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

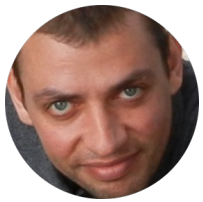

Andreas Pedersen *


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)

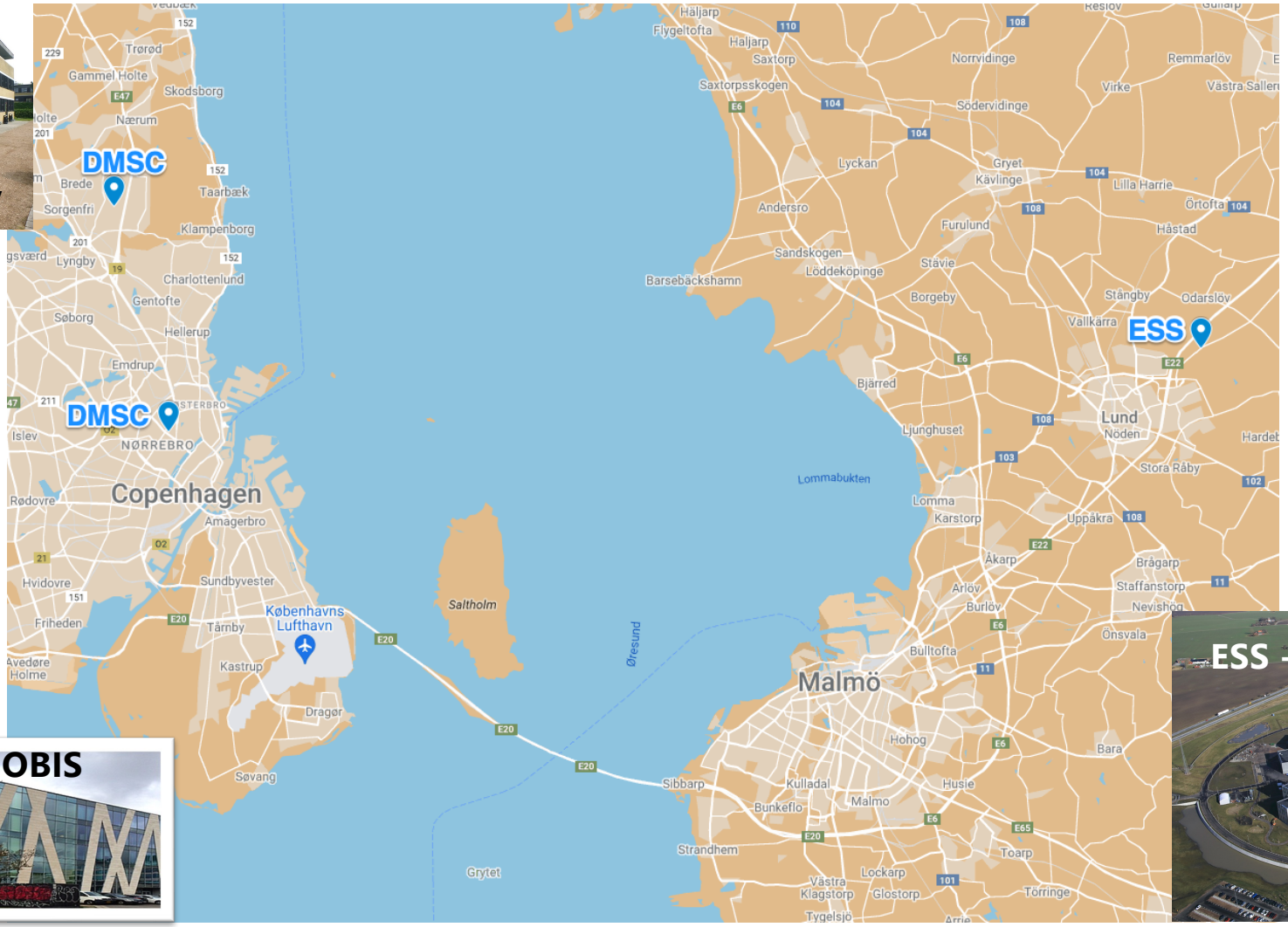
*/** "new" contract

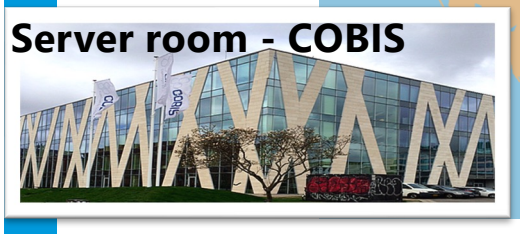
Scope

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

Scipp SWAT Modelling

DMSC –Lyngby/Copenhagen – ESS/LUND

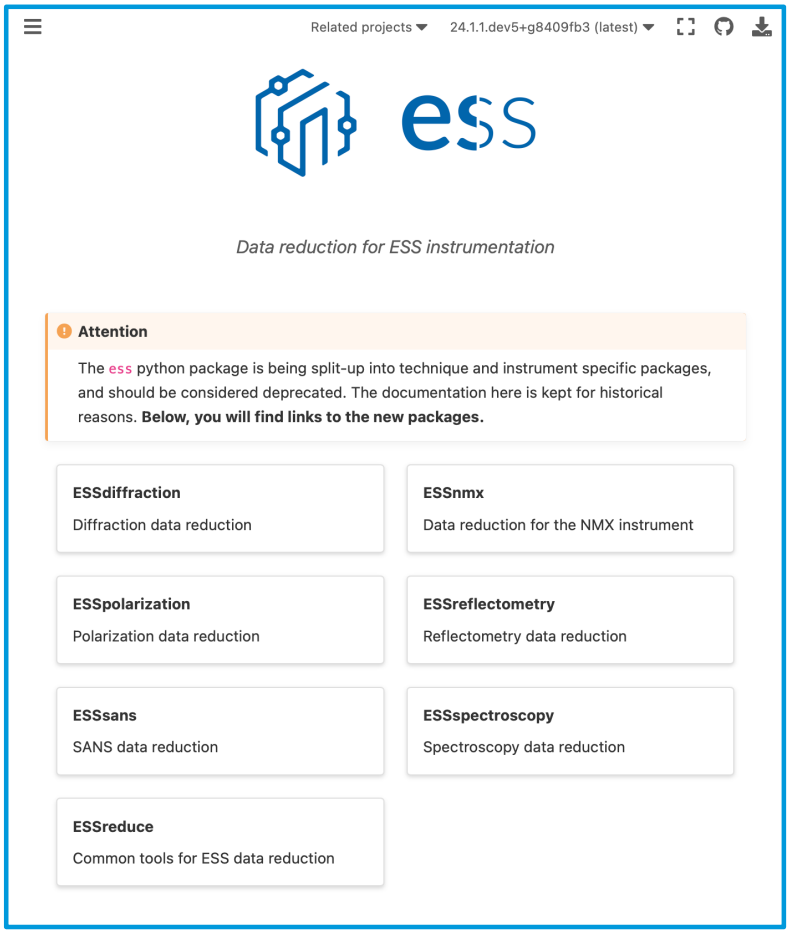




Scipp – Updates 1

General activities

1. New team member joined
2. Sciline – a workflow manager
3. **A lot of new instrument specific packages**
4. Beamlime – 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

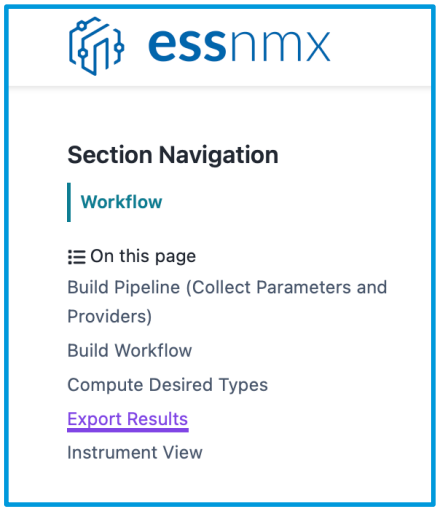


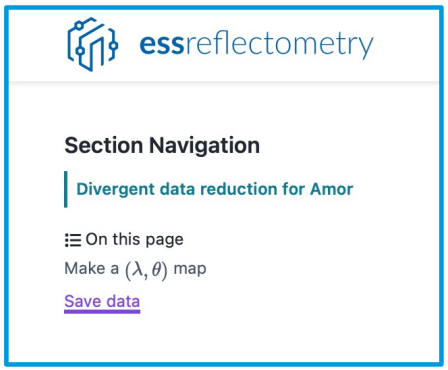
Scipp – Updates 2

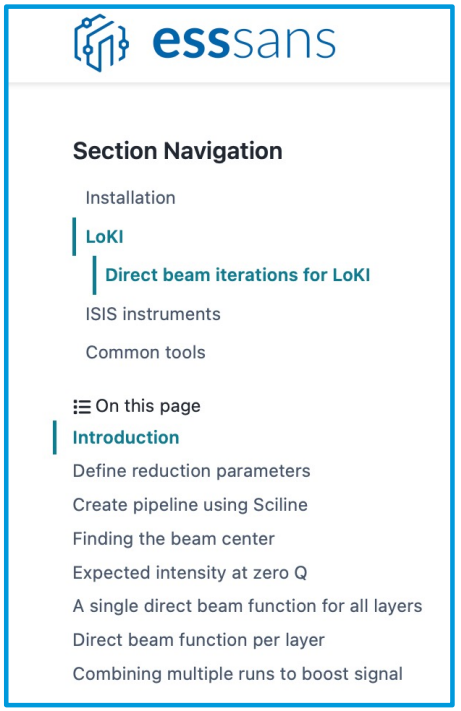
New instrument specific packages (breaking ess pacakge apart)

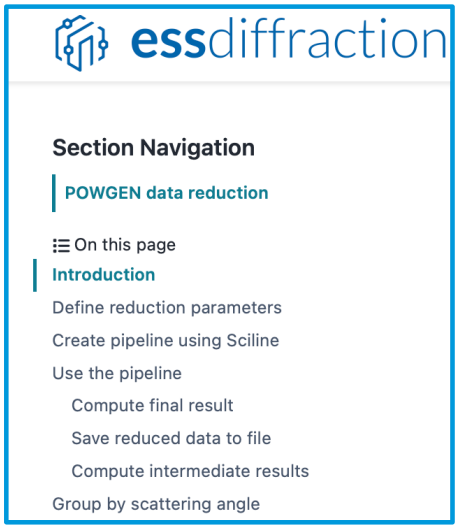
- ❑ Sciline
- ❑ ESSreduce

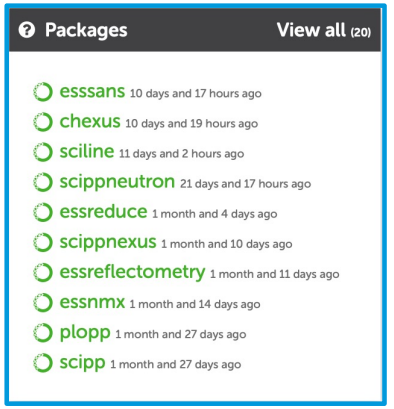
- ❑ ESSsans
- ❑ ESSnmx
- ❑ ESSdiffraction
- ❑ ESSreflectometry
- ❑ ESSpolarization
- ❑ ESSspectroscopy*
- ❑ ESSimaging*





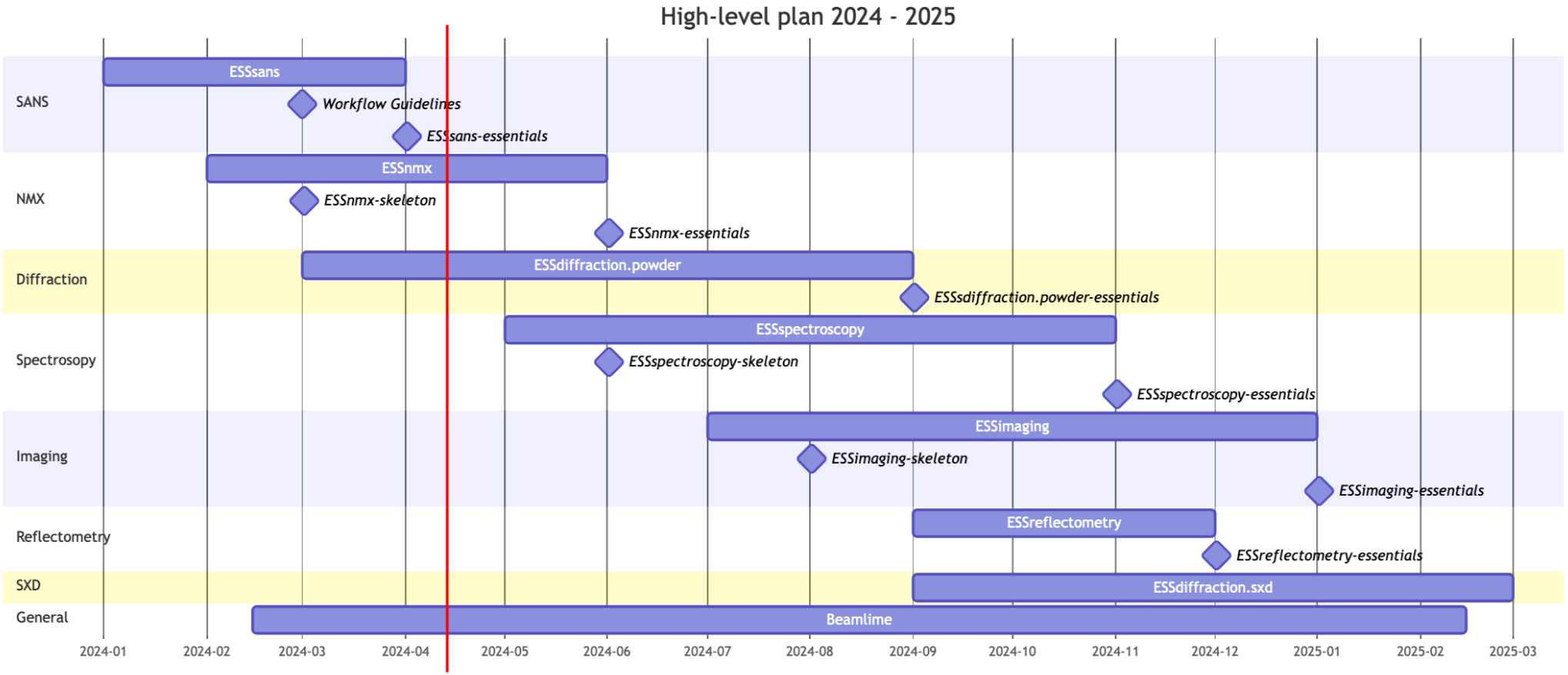






Scipp – Updates 3

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



Scipp – Updates 4

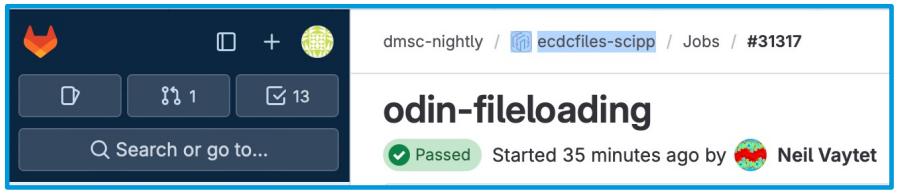
General (follow up on Requirements from the IDS from last STAP)

- 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



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

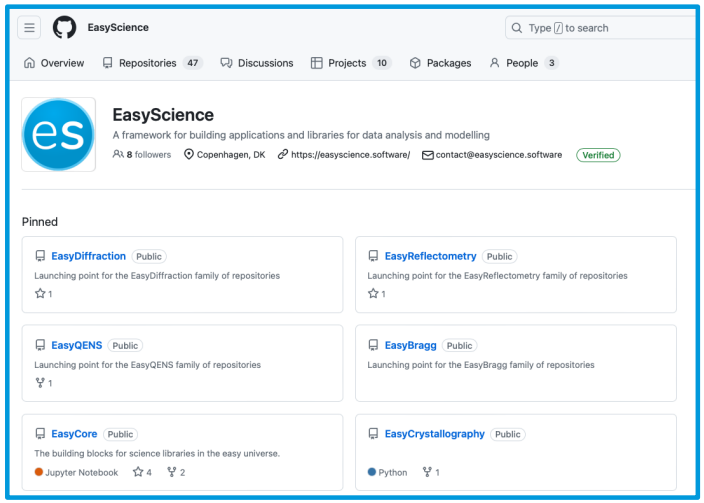
common.py 1.06 KiB

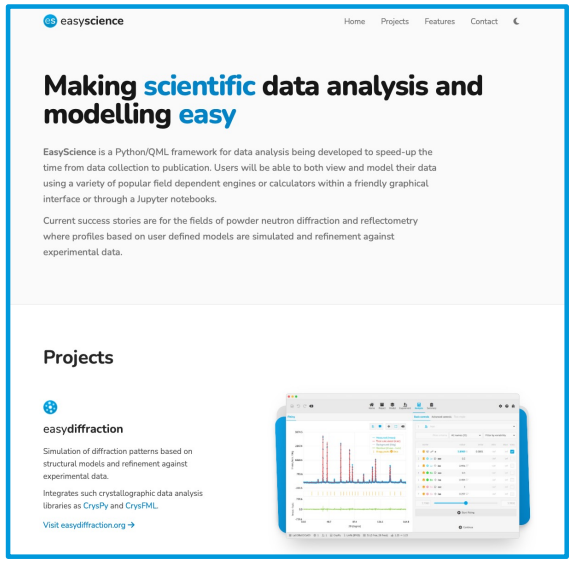
```python
# SPDX-License-Identifier: BSD-3-Clause
# Copyright (c) 2024 Scipp contributors (https://github.com/scipp)
import glob
import os
import shutil

import scippnexus as sx


def find_latest_file(
    instrument: str, path: str = "/ess/data/coda/2024/616254/raw"
) -> str:
    recent_files = sorted(glob.glob(os.path.join(path, "*.hdf")))[-10::][::-1]
    print(recent_files)
    for file in recent_files:
        print(f"Copying file {file} to local folder.")
        local_copy = file.split("/")[-1]
        shutil.copy(file, local_copy)
        try:
            with sx.File(local_copy, "r") as f:
                instrument_in_file = f["/entry/instrument/name"][()]
                if instrument_in_file == instrument:
                    print(f"Found {instrument} file: {local_copy}")
                    return local_copy
            print(
                f"File instrument is {instrument_in_file}, but {instrument} was "
                "requested. Skipping file."
            )
        except OSError:
            print(f"File {file} could not be opened.")
            continue
```

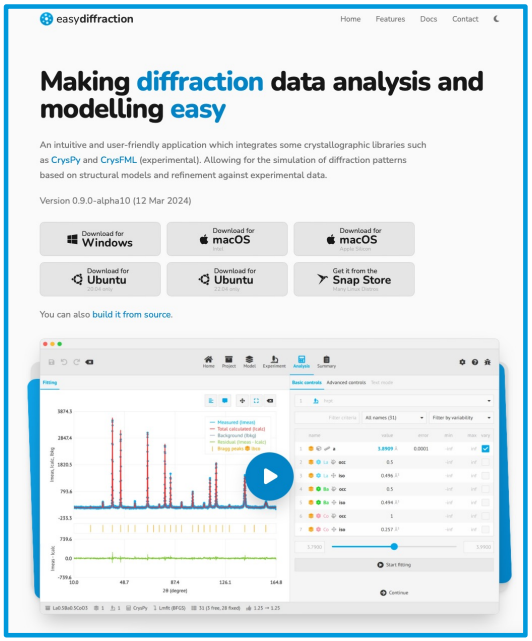
Data Analysis – Updates 1

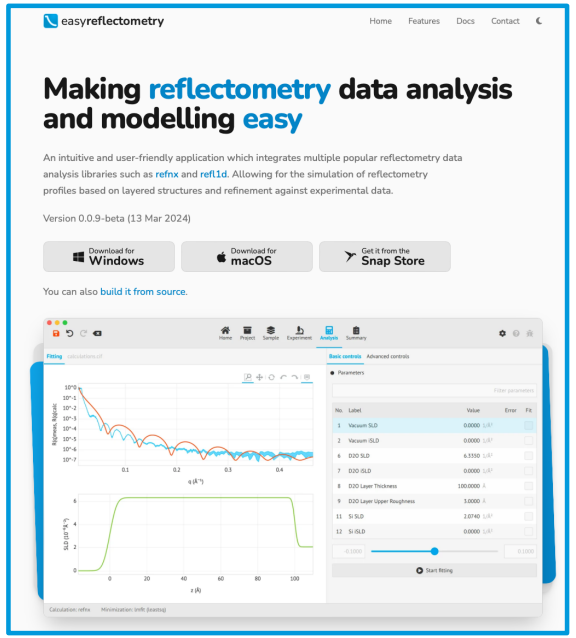
In-house projects

- ❑ EasyScince
- ❑ EasyDiffractionApp – EasyDiffractionLib
- ❑ EasyReflectometryApp – EasyReflectometryLib
- ❑ EasyCore
- ❑ EasyCrystallography









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)

❑ **Reflectometry**

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

❑ **Diffraction**

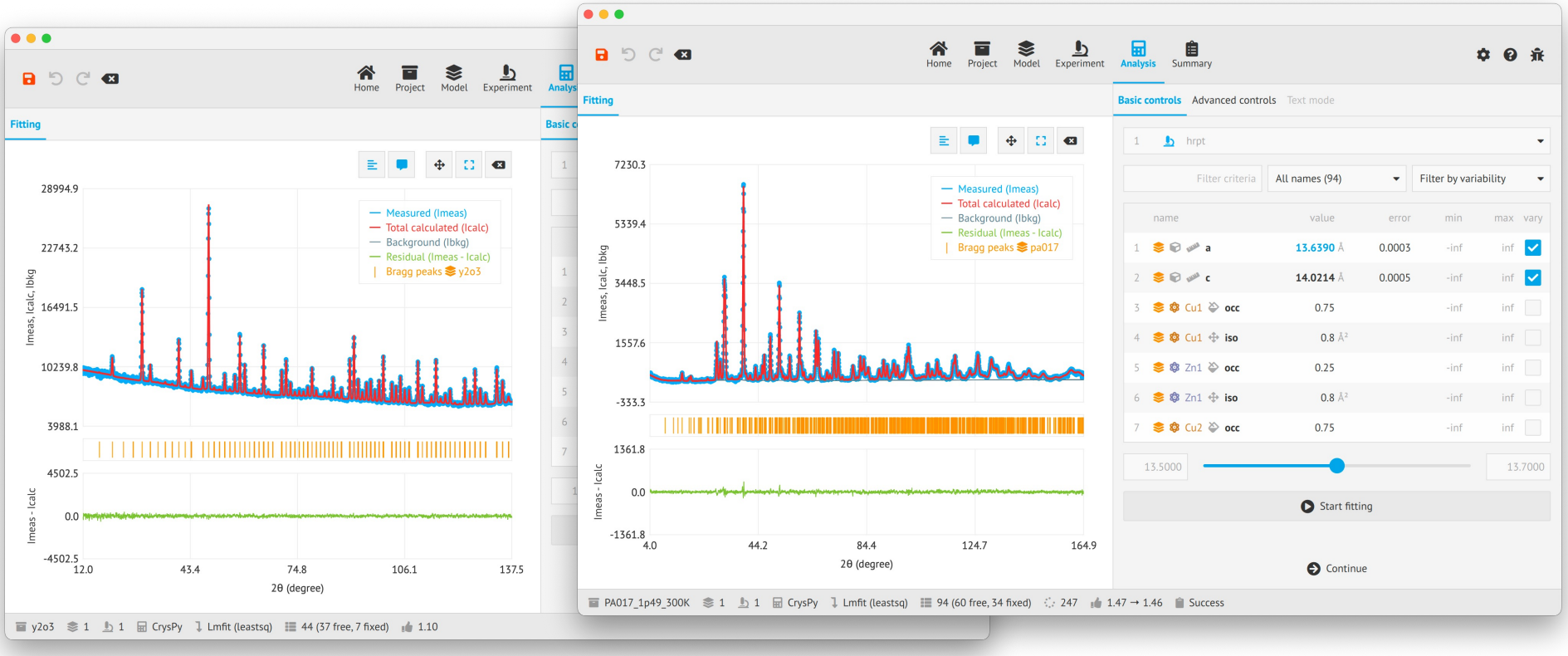
❑ Work has started to bring the EasyDiffraction application (version 0.9.0-beta) back into the EasyScience framework.

❑ 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.

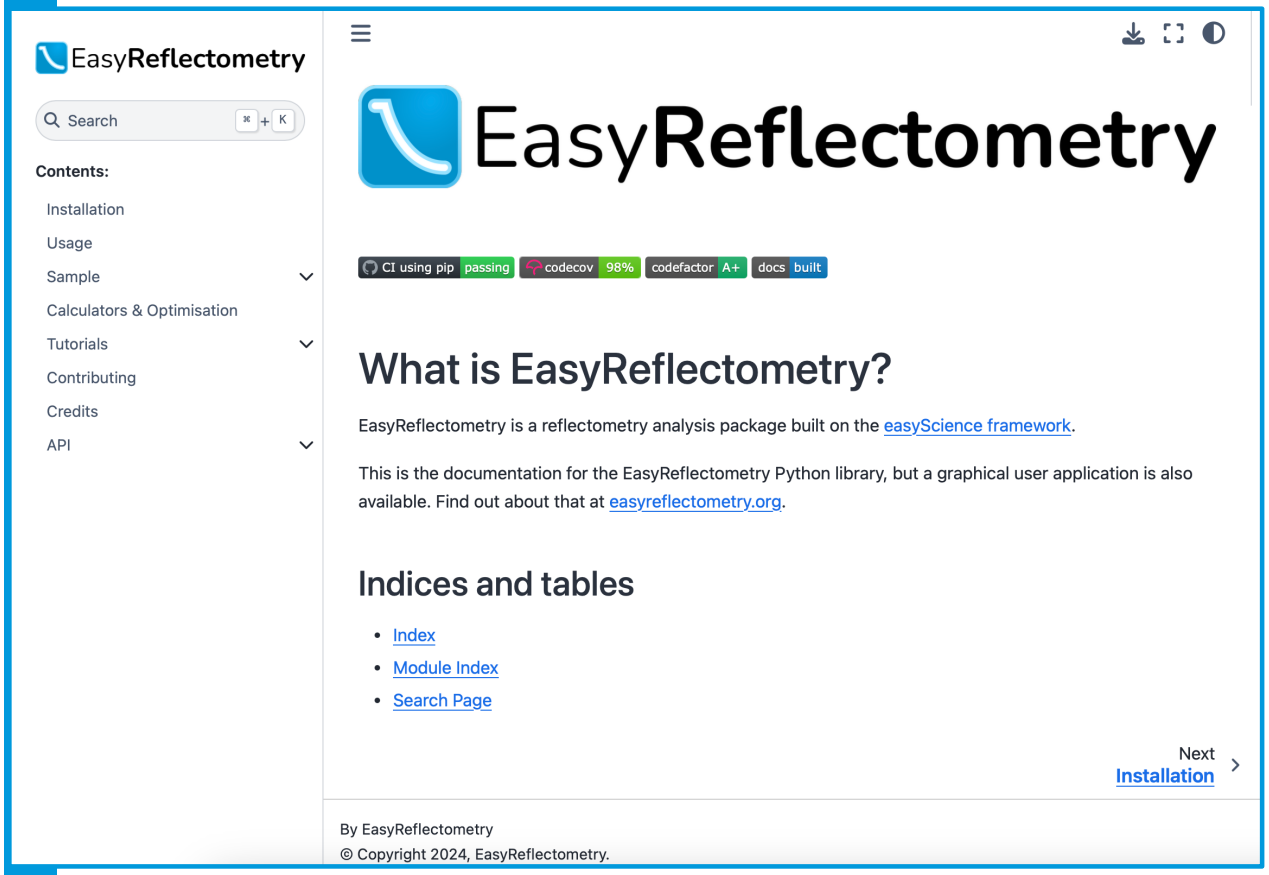
Data Analysis – Updates 5

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

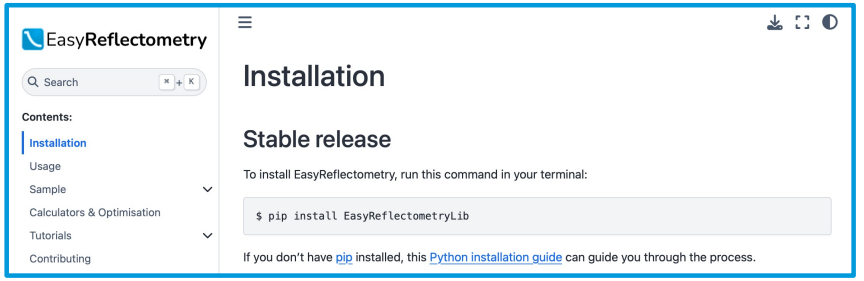


Data Analysis – Updates 6

EasyReflectometryLib - Documentation

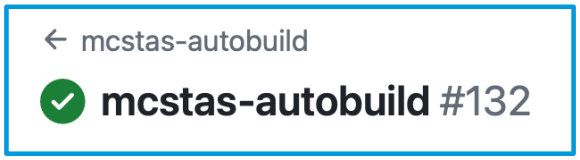


- ❑ Now installable with pip
- ❑ New slightly redesigned doc pages
- ❑ For better usability
- ❑ E.g. new search function included

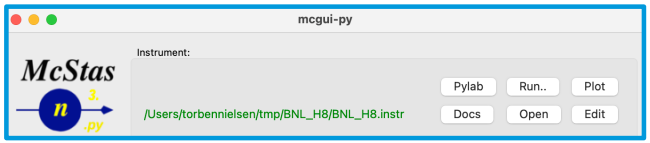


Instrument modelling – Update 1

McStas etc. updates



- ❑ 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)



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

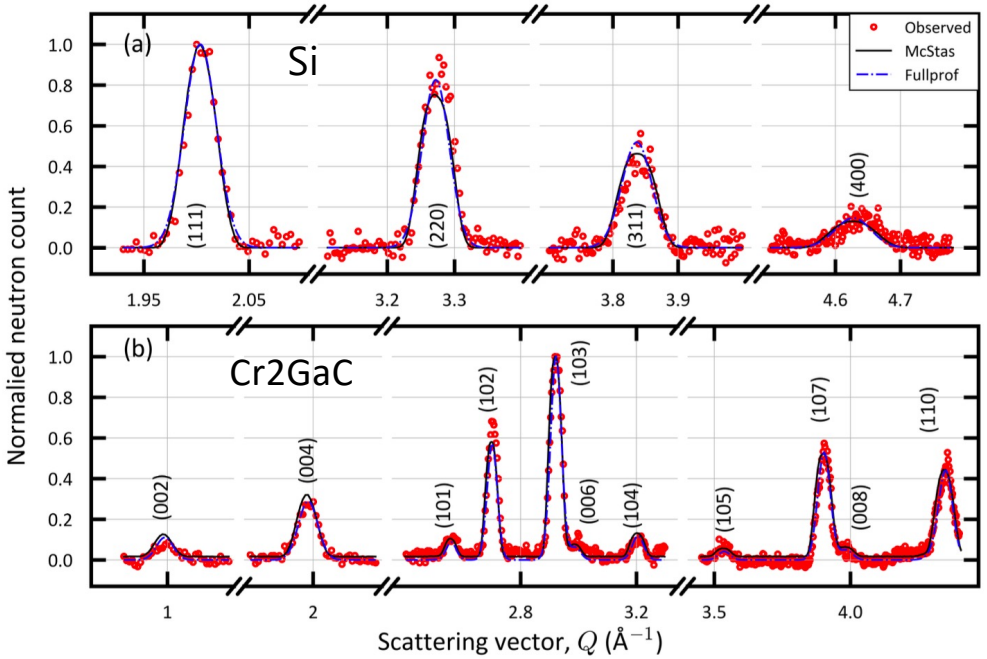


Figure 3: Observed (symbols) and calculated (lines) neutron powder diffraction pattern of (a) Si and (b) Cr2GaC using the KANDI-II diffractometer (2.47 Å). Solid line indicates a calculation performed using McStas, while dash-dotted line represents a Rietveld refined profile calculated using FULLPROF. 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

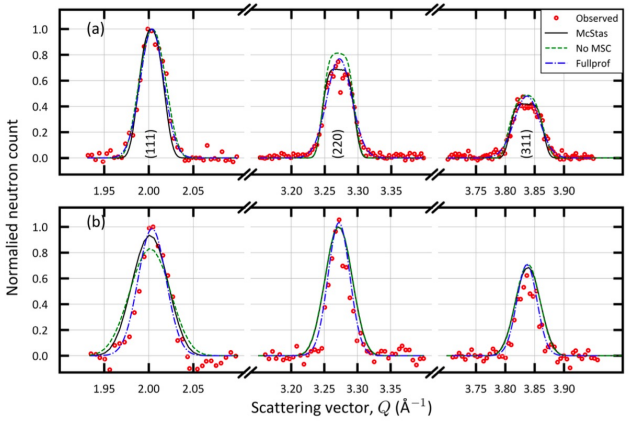


Figure 4: Observed (symbols) and calculated (lines) neutron diffraction patterns of Si powder using the KARL diffractometer with (a) PG monochromator (2.421 Å) and (b) Cu monochromator (0.98 Å). Solid line indicates a calculation performed using McStas, while dash-dotted line represents a Rietveld refined 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 **25th anniversary of the McStas** package
- An event at **DMSC** where all previous developers were invited

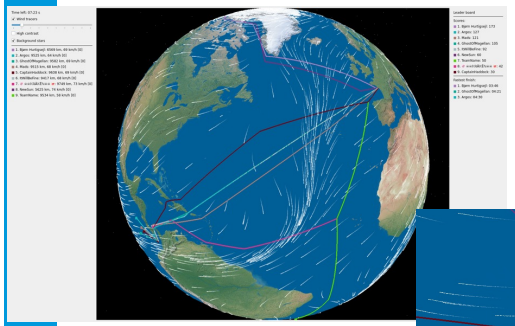
- It was decided to host another **DMSC summer school** in September **2024**.
- Due to the success of last year's school, it was chosen to keep changes to the format minimal, though with the ambition of **expanding the number of students from 14 to 20**.

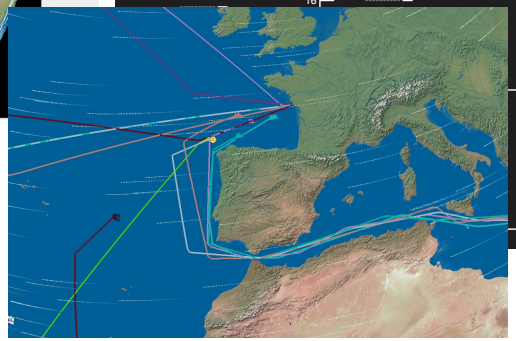
DMSC - python AI tournaments

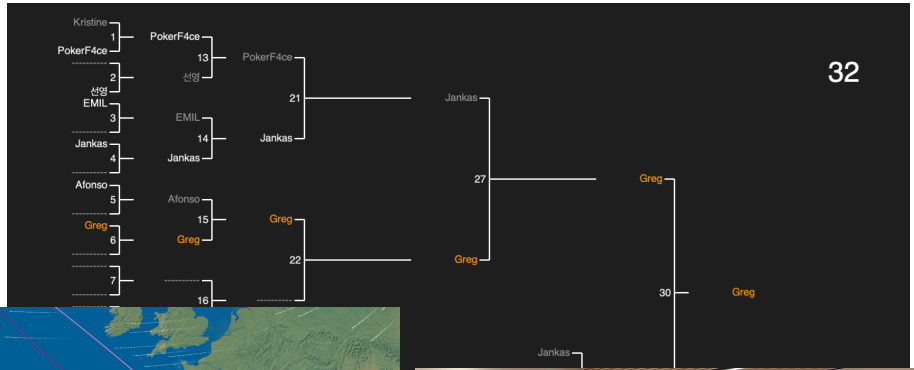
Open for all

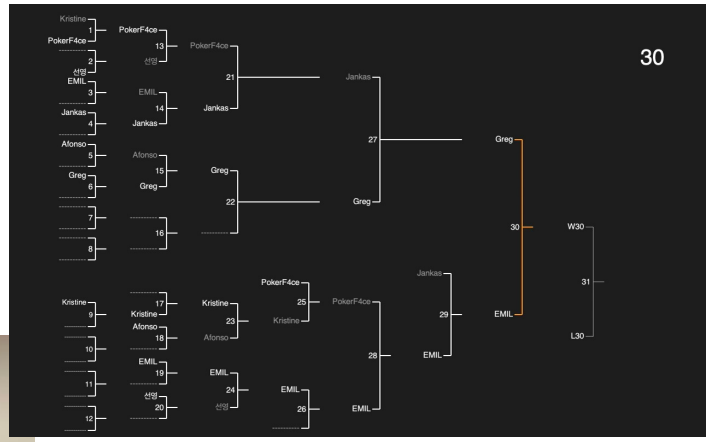
- December 2023
- VendéeGlobe results:
  - 1st: Jan-Lukas
  - 2nd: Greg
  - 3rd: Mads

- 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 ?