



# DREAM data processing

Simulation, data reduction, analysis, curation:  
one-year plan

Diffraction STAP Autumn 2024

Céline Durniak

Instrument Data scientist for diffraction

# DREAM data processing

## Current status – What's available



### Instrument simulation

- GEANT4 models of all detectors (full-scope configuration)
- McStas model in High Flux and High Resolution configurations

### NeXus and ancillary files

- added simulated detector data
- stored on Scicat
- draft of calibration and reduced file format (hdf5)

### Reduction

Powder Diffraction data reduction workflows in Scipp online documentation (using Sciline)

### Analysis

Test with EasyDiffraction (Jupyter notebooks) and GSAS-II (GUI and Jupyter notebooks) for Powder Diffraction

### User interface

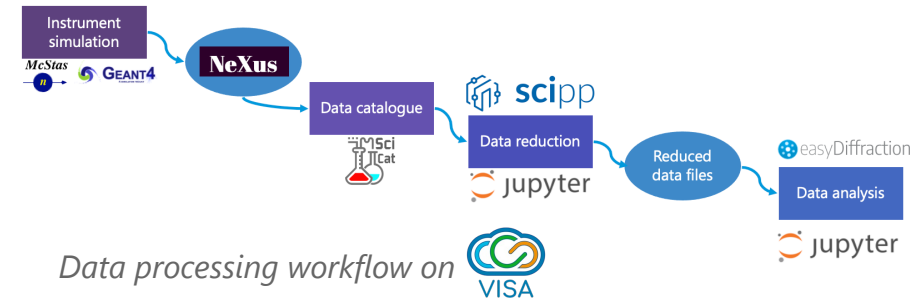
Test of workflow on VISA: proposal → analysed data

### Instrument control

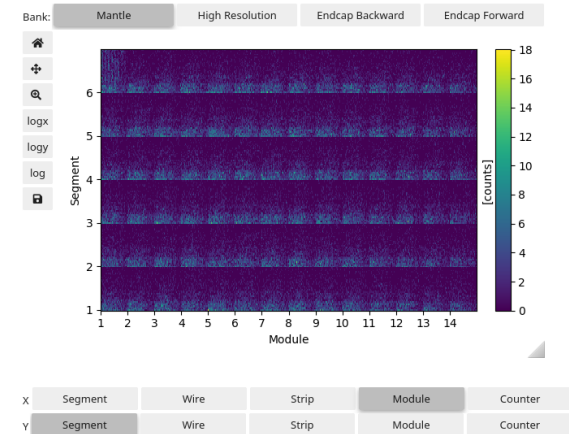
- Draft of plots of DREAM detectors
- Continuous Data (CODA) data pipeline from detectors to NeXus file and Scicat (*random data*)

### Data catalogue

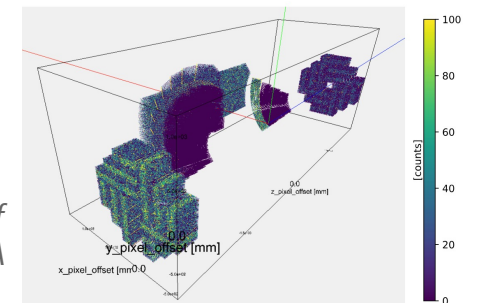
Definition of searchable metadata



Data processing workflow on VISA



2D DREAM detector view:  
selection of bank  
and 2 of its sub-  
elements as x, y axes



3D instrument view in Scipp of  
NeXus file generated by CODA  
pipeline

# DREAM data processing



One-year plan: commissioning, preparation for First Science and User program

## Instrument simulation

- fix bug in High Resolution configuration
- optimize chopper settings for High-Flux and intermediate configurations
- simulations for **Single Crystal Diffraction** and **PDF**

## Instrument control

plots related to NICOS: detectors' display in "more user-friendly units"

## Raw NeXus event files

finalize ESS DREAM NeXus files:  
*add monitor data and other metadata*

## Reduction

- **powder Diffraction:** WFM
- finalize format of calibration and reduced files (hdf5 → cif, ascii)
- **PDF** data reduction
- data reduction for **polarized data** (Annika)
- start work on **Single Crystal Diffraction** data reduction

## Analysis

- analysis of DREAM data with EasyDiffraction (GUI and Jupyter notebooks)
- analysis with other standard diffraction software (GSAS-II, FullProf...)
- **EasyDiffraction**  
general features (constraints, excluded regions, multiple datasets)  
user experience (performance, documentation)  
support **ToF single crystal diffraction**

## Miscellaneous

- Python and Scipp **training** for instrument teams
- **demo** of Powder Diffraction data processing pipeline in VISA to instrument teams
- **documentation:** tutorials (document, Jupyter notebooks) / videos for data reduction and analysis (simple cases)

## Interfaces for data processing pipeline

**real time** data reduction: Event Formation Unit using simulated data

## Archiving

finalize list of searchable metadata



# DREAM data processing

## Focus on analysis with other software

- 1D profile saved as xye file
  - can be loaded in **FullProf**, **GSAS-II**, **EasyDiffraction**
  - TO DO: Check compatibility in **Jana2020** and **TOPAS**
  
- Instrument file
  - Skeleton done for **GSAS-II** and **EasyDiffraction** (CIF)
  - TO DO for **FullProf**, **Jana2020** and **TOPAS**



# Questions

## From IDS to STAP

- format of reduced files: XYE, CIF, hdf5\*
- data analysis software to provide reduced files for:  
GSAS-II, FullProf, Jana, MAUD, Topas, ...

*\* Note that scripts will be available to convert hdf5 to other formats. Hdf5 format is convenient to store data and metadata in a single entity*