EUROPEAN
SPALLATION
SOURCE

DMSC STAP

Updates from DRAM

TORBEN NIELSEN

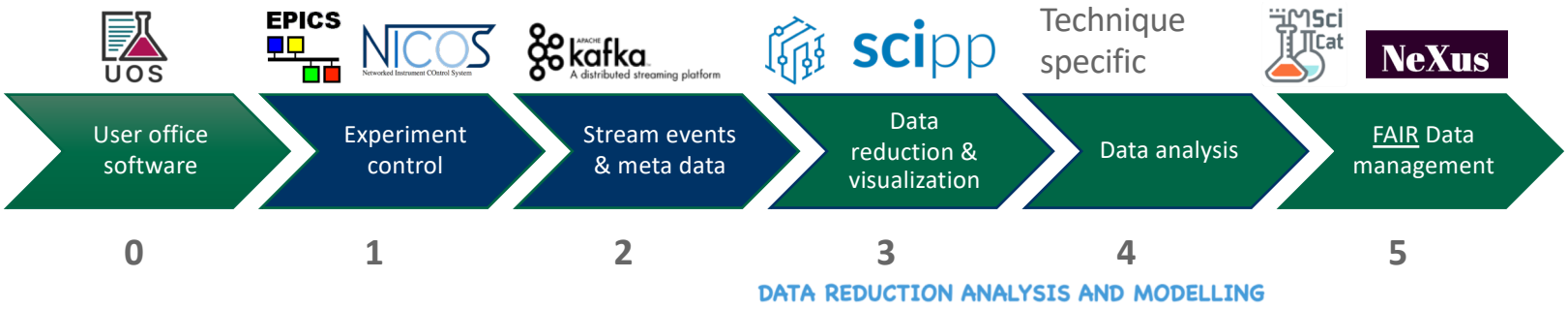
APRIL 2023

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**

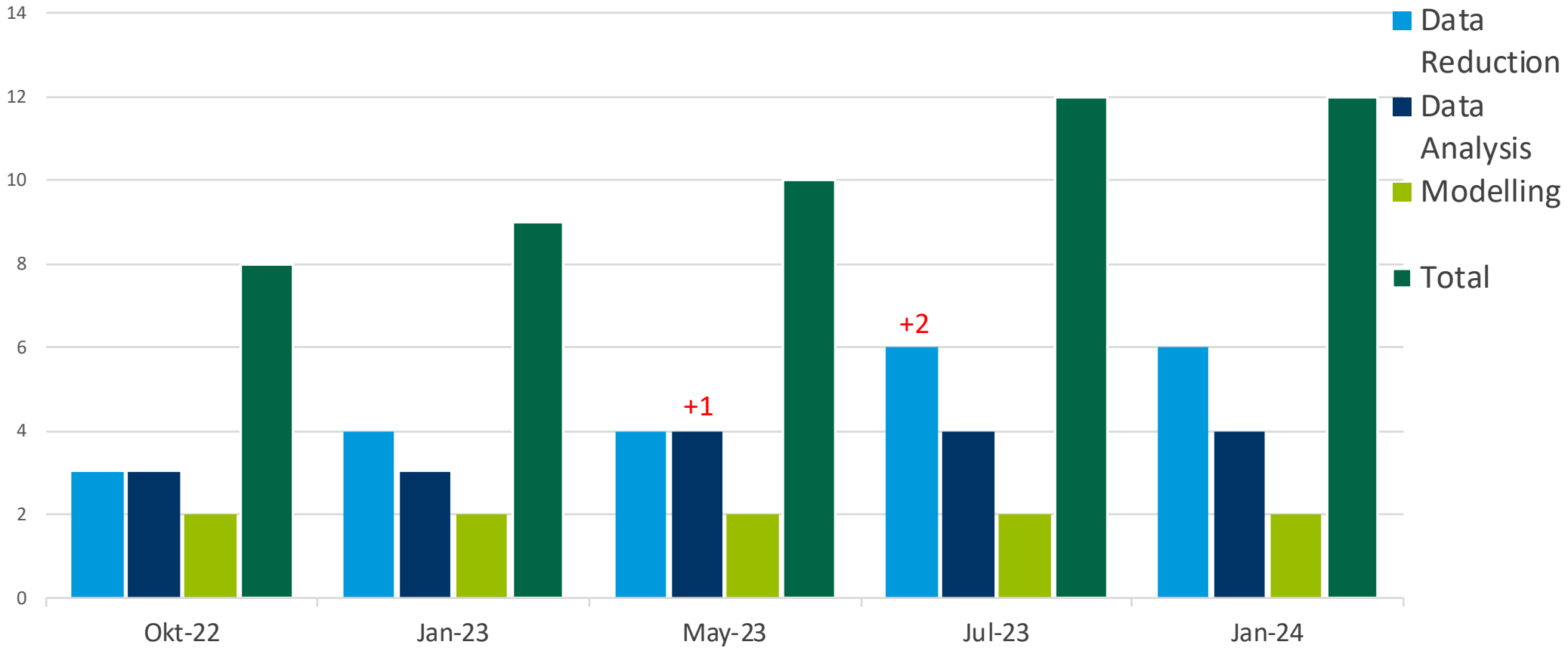
Scope

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

P0 – 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	○	●	●	○								
beamlime	○	○	○	●								
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	easyQENSApp	easyBraggLib	easyBraggApp	easyTexLib	easyTexApp
Simon H	●		●					○					
Piotr R		○		●	●		○		●	○			
Andrew S		●		●	●				●	○	○	○	○
Dev4										●	●		
Andrew M*		○				●	●						
Søren S*										○			
Celine D*								○					
Thomas K**										○			

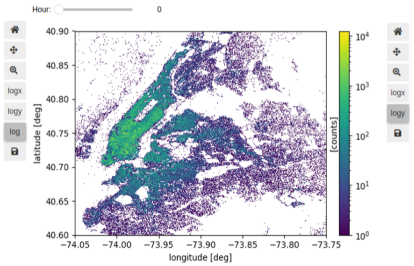
● main responsible
○ backup

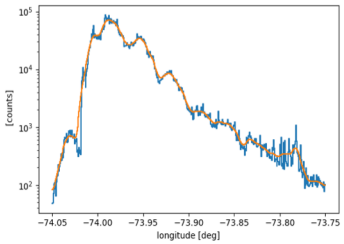
Scipp – Updates 1

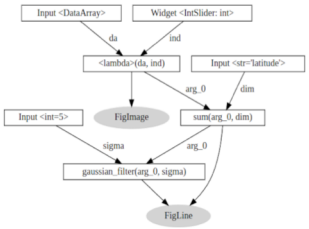
- **New Scipp developer:** Sunyoung Yoo started Jan 2nd 2023
- **NeXus:** We have encountered some performance issues when working with files from YMIR, BIFROST, and DREAM. Specifically, small files with many groups and datasets were affected.
- **NeXus:** Finally, we are working with ECDC to weed out 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.

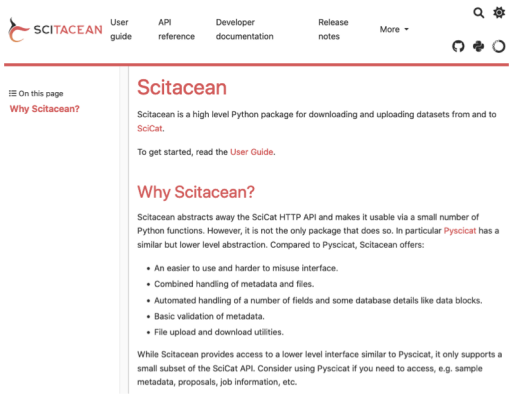
Scipp – Updates 2

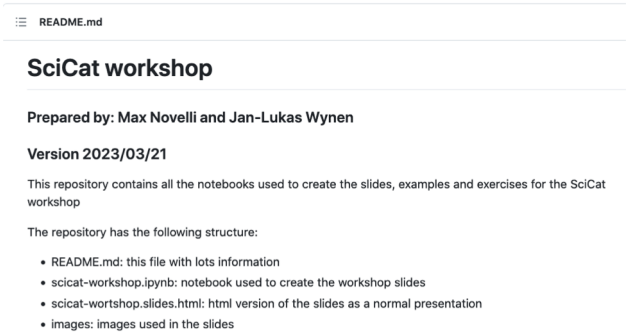
```
# file, scippnexus, scippnexus.v2, speedup
2023/DREAM_baseline_all_dets.nxs          1.99   2.02  1x
2023/BIFROST_873855_00000015.hdf          5.95   0.74  8x
2023/DREAM_mccode.h5                      2.79   0.77  4x
2023/LOKI_mcstas_nexus_geometry.nxs       0.17   0.05  4x
2023/NMX_2e11-rechunk.h5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

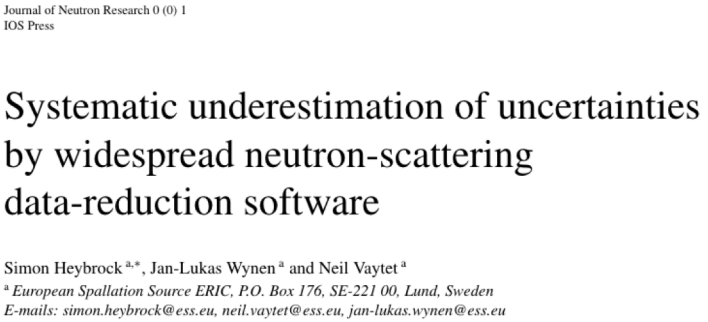






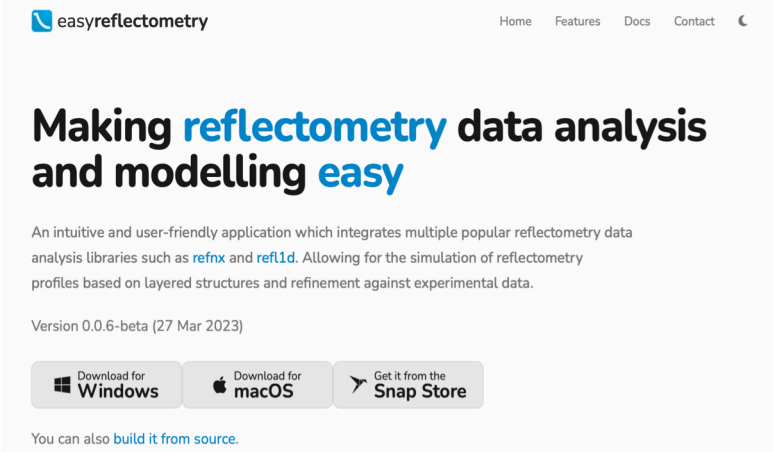






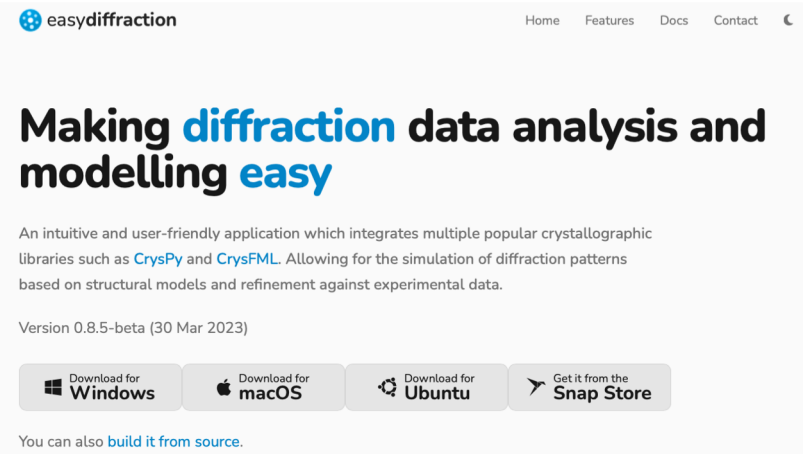
Data Analysis – Updates 1

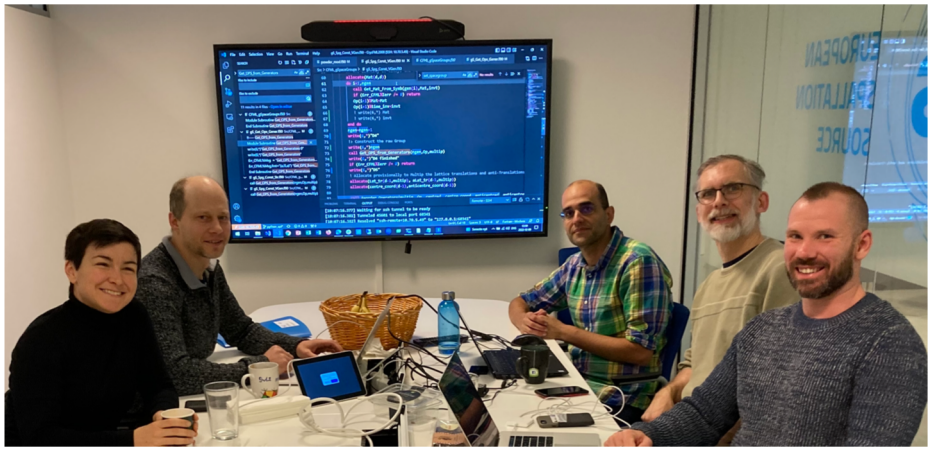
- **Staff:** About to start recruitment of extra developer for data analysis
- **EasyReflectometry:** A new release with improvement for file loading, plotting, continuous integration setup as well as distributing snapcast images for installation on Linux platforms.
- **EasyReflectometry:** In addition,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



Data Analysis – Updates 2

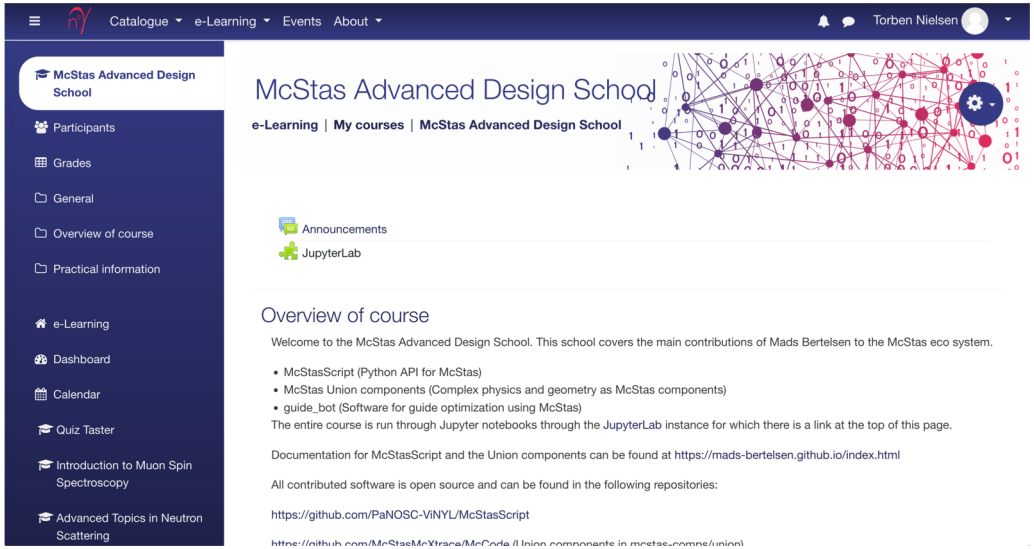
- **EasyDiffraction:** One track is related to the usage of the crystallographic libraries CrysPy and CrysFML, while the second track is related to the internals of EasyDiffraction for improving the UX.
- **EasyDiffraction:** We have established monthly video meetings with the ILL team (ER & NK) and 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.

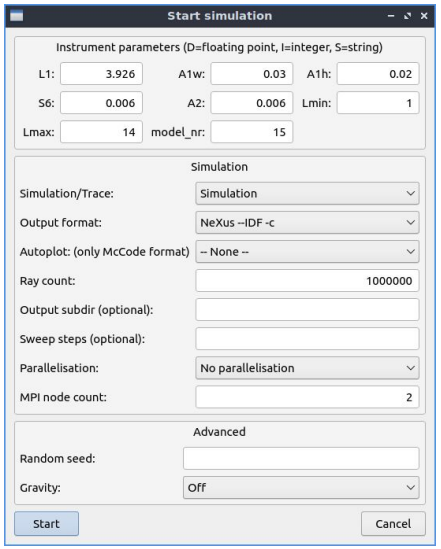


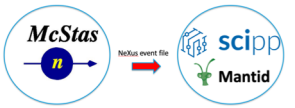


Modelling – Updates 1

- **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)

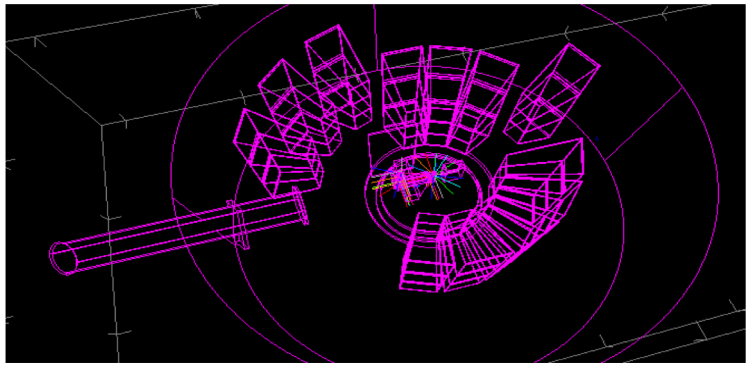


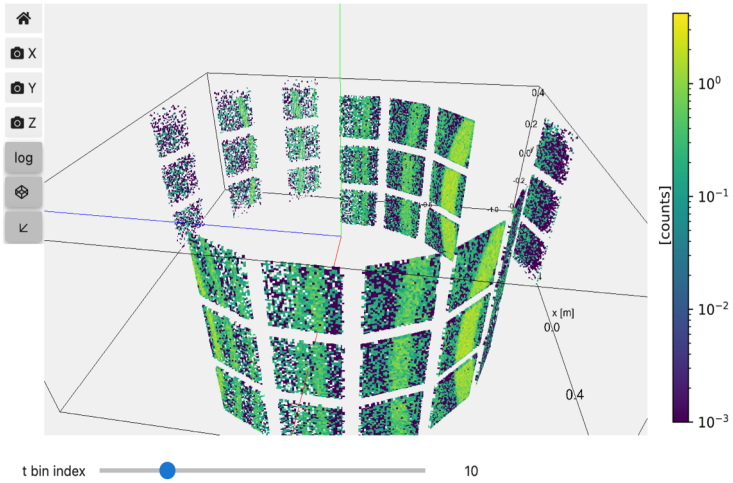


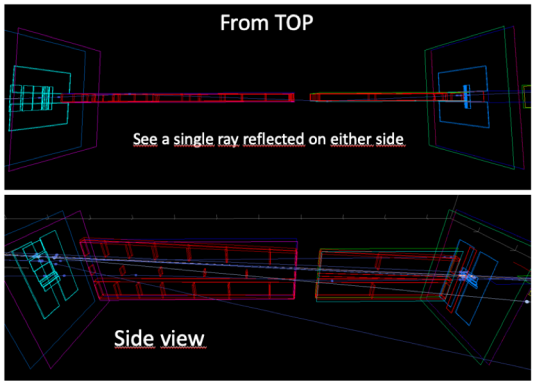


Modelling – Updates 2

- **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

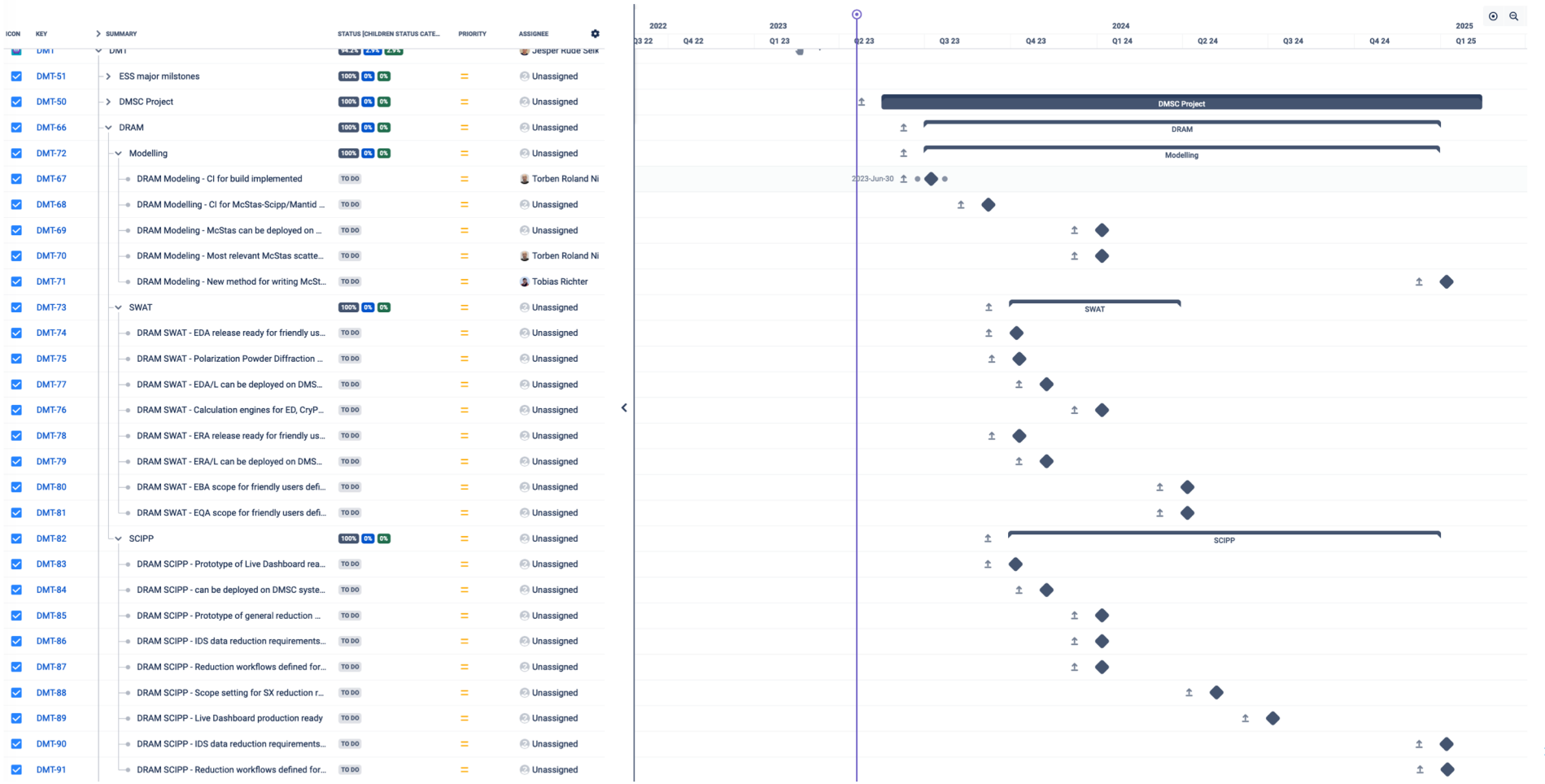






Plans and Milestones

Jira BigPicture



ICON	KEY	SUMMARY	STATUS [CHILDREN STATUS CATE...	PRIORITY	ASSIGNEE
	DMT	DMT			Jesper Rude Selt
	DMT-51	ESS major milstones	100% 0% 0%	=	Unassigned
	DMT-50	DMSC Project	100% 0% 0%	=	Unassigned
	DMT-66	DRAM	100% 0% 0%	=	Unassigned
	DMT-72	Modelling	100% 0% 0%	=	Unassigned
	DMT-67	DRAM Modeling - CI for build implemented	TO DO	=	Torben Roland Ni
	DMT-68	DRAM Modelling - CI for McStas-Scipp/Mantid ...	TO DO	=	Unassigned
	DMT-69	DRAM Modeling - McStas can be deployed on ...	TO DO	=	Unassigned
	DMT-70	DRAM Modeling - Most relevant McStas scatte...	TO DO	=	Torben Roland Ni
	DMT-71	DRAM Modeling - New method for writing McSt...	TO DO	=	Tobias Richter
	DMT-73	SWAT	100% 0% 0%	=	Unassigned
	DMT-74	DRAM SWAT - EDA release ready for friendly us...	TO DO	=	Unassigned
	DMT-75	DRAM SWAT - Polarization Powder Diffraction ...	TO DO	=	Unassigned
	DMT-77	DRAM SWAT - EDA/L can be deployed on DMS...	TO DO	=	Unassigned
	DMT-76	DRAM SWAT - Calculation engines for ED, CryP...	TO DO	=	Unassigned
	DMT-78	DRAM SWAT - ERA release ready for friendly us...	TO DO	=	Unassigned
	DMT-79	DRAM SWAT - ERA/L can be deployed on DMS...	TO DO	=	Unassigned
	DMT-80	DRAM SWAT - EBA scope for friendly users defi...	TO DO	=	Unassigned
	DMT-81	DRAM SWAT - EQA scope for friendly users defi...	TO DO	=	Unassigned
	DMT-82	SCIPP	100% 0% 0%	=	Unassigned
	DMT-83	DRAM SCIPP - Prototype of Live Dashboard rea...	TO DO	=	Unassigned
	DMT-84	DRAM SCIPP - can be deployed on DMSC syste...	TO DO	=	Unassigned
	DMT-85	DRAM SCIPP - Prototype of general reduction ...	TO DO	=	Unassigned
	DMT-86	DRAM SCIPP - IDS data reduction requirements...	TO DO	=	Unassigned
	DMT-87	DRAM SCIPP - Reduction workflows defined for...	TO DO	=	Unassigned
	DMT-88	DRAM SCIPP - Scope setting for SX reduction r...	TO DO	=	Unassigned
	DMT-89	DRAM SCIPP - Live Dashboard production ready	TO DO	=	Unassigned
	DMT-90	DRAM SCIPP - IDS data reduction requirements...	TO DO	=	Unassigned
	DMT-91	DRAM SCIPP - Reduction workflows defined for...	TO DO	=	Unassigned

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

ES: EasyScience – EDA: EasyDiffractionApp – ERA: EasyReflectionApp – EQA: EasyQENSApp – EBA: EasyBraggApp

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 seprarate 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 somehere (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 nvaytet merged 63 commits into main from beam_centre_finder last month

ess

Search the docs ...

GETTING STARTED

Installation

INSTRUMENTS

Amor

Loki

External Instruments

TECHNIQUES

Diffraction

Reflectometry

SANS

Beam center finder

Related projects | 23.4.0 (latest)

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')
```

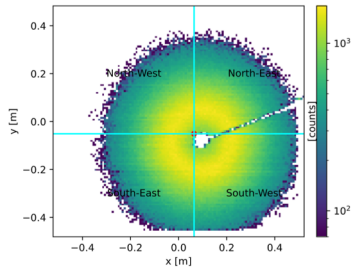
Renamed dimensions:
Q <- wavelength
Steps:
Compute (scattered beam) =

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.axvline(xc.value, color='cyan')
      p.ax.axhline(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
```

[10]:



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 ?