

# Instrument Data Scientist for Diffraction

**DREAM and MAGIC** 

# Agenda



- 1 Updates from Lund
- 2 SWOT analysis of Diffraction project
- 3 Plans and schedule
- 4 Status of Diffraction pipelines
- 5 Conclusion

## Diffraction @ ESS

#### News from Lund

### Staff

#### Instrument

#### **DREAM** (Tranche 1)

- *Science cases*: <u>Powder diffraction</u>, Single crystal, PDF, SANS, polarized cold neutrons
- Endcap detectors tested at Utgård and installed at ESS
   MAGIC (among first 8 instruments)
- Science cases: polarised single crystal diffraction
- installation started

### DREAM

#### KEAWI

- Mikhail Feygenson: DREAM instrument scientist
  - → head of Diffraction & Imaging division
- Florence Porcher: Project scientist for DREAM in Lund

#### MAGIC

- No scientific staff in Lund
- Instrument scientist to be recruited



Visit at Utgård



Installation of endcap detectors



MAGIC cave

# Progress for DREAM & MAGIC

### **SWOT** analysis



#### **Successes / achievements**

- good communication with DREAM instrument team through weekly meetings
- instrument simulation for DREAM (McStas/GEANT4)
- simple reduction pipeline for Powder Diffraction for DREAM using Sciline
- JIRA boards for cold, hot commissioning, first science

#### **Failures / setbacks**

- WFM stitching
- no final design for raw NeXus file (mask, storage of instrument geometry)

- DREAM test datafiles collected by ESS detector group (Utgård) → commissioning tools
- beamtime at SXD ISIS
- ErUM data project: (PhD) on IA tools to identify phases in diffraction patterns
- post doc to develop polarisation reduction workflow
- discussions on First Science during Diffraction STAPs

#### **Opportunities / accelerating measures**

- new instrument scientists to be recruited (replacements for Mikhail and Xavier)
- no scientific staff on site for MAGIC
- no ToF support in new version of EasyDiffraction
- align priorities between teams & keep JIRA boards up to date

Threats / risks

### Plans & schedule

### Major milestones or Gantt chart



#### Three medium-term milestones

- 1. Powder diffraction processing pipeline
- 2. PDF processing pipeline
- 3. Real-time powder diffraction processing pipeline

Monthly report (Confluence page)

#### **JIRA boards for DREAM and MAGIC**

- DMSC tasks for cold commissioning, hot commissioning, first science

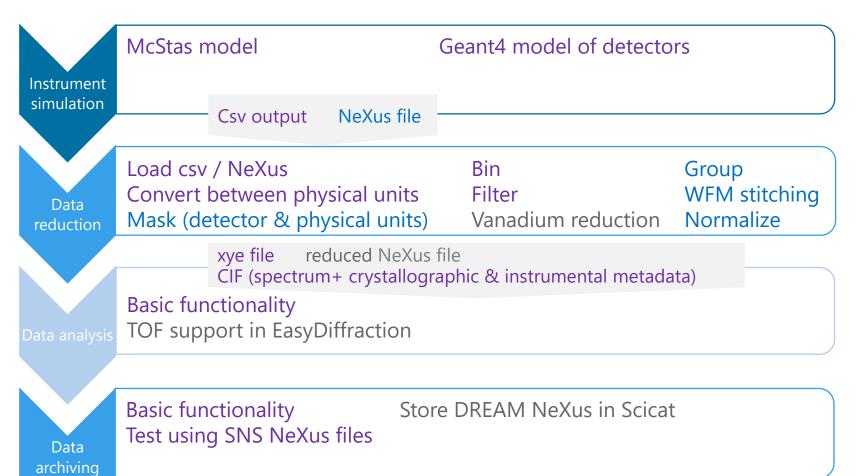


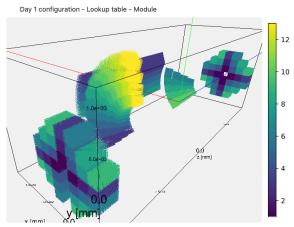
- Discussions about First Science for DREAM during Diffraction STAP (Oct 2023 and April 2024)

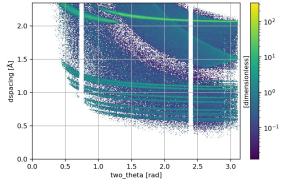
# Data pipeline status

### Powder Diffraction









# Data pipeline status

### PDF



Instrument	McStas model	Geant4 model of detectors
Instrument simulation	Csv output NeXus file	
Data reduction	Load csv / NeXus Convert between physical units Mask (detector & physical units)	Bin, Filter Group FFT WFM stitching "PDF" corrections Normalize
Data analysis	xye file reduced NeXus file CIF (spectrum+ crystallographic & instrumental metadata)  Basic functionality Notebook using DREAM data Notebook using test data and diffpy library	
Data archiving		

Legend: Done In progress To do

# Concluding remarks

### Diffraction @ ESS – IDS point of view



- Some progress in the development of the data processing pipelines
- Uncertainty related to move to DTU
  - no clear definition of IDS role,
  - connection to ECDC and instrument teams
  - daily commute
- High staff turnover → uncertainty in distribution of work and preserving expertise