



**EUROPEAN
SPALLATION
SOURCE**



DMSC STAP

Updates from DRAM

TORBEN NIELSEN

APRIL 2023



Agenda



- 0. DRAM

- 1. Staffing

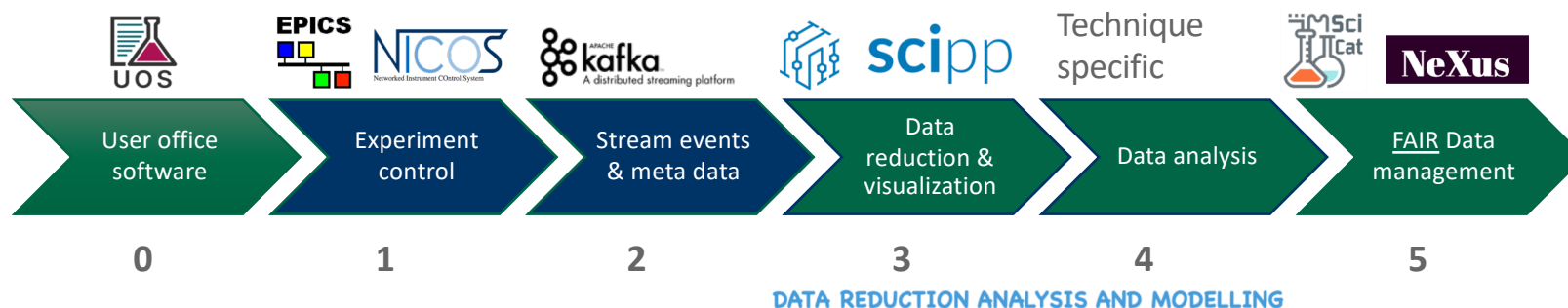
- 2. Achievements since last STAP

- 3. Plans and Milestones for 2023

- 4. Concerns

DMSC Scope for scientific computing

Support users with scientific computing at modern open science facility



Including

- Compute infrastructure
- Remote access to compute infrastructure & services
- Live data reduction and visualization
- Live analysis for some techniques

Plus

- Support for and with instrument simulations
- User support for scientific computing (Instrument Data Scientists)
- Materials and molecular modelling and simulations (not prioritised so far)

Services for ESS users



High level plans



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
 - possibly also QENS and TOF imaging
 - But always in combination with other libraries (backengines)
- **SasView** for SANS
- **PACE** for spectroscopy
- **MuhRec** for Tomography. (But now there is also a good commercial solution)

Data modelling

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

DRAM

Data Reduction, Analysis and Modelling



Simon Heybrock



Neil Vaytet



Jan-Lukas Wynen



Sunyoung Yoo



Piotr Rozyczko



Simon Ward



Andrew Sazonov



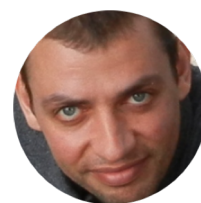
Peter Willendrup



Mads Bertelsen



Justin Bergmann*



Thomas Kittlemann**

Scope

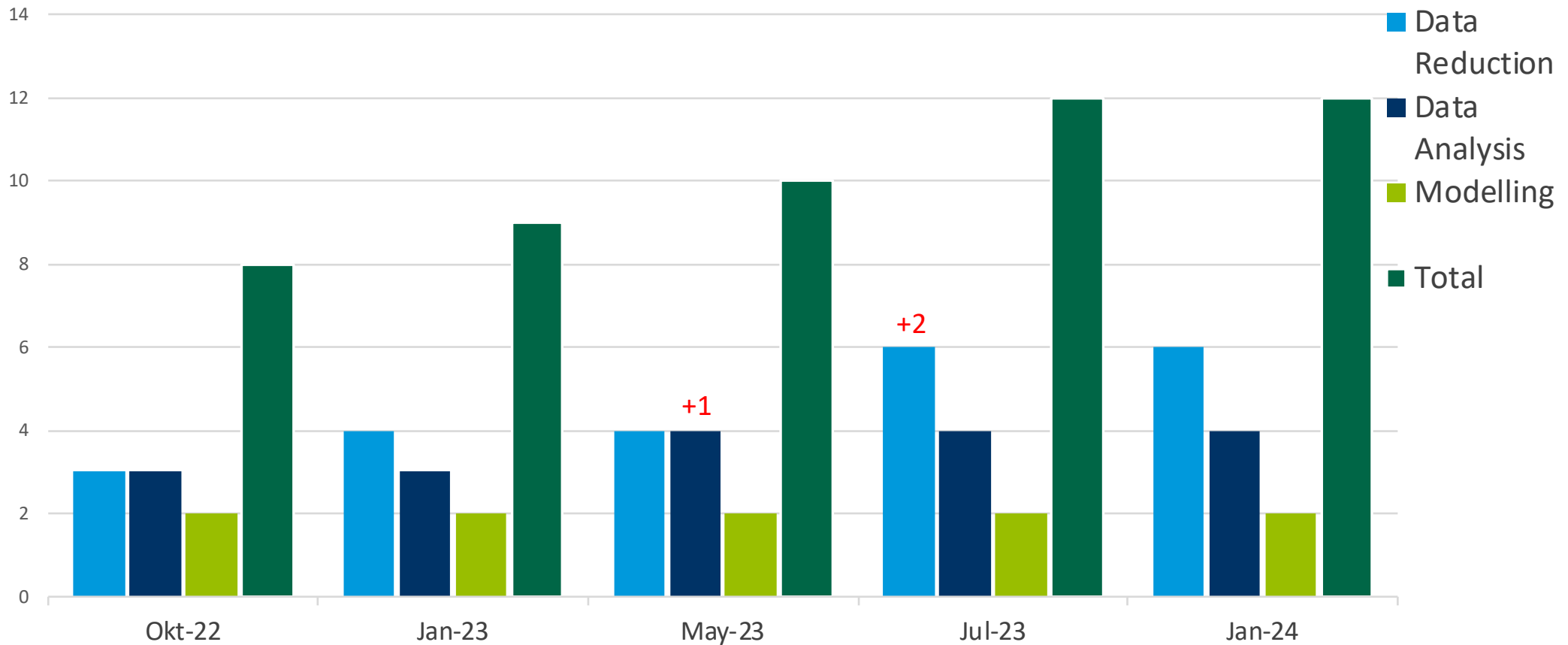
The DRAM group is responsible for providing the data reduction, analysis and modelling soft-ware for all instruments at ESS.

- ❑ 3 teams (11 persons)
 - ❑ Data Reduction (scipp)
 - ❑ Data Analysis (SasView, SpinW, EasyScience, external collaborations)
 - ❑ Modelling (McStas++, pan-learning.org, DetectorGroup , NMX)

DRAM - staff profile – Updated April 2023



PO – spring 2022



DRAM

	Simon H	Neil	Jan-Lukas	Sunyoung	Piotr	Simon W	Andrew S	Peter	Mads	Justin**	Wojtek*	Andrew M*	Gregory T*
Data Reduction (scipp)	●	●	●	●									
Data Analysis (easyScience)					●	●	●			○	○	○	
SpinW						●							
Pace-Project						●							●
SasView					●						●		
Modelling (McStas)								●	●				
pan-learning.eu								●					
Teaching	●	●	●	●	●	●	●	●	●	○	●	●	●

Data Reduction

scipp

	Simon H	Neil	Jan-Lukas	Sunyoung	Piotr	Simon W	Andrew S	Peter	Mads	Justin**	Wojtek*	Andrew M*
scipp (core)	●	●	●	●								
scippnexus	●	○	○	○								
plopp	○	●	○	○								
scippneutron	●	●	●	○								
ess	○	●	●	○								
beamline	○	○	○	●								
scitation	○	○	●	○								

- main responsible
- backup

Modelling

McStas – Digital Twins

	Simon H	Neil	Jan-Lukas	Sunyoung	Piotr	Simon W	Andrew S	Peter	Mads	Justin**	Wojtek*	Andrew M*
Mcstas (core)								●	○			
McStasScript									●			
Union								○	●			
Guide-Bot									●			
PaNOSC								●	●			
HIGHNESS									●			
pan-learning								●	○			
Moodel								●				

- main responsible
- backup

DRAM – easyScience

	easyCore	easyApp	easyCrystal	easyDiffLib	easyDiffApp	easyRefLib	easyRefApp	easyQENSLib	easyQENSAApp	easyBraggLib	easyBraggApp	easyTexLib	easyTexApp
Simon H	●		●					○					
Piotr R		○		●	●		○		●	○			
Andrew S		●		●	●				●	○	○	○	○
Dev4										●	●		
Andrew M*		○				●	●						
Søren S*										○			
Celine D*								○					
Thomas K**										○			

- main responsible
- backup

Scipp – Updates 1

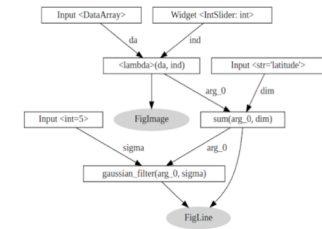
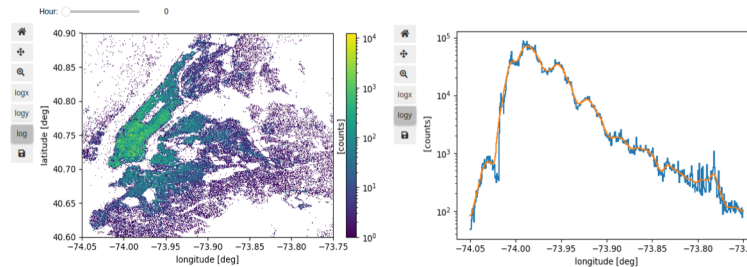


- ❑ **New Scipp developer:** Sunyoung Yoo started Jan 2nd 2023
- ❑ **NeXus:** We have encountered some performance issues when working with files from YMIR, BIFROST, and DREAM. Specifically, small files with many groups and datasets were affected.
- ❑ **NeXus:** Finally, we are working with ECDC to weed out various smaller issues with the NeXus files written by ESS, to ensure that the files are valid and interpretable.
- ❑ **Plopp:** We have re-implemented Scipp's plotting as a separate Python project based on Scipp. Plopp has been consolidated over the past 6 months.
- ❑ **Scitacean:** In collaboration with SWAP, we have begun the development of Scitacean, a Python package for interaction with SciCat.
- ❑ **Scitacean:** Workshops for DMSC staff – “Howto use Scitacean(SciCat)”
- ❑ **IDS requirements:** We have initiated the process of defining more detailed requirements from the IDS. The goal is to move from the current high-level lists of things that need to be done to concrete and actionable requirements.
- ❑ **IDS requirements:** To this end, after a kickoff meeting with the IDS, we have defined a template that can be used to describe requirements at a level of detail where we can begin working on them and include them in more detailed planning.

Scipp – Updates 2



# file, scippnexus, scippnexus.v2, speedup			
2023/DREAM_baseline_all_dets.nxs	1.99	2.02	1x
2023/BIFROST_873855_00000015.hdf	5.95	0.74	8x
2023/DREAM_mccode.h5	2.79	0.77	4x
2023/LOKI_mcstas_nexus_geometry.nxs	0.17	0.05	4x
2023/NMX_2e11-rechunk.h5	7.52	2.05	4x
2023/YMIR_038243_00010244.hdf	3.12	0.11	28x



SCITACEAN User guide API reference Developer documentation Release notes More

On this page
Why Scitacean?

Scitacean

Scitacean is a high level Python package for downloading and uploading datasets from and to SciCat.

To get started, read the [User Guide](#).

Why Scitacean?

Scitacean abstracts away the SciCat HTTP API and makes it usable via a small number of Python functions. However, it is not the only package that does so. In particular *Physicat* has a similar but lower level abstraction. Compared to *Physicat*, Scitacean offers:

- An easier to use and harder to misuse interface.
- Combined handling of metadata and files.
- Automated handling of a number of fields and some database details like data blocks.
- Basic validation of metadata.
- File upload and download utilities.

While Scitacean provides access to a lower level interface similar to *Physicat*, it only supports a small subset of the SciCat API. Consider using *Physicat* if you need to access, e.g. sample metadata, proposals, job information, etc.

README.md

SciCat workshop

Prepared by: Max Novelli and Jan-Lukas Wynen

Version 2023/03/21

This repository contains all the notebooks used to create the slides, examples and exercises for the SciCat workshop

The repository has the following structure:

- README.md: this file with lots of information
- scicat-workshop.ipynb: notebook used to create the workshop slides
- scicat-workshop.slides.html: html version of the slides as a normal presentation
- images: images used in the slides

Journal of Neutron Research 0 (0) 1
IOS Press

Systematic underestimation of uncertainties by widespread neutron-scattering data-reduction software

Simon Heybrock^{1,*}, Jan-Lukas Wynen¹ and Neil Vaytet¹
¹ European Spallation Source ERIC, P.O. Box 176, SE-221 00, Lund, Sweden
 E-mails: simon.heybrock@ess.eu, neil.vaytet@ess.eu, jan-lukas.wynen@ess.eu

Data Analysis – Updates 1



- ❑ **Staff:** About to start recruitment of extra developer for data analysis
- ❑ **EasyReflectometry:** A new release with improvement for file loading, plotting, continuous integration setup as well as distributing snapcast images for installation on Linux platforms.
- ❑ **EasyReflectometry:** In addition, work has been put into updating the EasyReflectometry roadmap.

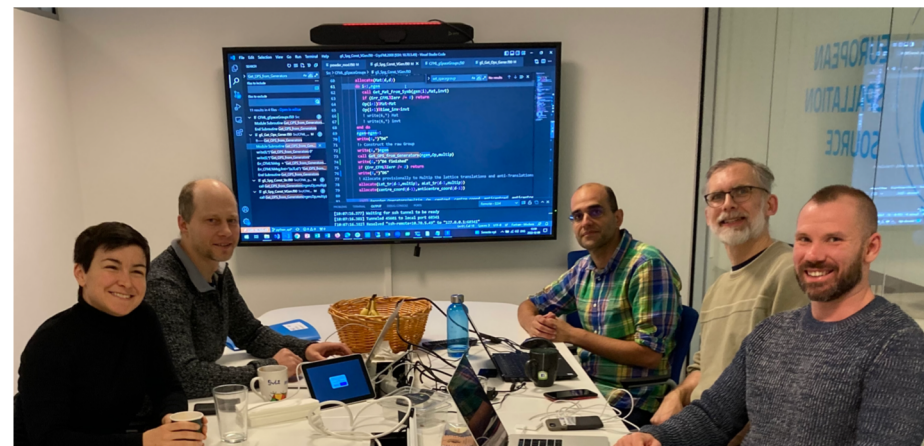
The screenshot shows the homepage of the EasyReflectometry website. At the top left is the 'easyreflectometry' logo. To the right are navigation links for 'Home', 'Features', 'Docs', and 'Contact'. The main heading reads 'Making reflectometry data analysis and modelling easy'. Below this is a descriptive paragraph: 'An intuitive and user-friendly application which integrates multiple popular reflectometry data analysis libraries such as [refnx](#) and [refl1d](#). Allowing for the simulation of reflectometry profiles based on layered structures and refinement against experimental data.' The version information 'Version 0.0.6-beta (27 Mar 2023)' is displayed. Three download buttons are present: 'Download for Windows', 'Download for macOS', and 'Get it from the Snap Store'. A link at the bottom says 'You can also [build it from source](#)'.

Data Analysis – Updates 2



- ❑ **EasyDiffraction:** One track is related to the usage of the crystallographic libraries CrysPy and CrysFML, while the second track is related to the internals of EasyDiffraction for improving the UX.
- ❑ **EasyDiffraction:** We have established monthly video meetings with the ILL team (ER & NK) and we also had a productive code hackathon with them at DMSC in December 2022. To continue the collaboration, another code hackathon is scheduled to be held in Grenoble in early summer 2023.

The screenshot shows the EasyDiffraction website homepage. At the top left is the 'easydiffraction' logo. Navigation links for 'Home', 'Features', 'Docs', and 'Contact' are visible. The main heading reads 'Making diffraction data analysis and modelling easy'. Below this, a paragraph describes the application as intuitive and user-friendly, integrating libraries like CrysPy and CrysFML. The current version is listed as 0.8.5-beta (30 Mar 2023). At the bottom, there are four buttons for downloading on Windows, macOS, Ubuntu, and the Snap Store. A link to 'build it from source' is also present.



Modelling – Updates 1



- ❑ **Staff:** PKW now 100% at DMSC (DTU In-Kind)
- ❑ **McStas:** UX, easier generation of event files for Scipp/Mantid
- ❑ **Teaching at KU:** McStas & McStasScript (pan-learning.org)

McStas Advanced Design School

e-Learning | My courses | McStas Advanced Design School

Announcements

JupyterLab

Overview of course

Welcome to the McStas Advanced Design School. This school covers the main contributions of Mads Bertelsen to the McStas eco system.

- McStasScript (Python API for McStas)
- McStas Union components (Complex physics and geometry as McStas components)
- guide_bot (Software for guide optimization using McStas)

The entire course is run through Jupyter notebooks through the JupyterLab instance for which there is a link at the top of this page.

Documentation for McStasScript and the Union components can be found at <https://mads-bertelsen.github.io/index.html>

All contributed software is open source and can be found in the following repositories:

<https://github.com/PaNOSC-VINYL/McStasScript>

https://github.com/McStasMcXtrace/McCode_II/blob/main/components_in_mcstas-union

Start simulation

Instrument parameters (D=float, I=int, S=string)

L1: 3.926 A1w: 0.03 A1h: 0.02

S6: 0.006 A2: 0.006 Lmin: 1

Lmax: 14 model_nr: 15

Simulation

Simulation/Trace: Simulation

Output format: NeXus -IDF -c

Autoplot: (only McCode format) - None -

Ray count: 1000000

Output subdir (optional):

Sweep steps (optional):

Parallelisation: No parallelisation

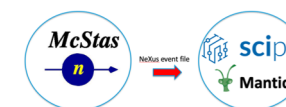
MPI node count: 2

Advanced

Random seed:

Gravity: Off

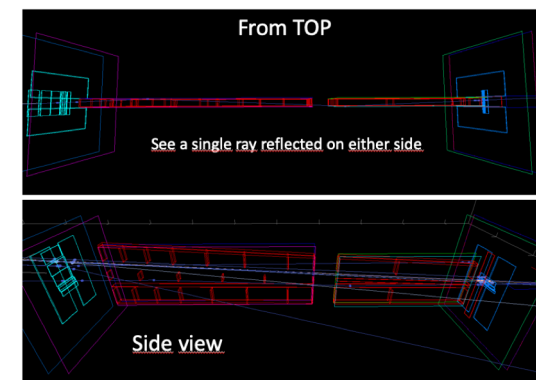
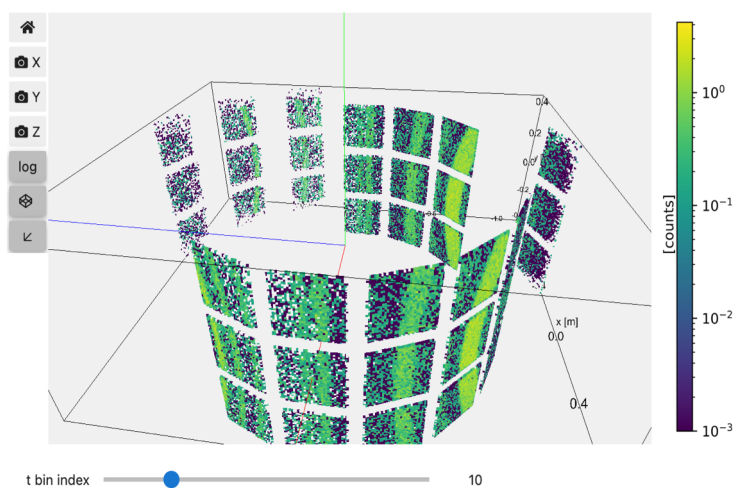
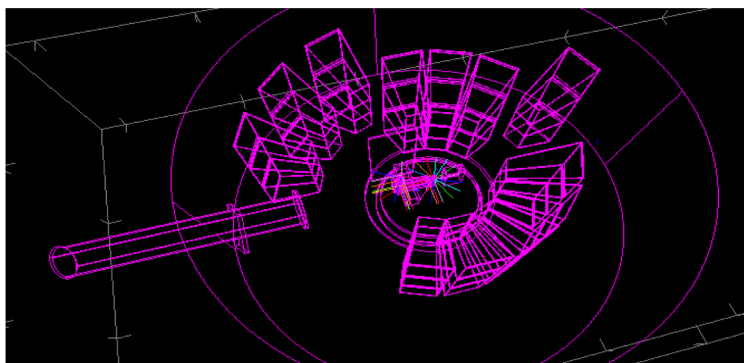
Start Cancel



Modelling – Updates 2

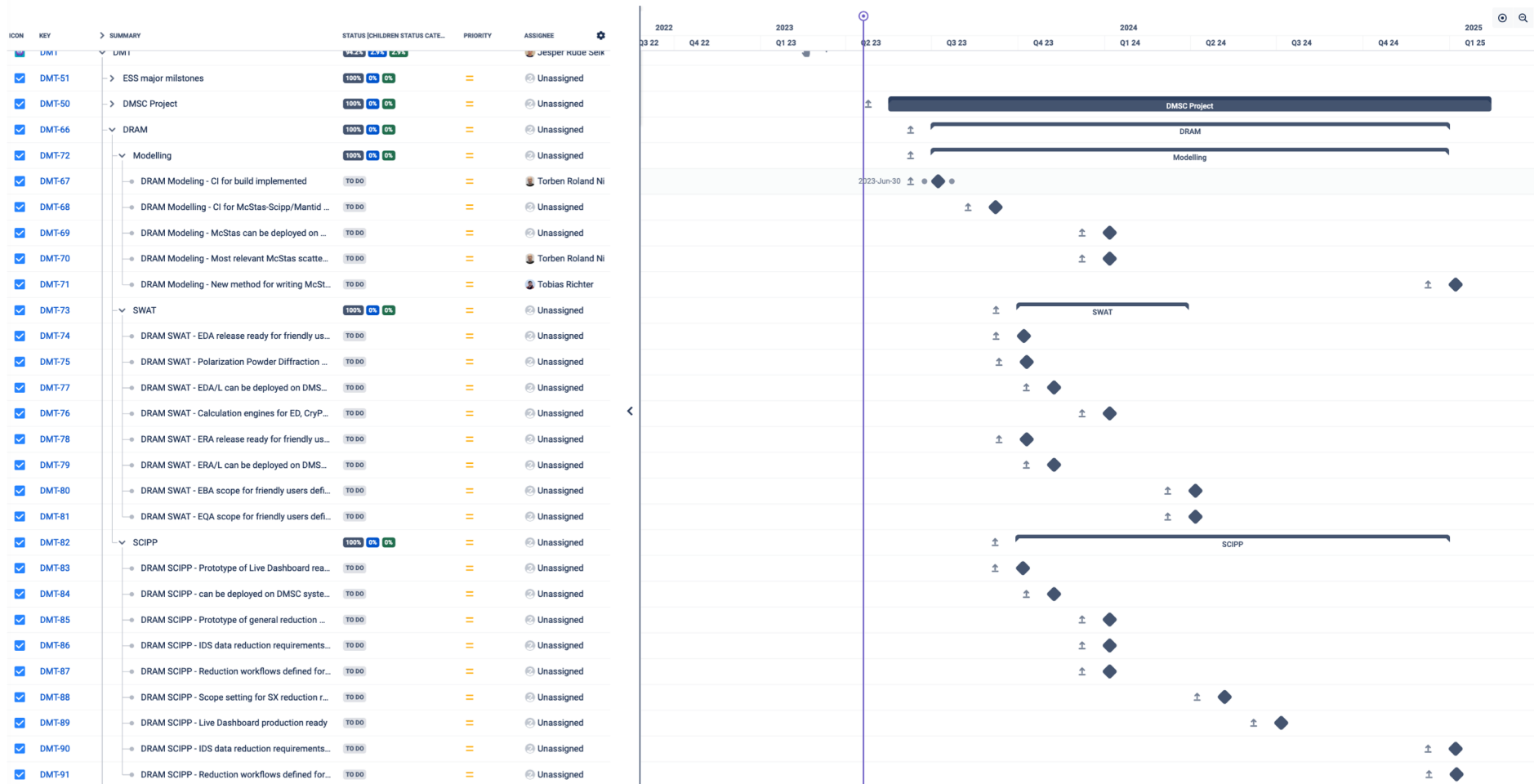


- ❑ J-PARC beam time: McStas support during test of new timepix-3 detector (at SENJU)
- ❑ Help FREIA instrument team: Slit systems for FREIA – Feasibility studies before procurement



Plans and Milestones

Jira BigPicture



Plans and Milestones



2023 – Scipp

Prototype of Live Dashboard ready	(ECDC)	2023-09-31
IDS data reduction requirements gathered for Phase HC-1 (2023)*	(IDS)	2023-12-31

2023 Data analysis

EDA release ready for friendly users to use & test	(IDS)	2023-09-31
Calculation engines for ED, CryPy & CrysFML, updated to latest versions	(ILL)	2023-12-31

2023 Modelling (McStas)

McStas intr files for instrument 1-9 updated and validated	(IDS)	2023-12-31
Most relevant McStas scattering kernels for instrument 1-9 identified	(IDS)	2023-12-31

General concerns, comments and aspirations



Scipp

- While work on initial requirements has started, we experience challenges in gathering concrete requirements.
- Among other reasons, the lack of actual ESS data files is a contribution to this.
- We will keep working with the IDS to ensure we can support them in the process of defining concrete requirements
- New approach seems to working in the right direction
 - E.g. LOKI “Beam Center Finder” part of this IDS-Scipp req. setup
 - Now in ess release 23.4.0

General concerns, comments and aspirations



Scipp – IDS requirements (LOKI)

Beam Center Finder

Created by Wojciech Potrzebowski, last modified on Feb 13, 2023

Requirement description

We would like to have a script that runs beam center finder algorithm. We assume that we run algorithm on isotropic well defined sample and to begin with we consider only rear panel (side panels will be considered later/as a separate requirement).

INPUT: all the files need for data reduction: sample, backgrounds, trans, monitors, etc.

OUTPUT: Beam center position x,y (and possibly z). The data should be logged somewhere (scicat), however in the first approximation we can also copy/paste numbers to data reduction notebooks

TEST DATA: LOKI detector test data (from March 2022) and SANS2D data for benchmarking

scipp / ess Public

Code Issues 18 Pull requests 4 Zenhub Discussions Actions

Beam centre finder #169

Merged nwaytet merged 63 commits into main from beam_centre_finder last month

Beam center finder

In SANS experiments, it is essential to find the center of the scattering pattern in order to allow symmetric summation of the scattering intensity around the beam (i.e. computing a one-dimensional $I(Q)$). As detector panels can move, the center of the beam will not always be located at the same place on the detector panel from one experiment to the next.

Here we describe the beam center finding algorithm, which uses a combination of a center-of-mass calculation and an iterative refinement on a computed scattering cross-section to find the center of the scattering pattern.

```
[1]: import scipp as sc
      from scipp.constants import g
      from ess import loki, sans
      from ess.sans import beam_center_finder as bcf
      from ess.logging import configure_workflow
      import plopp as pp

[2]: logger = configure_workflow('sans_beam_center_finder', filename='sans.log')
```

renamed dimensions:
Q <- wavelength
Steps:
Compute (scattered beam) =

Making 4 quadrants

We divide the panel into 4 quadrants.

```
[10]: p = image.plot(norm='log', aspect='equal')
      p.ax.plot(xc.value, yc.value, 'o', color='red', ms=5)
      p.ax.axline(xc.value, color='cyan')
      p.ax.axline(yc.value, color='cyan')
      dx = 0.25
      p.ax.text(xc.value + dx, yc.value + dx, 'North-East', ha='center', va='center')
      p.ax.text(xc.value - dx, yc.value + dx, 'North-West', ha='center', va='center')
      p.ax.text(xc.value - dx, yc.value - dx, 'South-East', ha='center', va='center')
      p.ax.text(xc.value + dx, yc.value - dx, 'South-West', ha='center', va='center')
      p
```

The plot shows a circular scattering pattern with a color scale from 10^2 to 10^3 counts. The axes are labeled x [m] and y [m], ranging from -0.4 to 0.4. The quadrants are labeled: North-East, North-West, South-East, and South-West.

General concerns, comments and aspirations



Data analysis

- Dependent on external calculation backends
 - Does requires extra man power
 - Can not support all. e.g. GSAS-II dropped in EasyDiffraction.

- SPOF (single point of failure)
 - Spread knowledge in team

- Bayesian data analysis
 - Update EasyCore, aligned with STAP comments from last meeting

DRAM – Summary



- ❑ **Staff:** We are consolidating the staff profile for DRAM in 2023.
- ❑ **Updates:** Good progress in the different team. Released several software packages.
- ❑ **Plans:** Started using BigPicture in Jira. (Holistic view of DRAM activities)



Finish presentation

Questions ?

