ISIS Facility Update

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Mantid User Meeting 2025

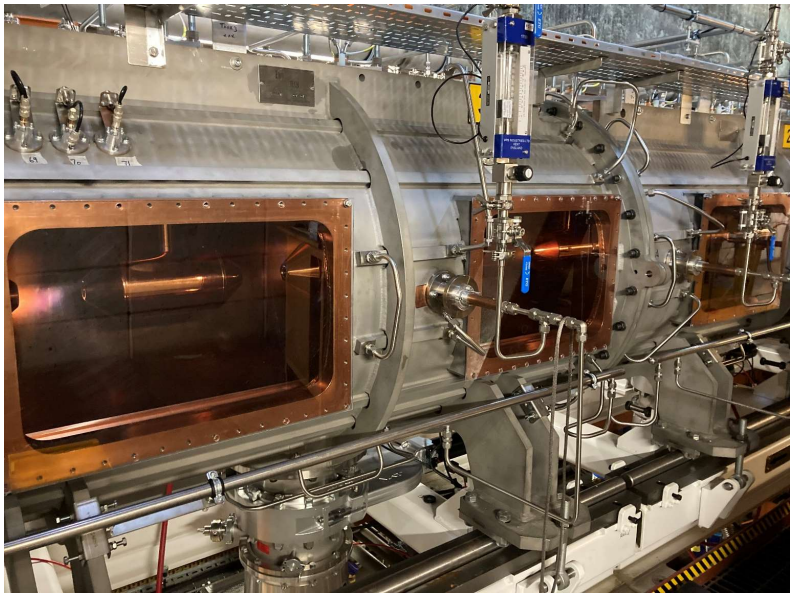
06/11/2025

What have we been up to since 2021?

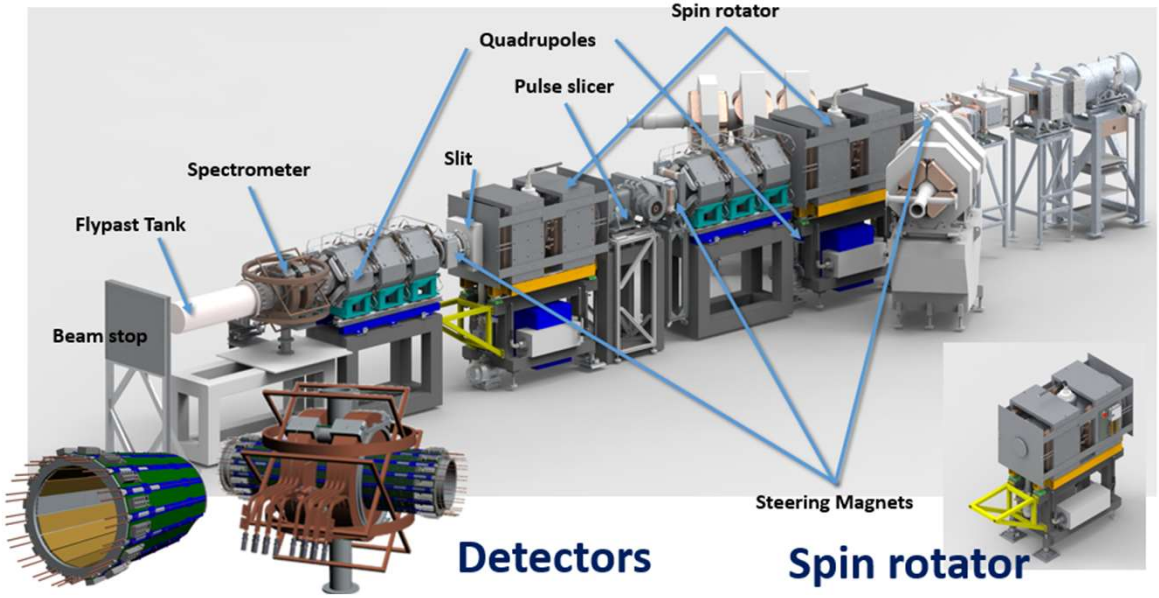
- The 2021/22 long shutdown
- Endeavor Programme
- New director
- Scientific software outside mantid
- Mantid Management
- Lots of new and improved mantid functionality!

The long shutdown

- ISIS is a 40 year old facility now, but parts are rather older.
- The long shutdown addressed two elements, the 40 year old TS1 target and the older linac tank 4.
- Tank 4 was replaced in time for beam to TS2 in April 2022.
- TS1 was back (sort of) in November 2022 but it took until well into 2023 to return to stable running.



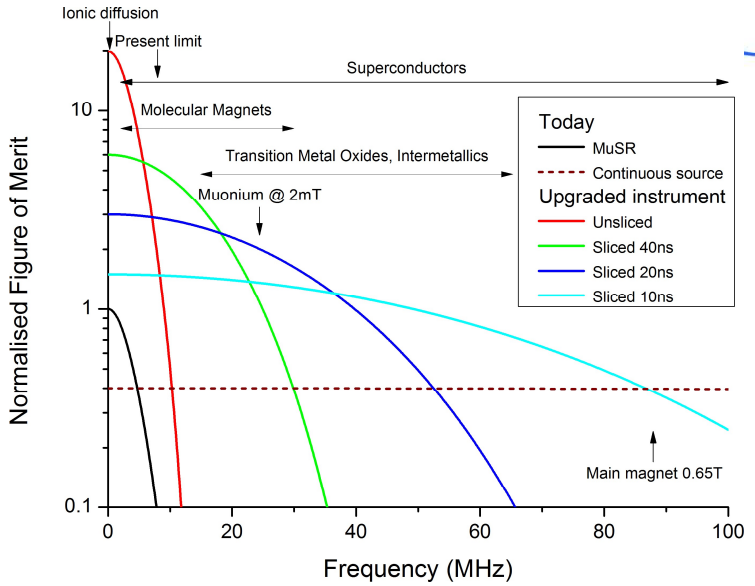
The endeavor programme, Phase 1, in implementation Super-MuSR



Super-MuSR

Order of magnitude gain in resolution and count rate

Target start early 2028



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The endeavor programme, Phase 1, in implementation Super-MuSR

HRPD-X

Significant increase in count rate (between 2.5 and 90 depending on angle).

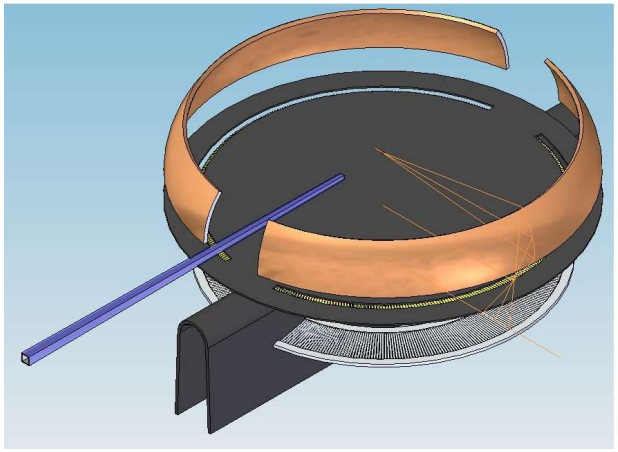
Target scientific commissioning in late 2027

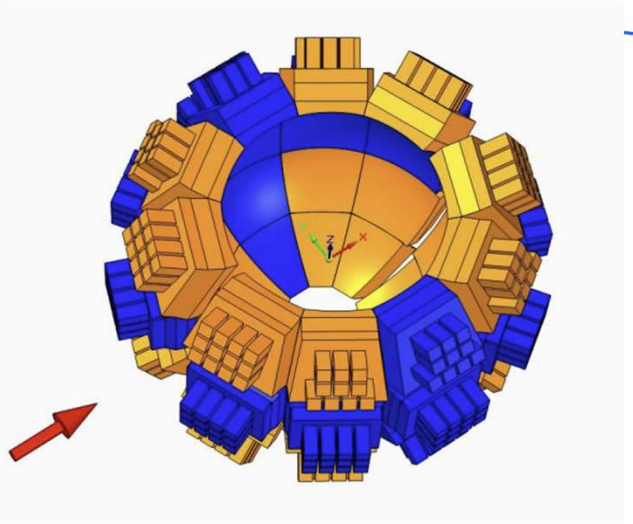
The endeavor programme, Phase 2 detailed design MUSHROOM, WISH-II and Sandals-II

- MUSHROOM is an indirect geometry spectrometer with 50-100x the count rate of LET for small single crystals

- WISH-II is a new single crystal diffractometer and major upgrade for WISH with polarization analysis.

- Sandals-II will increase count rate by a factor 3 and make it simpler to use complex sample environment

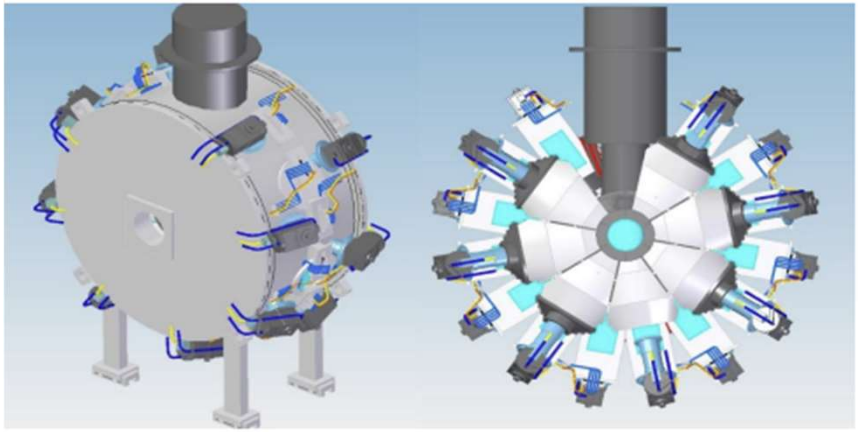




The endeavor programme, Phase 2b OSIRIS+,TOSCA+

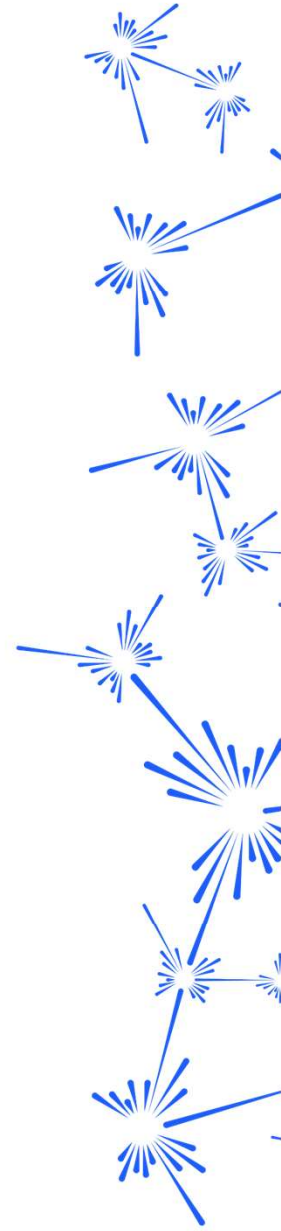
- TOSCA+ will deliver an order of magnitude increase in count rate over the present day instrument. It will also decrease the high energy background and deliver a new sample changer to exploit the count rate gains.

- OSIRIS+ is a guide replacement that is expected to increase flux at sample by around 10. There will be a new slit system allowing us to control the divergence profile at the sample. The OSIRIS Si analyser project is separate to endeavor.



The endeavor programme, Phase 3, being selected

- We aim to finalise the phase 3 instruments in early 2026.
- Likely to be two new build instruments or 1 new build and a number of modest instrument upgrades and refreshes.
- A number of different instruments still being considered.



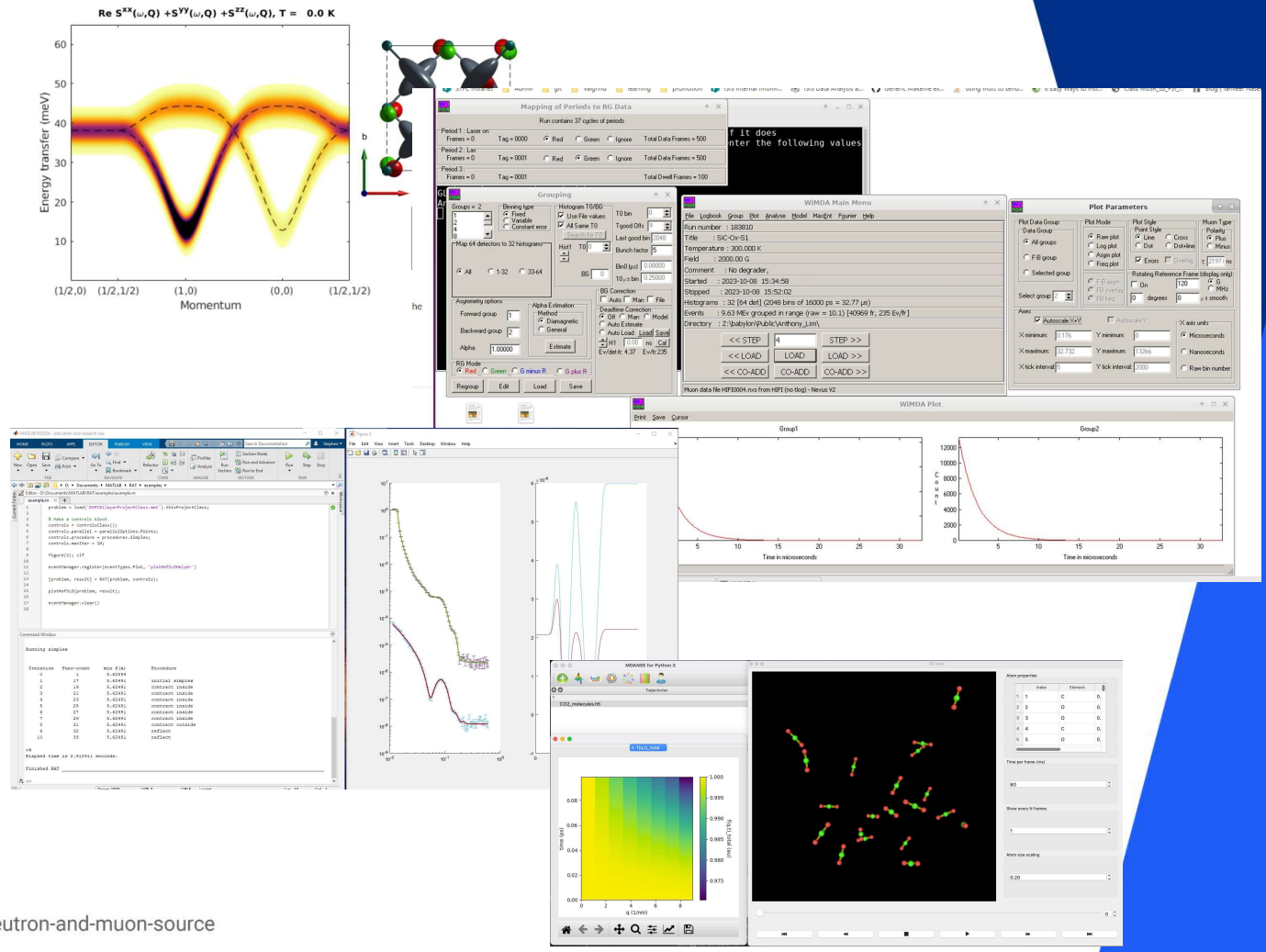
New director

- ISIS apparently changes leaders just before a mantid user meeting.
- We have said farewell to Roger Eccleston who is now head of STFC national Laboratories.
- We welcome Sarah Rogers as our new director. Sarah will be particularly well known to the SANS community and she has recently served as division head for Materials and Engineering at ISIS.

Slide from 2021 user meeting above

Software that takes mantid output as an input

- Sasview
- MDANSE
- MDANSE
- PACE
- RAT
- SpinW



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Mantid updates

Quite a lot to cover

- There have been 12 releases since our last meeting! Not going to cover everything.
- Major item changes to the way scientists and developers interact/prioritise projects.
- Some highlights from the most recent releases

Release Notes

- v6.15.0
- v6.14.0
- v6.13.1
- v6.13.0
- v6.12.0
- v6.11.0
- v6.10.0
- v6.9.1
- v6.9.0
- v6.8.0
- v6.7.0
- v6.6.0
- v6.5.0
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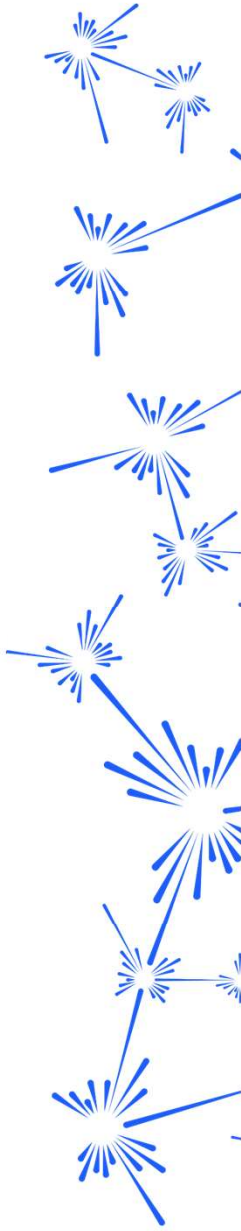
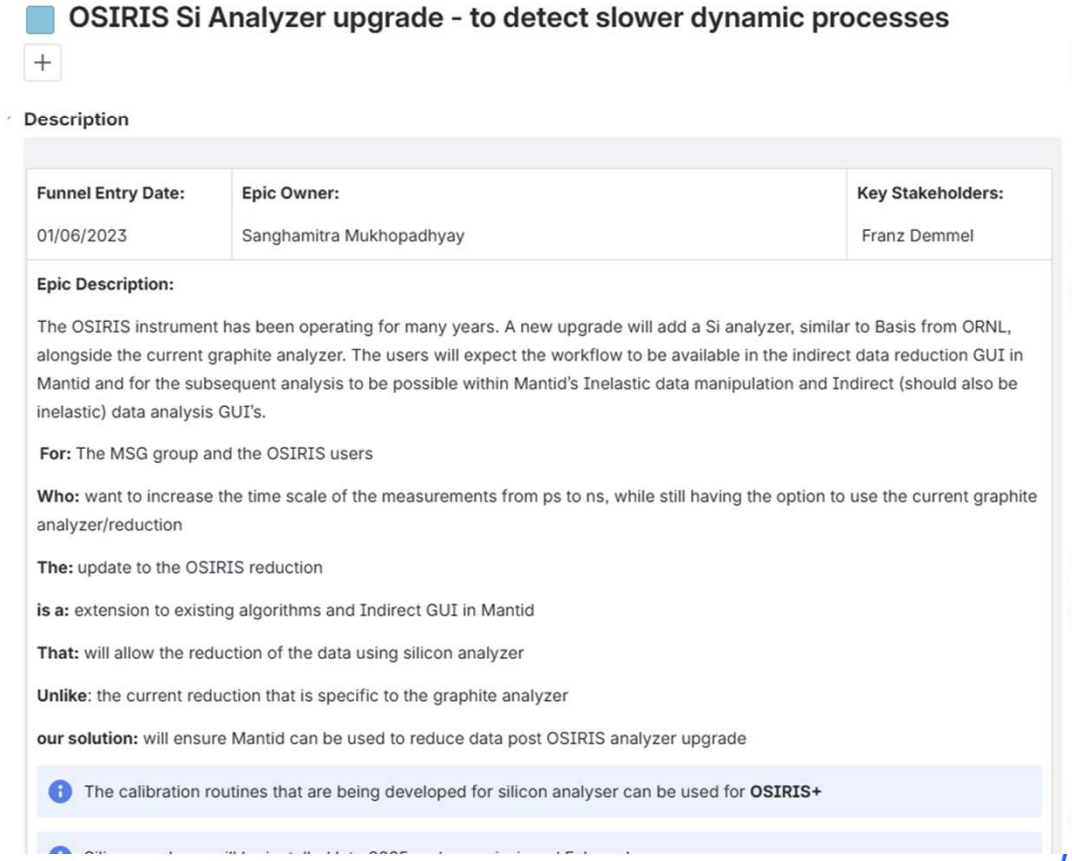


EPICS

- It was felt within ISIS that large items of work in mantid never really got finished.
- On exploring this it turned out there were a number of reasons, some was wrong, some was big projects being snuck in as BAU and some was no clear steer about what was important.
- We now have two workstreams. BAU and EPICS.



OSIRIS Si Analyzer upgrade - to detect slower dynamic processes

Description

Funnel Entry Date:	Epic Owner:	Key Stakeholders:
01/06/2023	Sanghamitra Mukhopadhyay	Franz Demmel

Epic Description:

The OSIRIS instrument has been operating for many years. A new upgrade will add a Si analyzer, similar to Basis from ORNL, alongside the current graphite analyzer. The users will expect the workflow to be available in the indirect data reduction GUI in Mantid and for the subsequent analysis to be possible within Mantid's Inelastic data manipulation and Indirect (should also be inelastic) data analysis GUI's.

For: The MSG group and the OSIRIS users

Who: want to increase the time scale of the measurements from ps to ns, while still having the option to use the current graphite analyzer/reduction

The: update to the OSIRIS reduction

is a: extension to existing algorithms and Indirect GUI in Mantid

That: will allow the reduction of the data using silicon analyzer

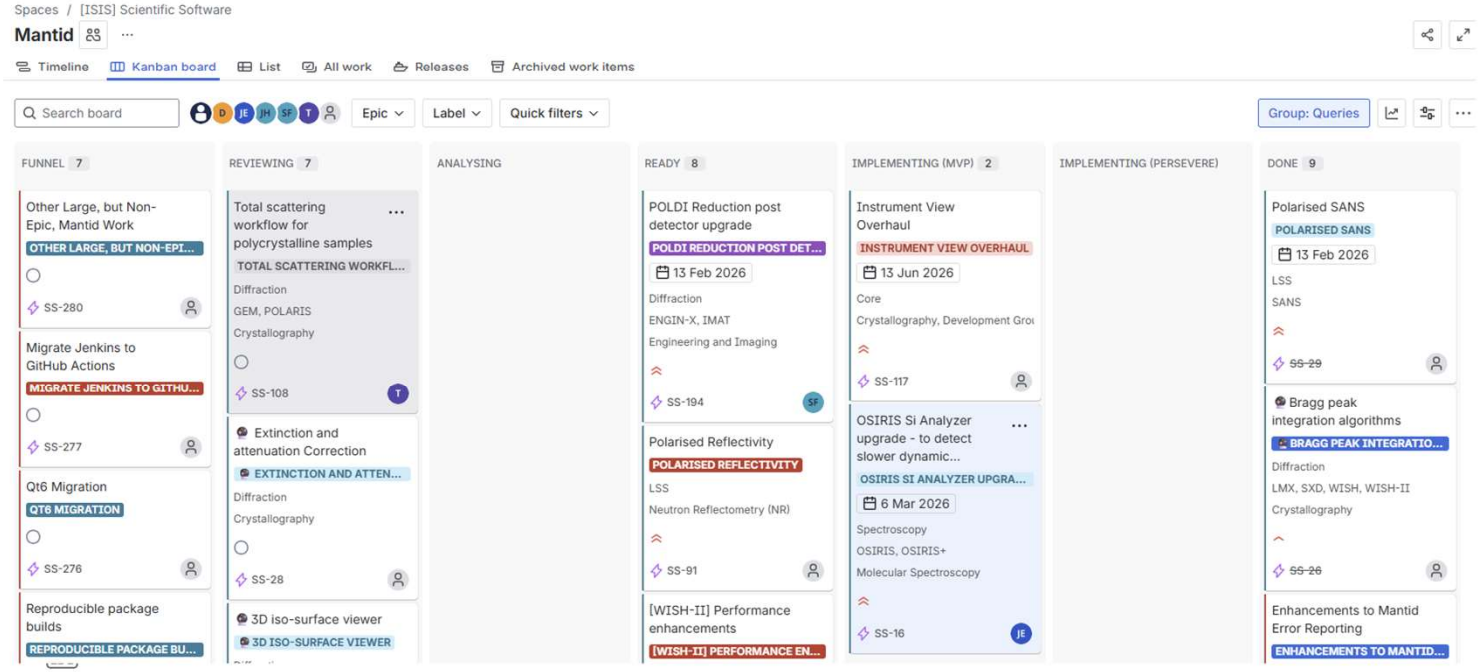
Unlike: the current reduction that is specific to the graphite analyzer

our solution: will ensure Mantid can be used to reduce data post OSIRIS analyzer upgrade

The calibration routines that are being developed for silicon analyser can be used for **OSIRIS+**

EPICS cont.

- An epic should be a substantive item of work requiring >0.1 FTE of effort. <= 0.1 is classed as BAU and is dealt with through direct interaction between developers and scientists.
- Once an epic is identified a short proposal is written with developers and scientists collaborating on it. The aim is for this to be about as burdensome as writing a beamtime proposal.
- These are then prioritized by a board with representatives from each of the science divisions and developers, they are also responsible for feeding back to the proposers.



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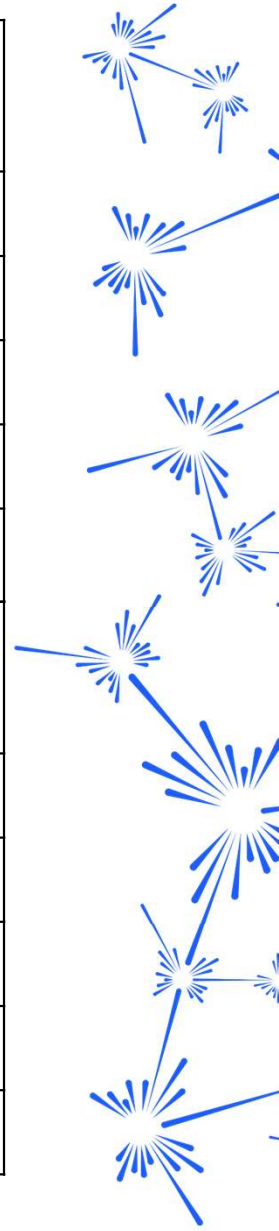
Crystallography

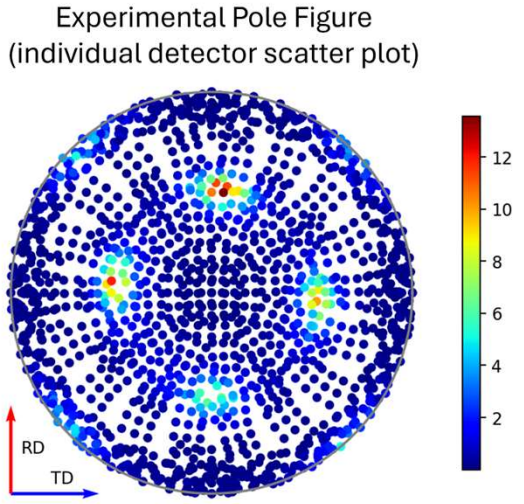
- Improvements to Bragg peak integration
  - Ways to visualize integration quality for existing algorithms,
  - Two new summation methods which work in TOF/detector space rather than Q
  - A new fitting integration approach.
  - Improvements to overlapping peaks to be worked on as BAU.
- Robust Bragg peak searches
  - New algorithms which work as well as those currently deployed on SXD
  - Slightly less total peaks but many less false positives.
  - Some further work required in speedup for endeavor instruments.

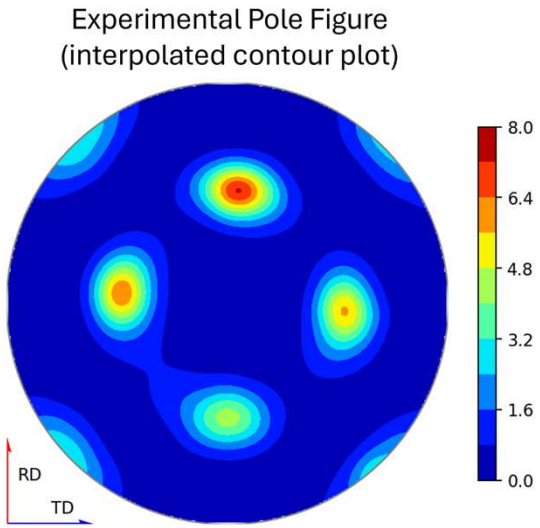
SXD2001	Number Peaks
Total	799
Total - Duplicates	704
Indexed (tol=0.15)	338
I/Sigma > 5	375
Indexed & I/sigma > 5	**274**
FindSXPeaksConvolve	Number Peaks
Total	302
Total - Duplicates	302
Indexed (tol=0.15)	281
I/Sigma > 5	259
Indexed & I/sigma > 5	**251**



Engineering

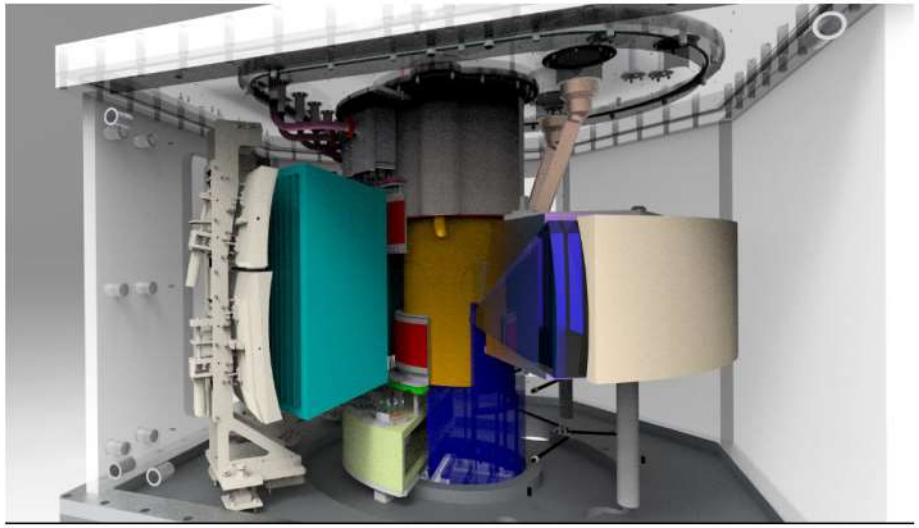
- Ongoing epics in collaboration with PSI engineering for Poldi@PSI and Engin-x@ISIS
- A new range of classes to support Pawley refinements.
- Texture analysis enabling preferential orientations to be extracted.





Spectroscopy

- Mslice is now available via conda as part of mantid workbench.
- Various improvements to vesuvio algorithms to bring them into the current mantid ecosystem
- Currently hard at work on the OSIRIS silicon analyser EPIC.
- Lots and lots of bug fixes and BAU improvements to direct and indirect workflows.

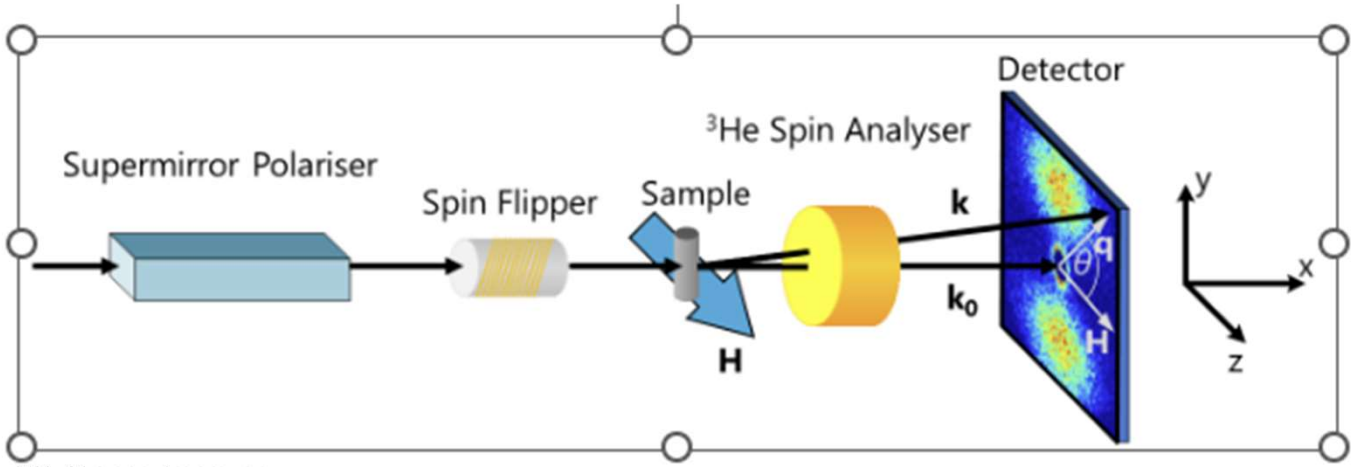


Reflectometry

- New save formats (ORSO)
- Addition of polarization corrections (underway)
- Changes to GUI and save standards to support this.

SANS

- Polarised SANS corrections
  - Calculating efficiency and transmission of beamline components
  - Calculation of and correcting for finite flipping ratio
  - Modification of SANS data files to hold the extra information



Core

- Enhancements to error reports. Should make the vast majority useful.
- Profiling data loading.
- Overhaul of instrument view (ongoing).
- Native ARM Mac OS