑ 2nd: Greg
  - ❑ 3rd: Mads

- ❑ AI Game: "Expression" March 2024
- ❑ <https://github.com/mads-bertelsen/expression>
- ❑ Visit of 7 students from Cambridge, and Mads Bertelsen was asked to prepare a 4 hour program that introduced the students to the work of DMSC with focus on simulations along with some entertainment in the form of a coding challenge (AI).



# Summary



## **Staff:**

- We have reached the P0 staff levels + one consultant

## **Overall:**

- Good progress / high productivity in the different teams





# Finish presentation

Questions ?

