DMSC activities related to Diffraction

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Contributors:

- Mikhail Feygenson, Florence Porcher (DREAM instrument scientists (IS))
- Irina Stefanescu (ESS detector group)
- Experiment Control and Data Curation (ECDC): NeXus, scicat
- Data Reduction, Analysis, and Modelling (DRAM): Scipp, EasyDiffraction, McStas

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1 Introduction

This document briefly describes the latest development activities by the Data Management and Software Centre (DMSC) related to Diffraction (since Autumn 2022). At this stage, these activities are mostly focused on DREAM. A section at the end of the document summarizes the status of the development of MAGIC. The work reported in this document has involved close collaborations between DMSC, the instrument teams to develop diffraction data processing, reduction and analysis at the European Spallation Source (ESS) and collaborations with other institutes.
Figure 1 shows the DMSC vision for the data workflow during an experiment, from running and steering the experiment, over to data acquisition and to data analysis and data management as the last steps. This brief document reports on activities related to:

- data reduction with Scipp
- data analysis with EasyDiffraction
- data recording with NeXus files
- data archiving with Scicat

In order to test parts of this pipeline, we rely on data from instrument simulations with McStas [1] or from existing instruments from other facilities. Activities related to these simulations are also reported in this document.

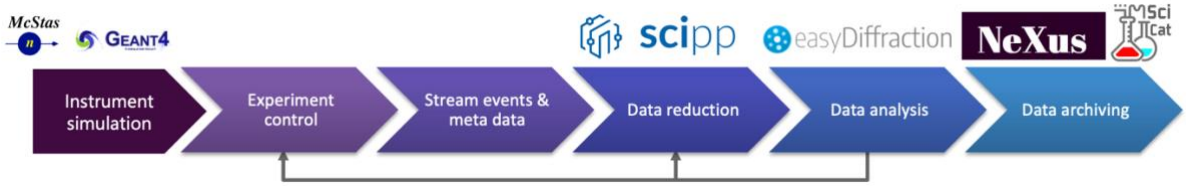

Figure 1: The DMSC data pipeline. Each chevron corresponds to a class of services needed for processing experimental data. The backward arrows show a mechanism to interact with the ongoing experiment based on feedback from the data reduction or analysis services. The software or frameworks are listed above the chevrons.

2 NeXus file

Contributors: ECDC, IDS, ESS detector group

ECDC has developed the skeleton of the ESS NeXus file for DREAM. Figure 2 shows the layout of the instrument in the NeXus Constructor (i.e., tool developed by ECDC for an easier maintenance of the NeXus files). This baseline file contains the description of the detectors (except the SANS detector), monitors, slits and choppers.

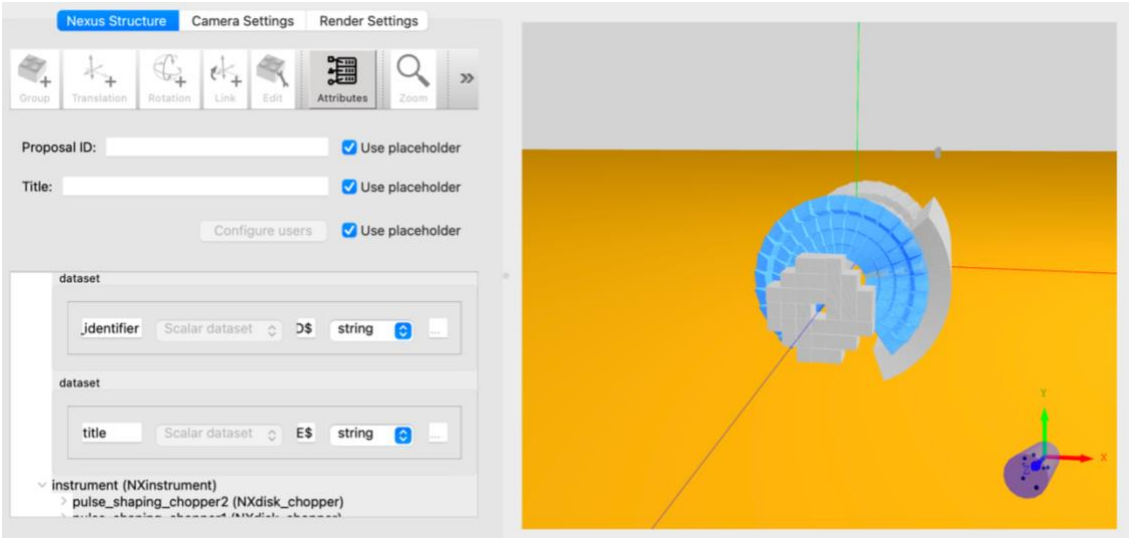

Figure 2: GUI of NeXus Constructor showing the layout of DREAM with the endcap forward detector highlighted in blue.

3 Instrument simulation with McStas

Contributors: DRAM, detector group, IS, IDS

DREAM

Experimental configurations

McStas models of DREAM up to the sample (i.e., without the 3D detectors) have been developed for the high-intensity and high-resolution configurations by the instrument scientists in collaboration with DMSC. These models developed for McStas versions 2.7.2 and 3.2 are stored on the DMSC gitlab repository.

Detectors

Because of the complex 3D geometry of the detectors of the ESS diffractometers, we rely on a combination of McStas + GEANT4 to get simulated data:

McStas is used up to the sample and the output file of this simulation is then used as input in GEANT4 [2] to deal with the detection of events by the 3D ^{10}B detectors. This work is done in collaboration with Irina Stefanescu. Figure 3 displays some of the DREAM detectors as simulated in GEANT4.

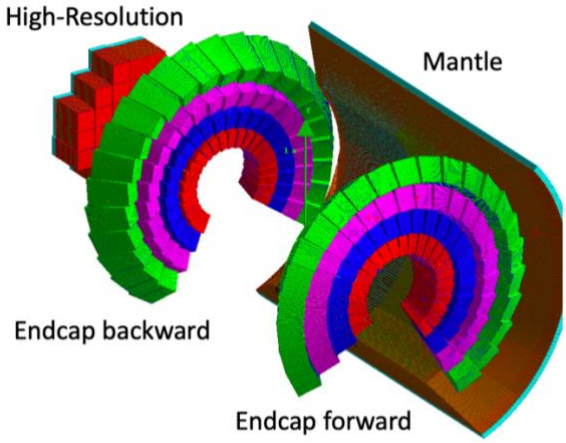

Figure 3: DREAM detectors in GEANT4. Note that the SANS detector has not been modelled in GEANT4 yet.

In parallel, a McStas model of DREAM has been implemented with a simplified 2D layout of the detectors (see Figure 4). This development enables to only rely on McStas to run simulations for testing / benchmarking.

Note: In order to share knowledge, I. Stefanescu also trained one of the DREAM ISs and the IDS on how to run McStas+GEANT4 simulations.

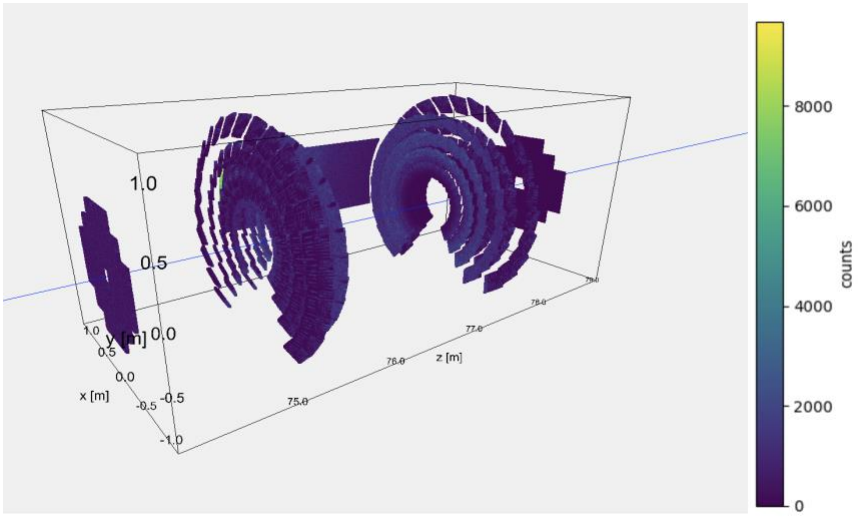

Figure 4: Instrument view in Scipp of the 2D implementation of DREAM detectors (simulation in High Flux configuration)

4 Reduction with Scipp

Contributors: IDS, IS, Detector group, DRAM

4.1 Documentation

The ISs, IDS and I. Stefanescu are working on a Data reduction document for DREAM, which will be available in CHESS after reviews. Its scope is to give a short theoretical background and to summarize the data reduction workflow for the scattering techniques covered by DREAM.

4.2 Software

Note: The NeXus file for DREAM mentioned in section NeXus file has not been used to test the reduction algorithms in scipp, except loading since it does not interface with neither McStas (2D detectors) nor GEANT4 (3D detectors).

There are already some algorithms to reduce Powder Diffraction data as described in scipp documentation, for example at https://scipp.github.io/scippneutron/tutorials/powder-diffraction.html. They use a set of POWGEN event NeXus files (Sample and Vanadium) available from Mantid's usage data.

As a temporary solution to develop the reduction workflow we use comma-separated-values-format files as output of GEANT4 simulations. Table 1summarizes the reduction steps currently available for Powder Diffraction and Figure 5 shows an example of data reduction from the raw data displayed in the 3D instrument view to a 2D contour plot for a subset of the detector as function of different physical units.

Loading	Event NeXus file, tabular data
Unit transformation	ToF ⇔ λ ⇔ d-spacing ⇔ Q & user-defined
Plotting	1D/2D/3D & Instrument view
Selecting	Masking, filtering
Grouping	Binning, histogramming, merging
Correcting	Normalization
Exporting	NeXus, XYE

Table 1: Overview of reduction steps for Diffraction available in Scipp

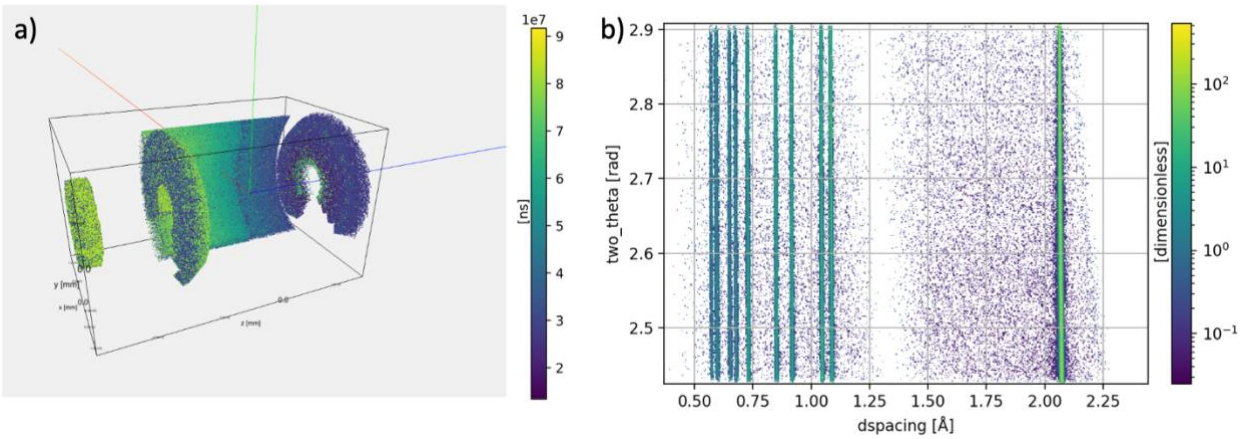

Figure 5: a) DREAM instrument view (the colors correspond to ToF) and b) 2D contourplot of reduced data for the endcap backward detector. The input was a csv file using a Diamond powder sample with the instrument in the High Flux configuration. The reduction steps were i) select endcap backward detectors, ii) convert ToF to d-spacing, iii) add 2θ coordinates, iv) normalize by Vanadium.

DREAM will use the Wavelength Frame Multiplication technique. Some algorithms are already implemented in ess [3]. Preliminary tests with data from V20 (test beamline at HZB) are on-going.
A recent implementation in Scipp enables to output data in a format compatible with EasyDiffraction and GSAS-II. Testing the interface between reduction and analysis and completing the data processing pipeline for Powder Diffraction are to be done shortly.

Other scattering techniques

For other scattering techniques covered by DREAM, we will adapt what has been done for other ESS instruments. For example, for LOKI in the case of SANS.

5 Analysis with EasyDiffraction

Contributors: DRAM, IDS

The latest release of EasyDiffraction supports the analysis of Pair Distribution Function (PDF) data using PDFfit library [4].
The developers' team collaborates with

- the Laboratoire Léon Brillouin and the Institut Laue Langevin on crystallographic libraries used by EasyDiffraction.
- Chalmers University on a joint Chalmers-MAX IV-ESS post doc project about statistical learning applied to diffraction data (neutrons and X-ray) and will make use of EasyDiffraction.

6 Data storage

Contributors: ECDC, IDS, IS

A set of NeXus datafiles from POWGEN has been added to Scicat in order to, in the near future, test its usage during data processing (see Figure 6) to, for example, retrieve raw data to be reduced, access to calibration files, searchable keywords.

Name	Size	Start Time	Type	Science Metadata	Proposal ID	Group
2021B Calibration V rod in PAC HR July13rd	4 GB	2023-02-21 Tue 11:50	raw	confluence_reference_page:[object Object] duration:10700.4189453125 s	276591	276591
2021B Calibration Si HR July13rd	975 MB	2023-02-21 Tue 13:46	raw	confluence_reference_page:[object Object] duration:8919.0625 s	276591	276591
2020B Calibration Empty PAC instrument HR July13rd	672 MB	2023-02-21 Tue 14:07	raw	confluence_reference_page:[object Object] duration:10710.869140625 s	276591	276591
MT PAC06 new at 300K CWL 0.8A	911 MB	2023-02-21 Tue 14:32	raw	confluence_reference_page:[object Object] duration:10683.75390625 s	276591	276591
2021B Long Calibration diamond HR on July13rd	12 GB	2023-02-21 Tue 14:35	raw	associated_empty_can_dataset:[object Object] associated_empty_instrument_dataset:	276591	276591
2021B Long Calibration diamond HR on July13rd after calibration	746 KB	2023-02-21 Tue 17:18	derived	comment:[object Object] experiment_identifier:		276591

Figure 6: Screenshot of Scicat webpage showing the POWGEN dataset (Powder Diffraction data.

7 Project management

Contributor: IDS

A JIRA dashboard listing DMSC tasks for DREAM data pipeline for cold, hot commissioning and First Science has been developed. Figure 7 shows an example of the tasks related to instrument simulation

for cold commissioning. For the next 18 months, 3 milestones have been defined and their progress will be tracked monthly by DMSC:

- *Milestone1:* Post-beamtime data processing workflow ready for 1D Powder diffraction at DREAM

User story: DREAM Instrument scientist and first friendly users should be able to reduce and analyse 1D powder diffraction data from DREAM simulated by McStas/GEANT4, stored in a NeXus file on Scicat. The user should also be able to store reduced data (with relevant metadata) and reduction script on Scicat.

- *Milestone2:* Post-beamtime data processing workflow for Pair Distribution Function at DREAM

User story: DREAM Instrument scientist and first friendly users should be able to reduce and analyse pair distribution function (PDF) data from DREAM simulated by McStas/GEANT4, stored in a NeXus file on Scicat. The user should also be able to store reduced data (with relevant metadata) and reduction script on Scicat

- *Milestone3:* Real-time data processing for 1D Powder diffraction for DREAM

User story: DREAM Instrument scientist and first friendly users should be able to reduce and analyse 1D powder diffraction data from DREAM simulated by McStas / GEANT4 in a real-time setting. The generated raw, reduced data and reduction script should be stored on scicat.

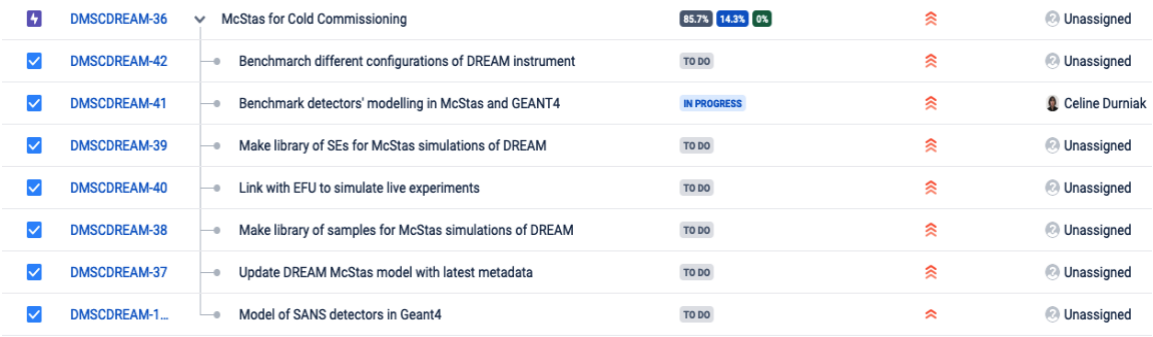

Figure 7: Screenshot of the EPIC and tasks for the development of instrument tools for DREAM cold commissioning

8 Collaborations

Contributors: IDSs / instrument teams / detector group

8.1 Internal collaborations

In addition to the activities mentioned above, there is a collaboration with Søren Schmidt, IDS for imaging and engineering diffraction, on common features for reduction and analysis workflows like WFM or texture analysis as well as with Wojtek Potrzebowski, IDS for SANS.

8.2 External collaborations

8.2.1 ORNL Diffraction Computing Instrument Scientists

Occasional meetings between the IDSs for Imaging and Diffraction and Computer Instrument Scientists (CIS) at ORNL (equivalent to Instrument Data Scientists at ESS) enable to share knowledge about the "IDS/CIS" position, which is new for both facilities and to discuss the development of software. The participants are responsible for the development of software covering a range of scattering techniques, such as Powder Diffraction, Engineering Diffraction, Single Crystal Diffraction, Diffuse scattering, and PDF.
The ICSs also provide test data from POWGEN, NOMAD, SNAPS and VULCAN that could be used in the ESS data processing workflow.

8.2.2 DREAM / POWTEX

The DREAM instrument scientists, I. Stefanescu and IDS started collaborating with the POWTEX team (Andreas Houben, Marina Ganeva, Jens Walter) [4] in January 2022.
The objectives were to:

- share knowledge and to collaborate on the development of software considering the similarities between both instruments (see Figure 8 for POWTEX and Figure 3 for DREAM).
- provide test data for a texture analysis software in development at Aachen university.

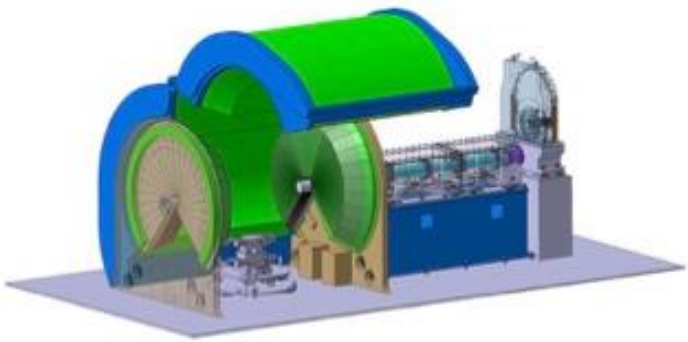

Figure 8: Part of POWTEX instrument, including detectors, choppers. Image from https://www.fzj.de/jcns/jcns-2/EN/Leistungen/NeutronScattering/Diffractometers/_node.html

These meetings are on a standstill but will resume once the "texture analysis" software can be demonstrated.

9 Status for MAGIC

MAGIC, polarised single-crystal diffractometer, is among the first eight instruments. The layout of detectors is less complicated than for DREAM. There is no MAGIC-specific development in progress at the moment. Below are listed some specific points as well as future plans related to this instrument.

Instrument simulation
The implementation of the model the detectors in GEANT4 is in progress (done by ESS detector group) and the updated McStas model will be provided by MAGIC Instrument Scientist.

Data reduction
All implementations in Scipp for DREAM can be applied to the MAGIC data workflow (i.e., loading files, unit conversions, plotting…).

The specific requirements for reduction have been discussed between the IDS and the instrument team. Their implementations will start shortly.

Project management: The IDS has also drafted commissioning plans for data reduction software for MAGIC. But a JIRA dashboard similar to the one for DREAM is being developed.

10 Other projects

10.1 Beamtimes

- DESY P03: scientific beamtime with Mikhail Feygenson (DREAM instrument scientist) and Caroline Curfs (ESS sample environment) to study magnetic nanoparticles (March-April 2023)
- ILL commissioning of D10+ and XtremeD (April 2023)

10.2 QENS

The IDS is an associated partner for the ErUM-data project *EvalSpek-ML: Entwicklung und Evaluierung von Machine-Learning-Algorithmen für die Analyse konvexkombinierter spektraler Daten (Development and evaluation of machine learning algorithms for the analysis of convex-combined spectral data)*, which started in March 2023 and is planning to use the QENS library (initially funded by SINE 2020 Workpackage10).

10.3 Research project

Collaboration with Defence Science and Technology Group, Edinburgh Australia on magnetostrictive thin films.

11 Communications

11.1 Internal communications

VISA and Scicat have been presented to the DREAM instrument team. Python training sessions have also started at the beginning of this year in order to learn the basics of Python and how to use Jupyter notebooks.
Monthly and quarterly meetings are scheduled with the DREAM and MAGIC instrument teams, respectively to update on the latest developments at DMSC.

11.2 External communications

Conferences

- Journées de la Diffusion Neutronique 2022: posters *(data processing at ESS and magnetic thin films)*
- ECNS 2023: poster *(QENS library)* and talk *(Instrument simulation and reduction for Powder Diffraction data at ESS)*

Paper

- Paper on QENS library to be submitted to EPJ Web of Conferences

12 Bibliography

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