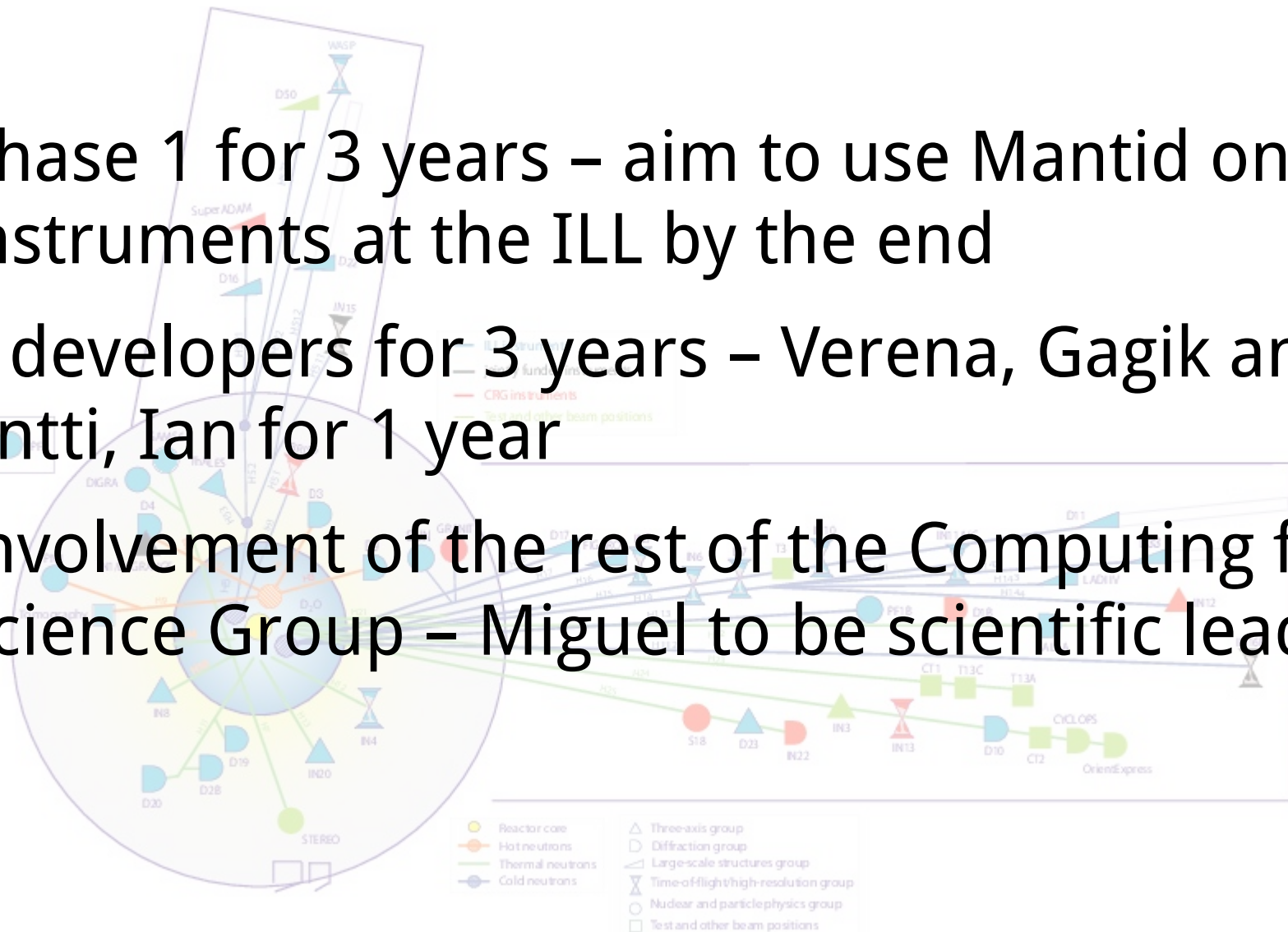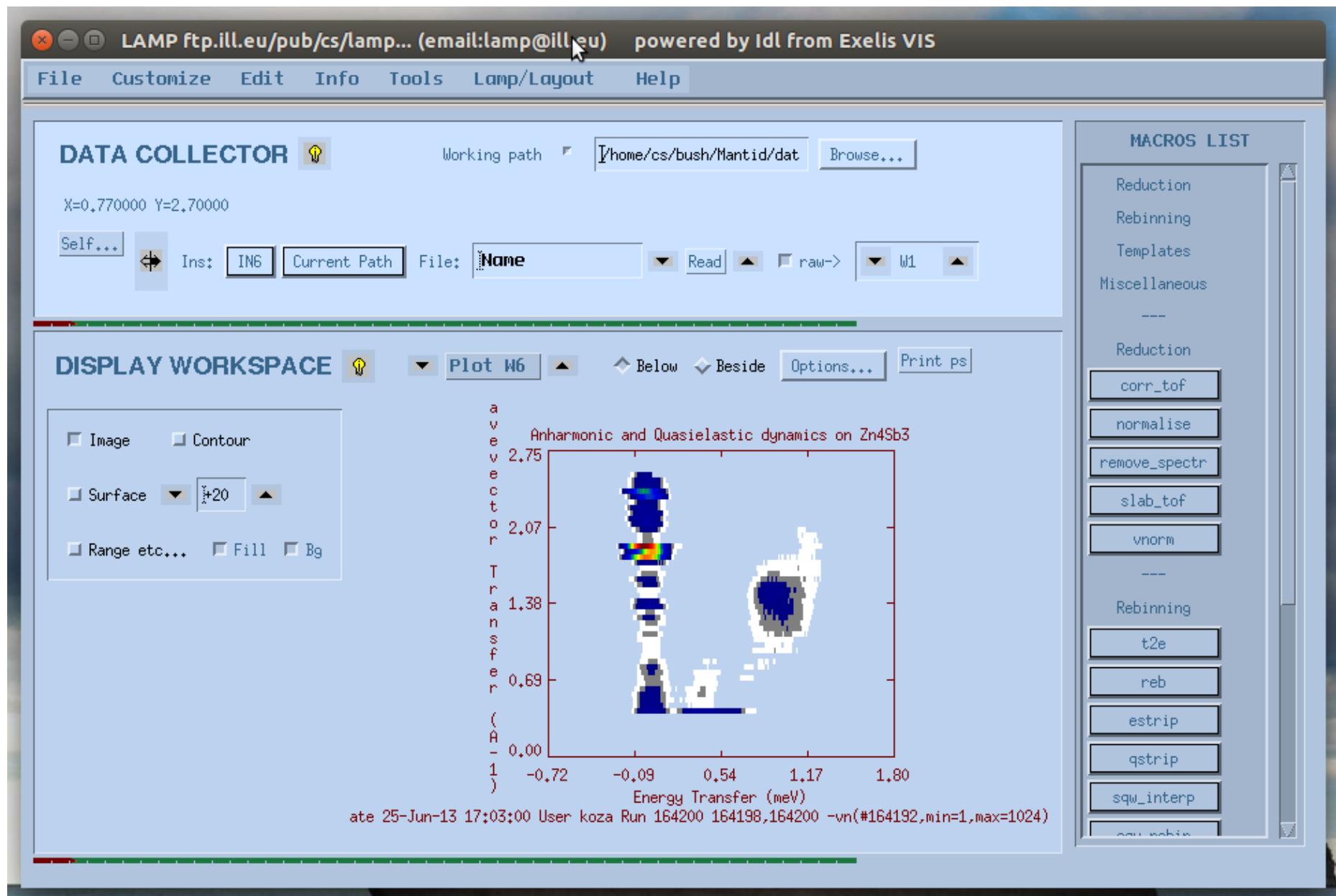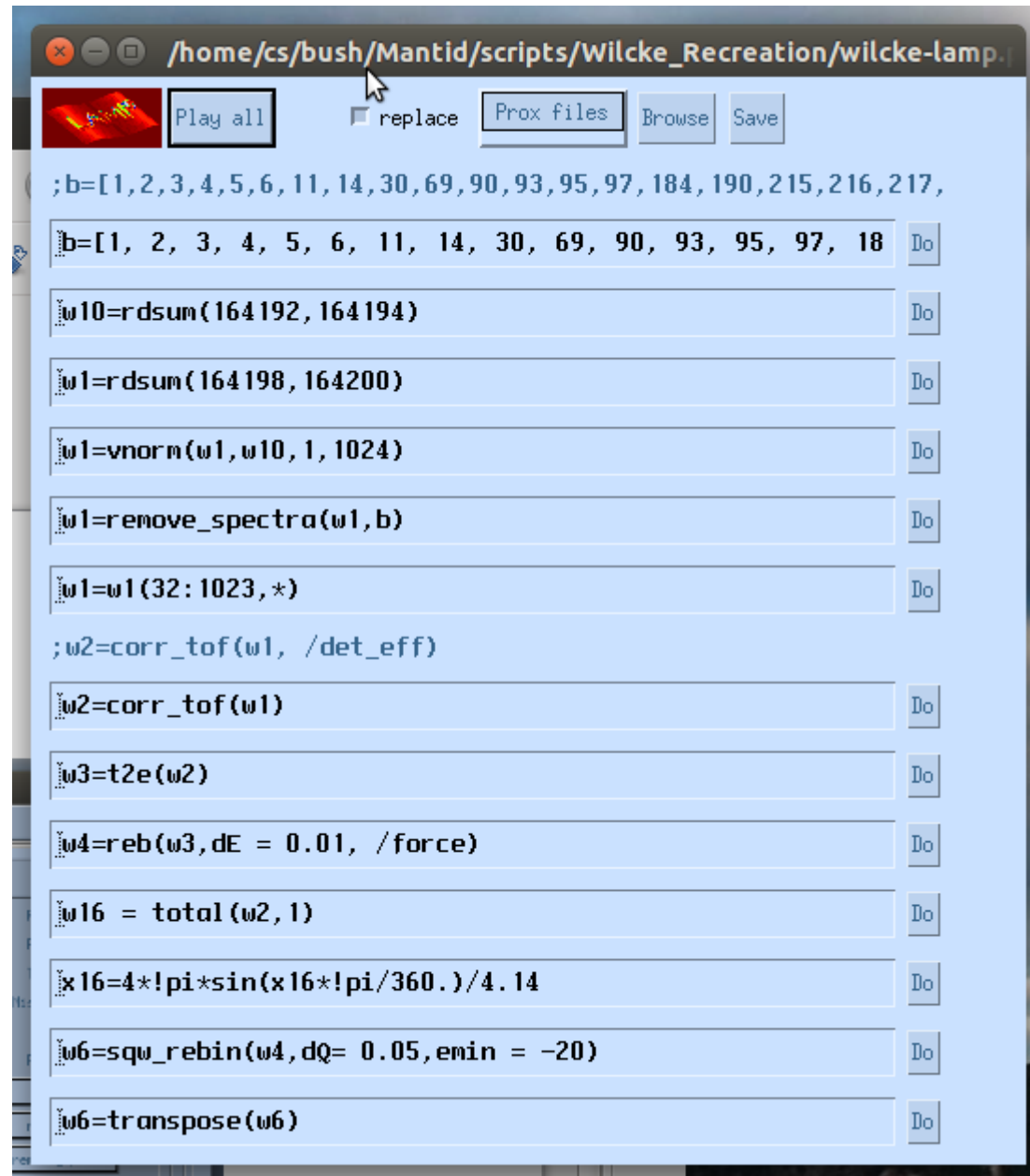# Mantid at the ILL

The Bastille Project

- Phase 1 for 3 years – aim to use Mantid on 20 instruments at the ILL by the end

- 3 developers for 3 years – Verena, Gagik and Antti, Ian for 1 year

- Involvement of the rest of the Computing for Science Group – Miguel to be scientific lead
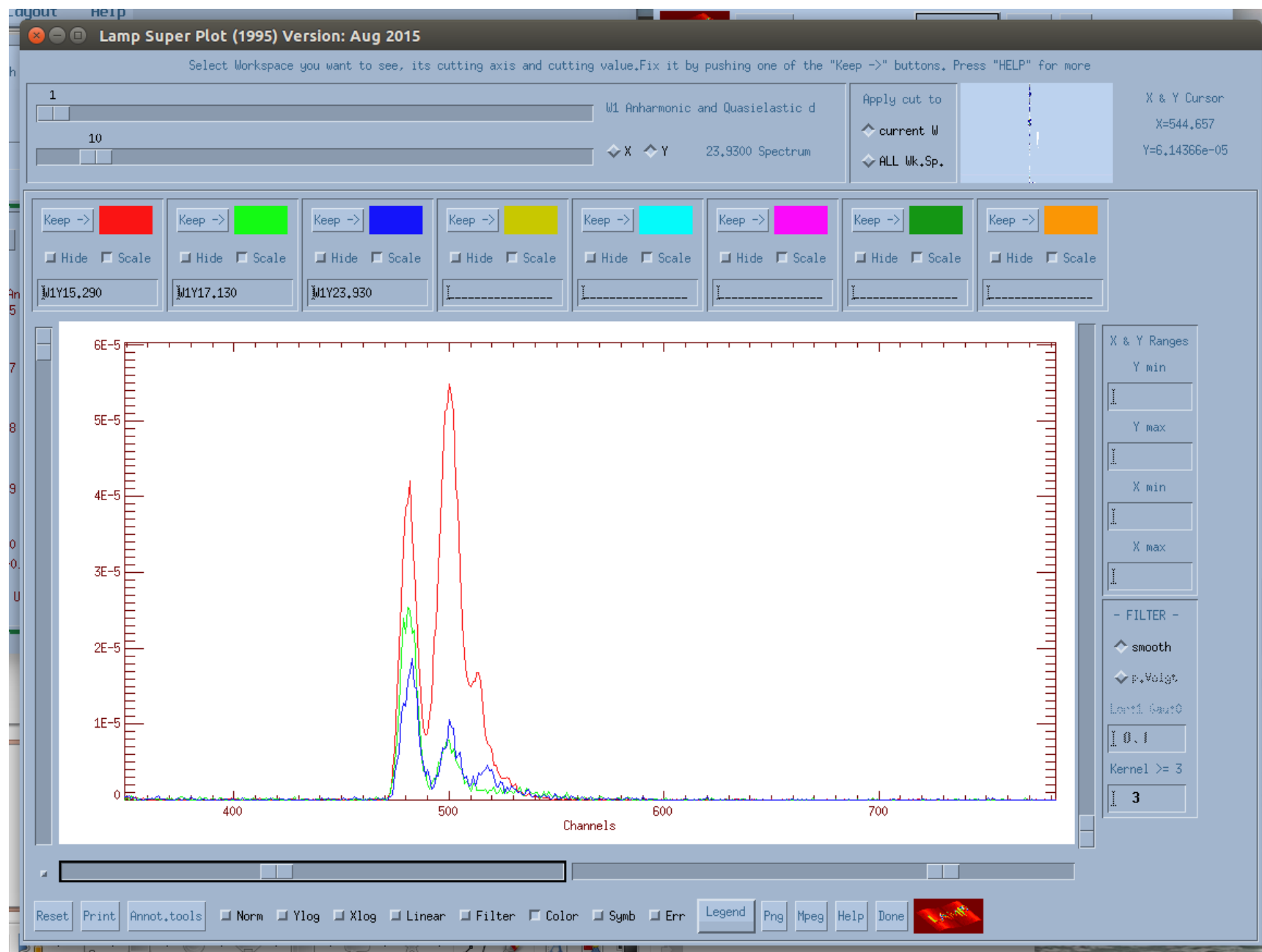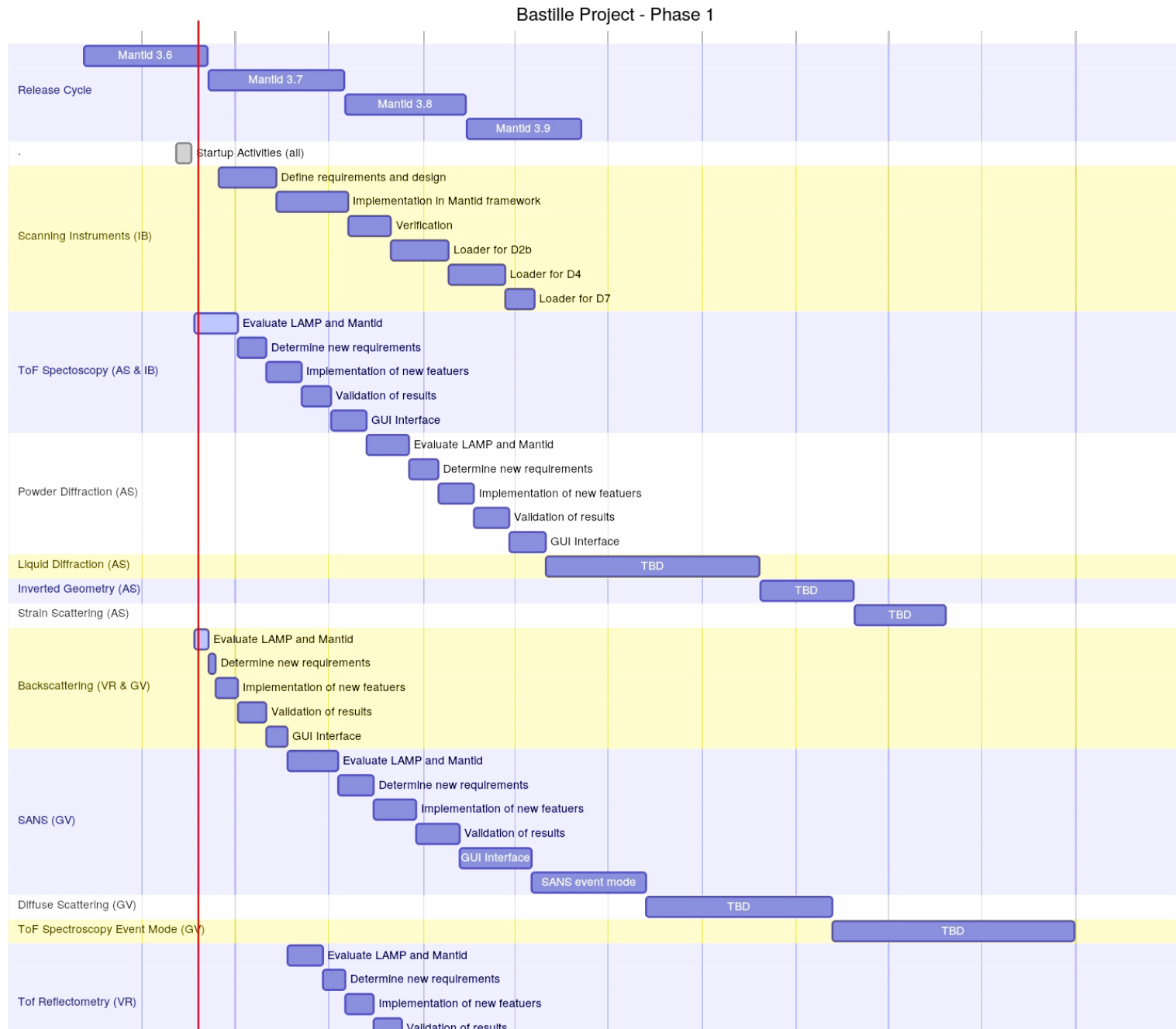
Lamp

Lamp

Lamp

Project Plan

- Antti & Ian – Time of Flight Spectroscopy

- Verena & Gagik – Backscattering Spectroscopy

- From September hope to have ToF and Backscattering in use

- Gagik, Antti and Verena to look at other technique areas

- Ian looking at simple scanning instruments

Bastille Project - Phase 1

Release Cycle
- Mantid 3.6
- Mantid 3.7
- Mantid 3.8
- Mantid 3.9

. Startup Activities (all)

Scanning Instruments (IB)
- Define requirements and design
- Implementation in Mantid framework
- Verification
- Loader for D2b
- Loader for D4
- Loader for D7

ToF Spectoscopy (AS & IB)
- Evaluate LAMP and Mantid
- Determine new requirements
- Implementation of new featuers
- Validation of results
- GUI Interface

Powder Diffraction (AS)
- Evaluate LAMP and Mantid
- Determine new requirements
- Implementation of new featuers
- Validation of results
- GUI Interface

Liquid Diffraction (AS) — TBD

Inverted Geometry (AS) — TBD

Strain Scattering (AS) — TBD

Backscattering (VR & GV)
- Evaluate LAMP and Mantid
- Determine new requirements
- Implementation of new featuers
- Validation of results
- GUI Interface

SANS (GV)
- Evaluate LAMP and Mantid
- Determine new requirements
- Implementation of new featuers
- Validation of results
- GUI Interface
- SANS event mode

Diffuse Scattering (GV) — TBD

ToF Spectroscopy Event Mode (GV) — TBD

Tof Reflectometry (VR)
- Evaluate LAMP and Mantid
- Determine new requirements
- Implementation of new featuers
- Validation of results

Mantid & TOF data reduction at ILL

- Aim: deliver a compelling replacement for LAMP
- Three instruments: IN4, IN5, IN6, BRISP
  - Initial focus on IN4 and IN6
- Some preliminary work already done

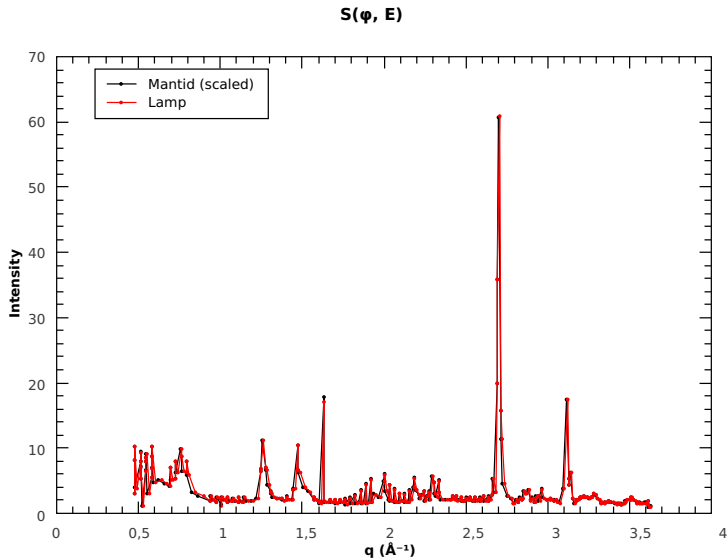# Comparison between Mantid & LAMP

- ▶ Identify & understand differences
- ▶ What is better, good enough, and what could be improved?
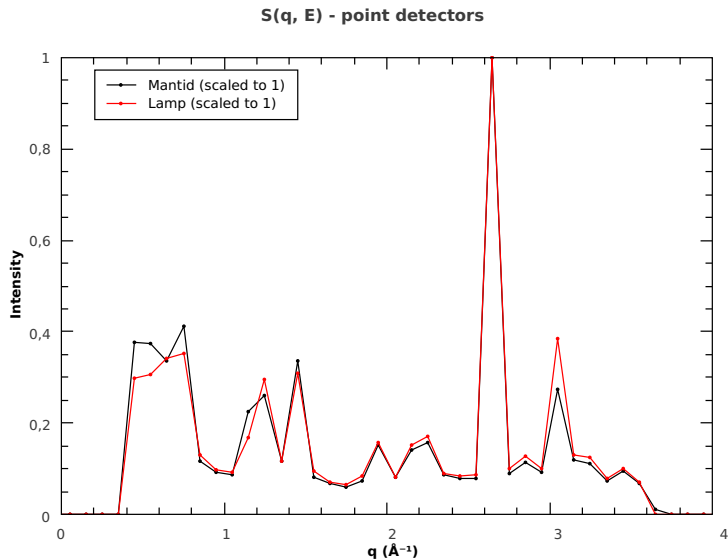
Comparison between Mantid & LAMP

Differences in:

- workflows
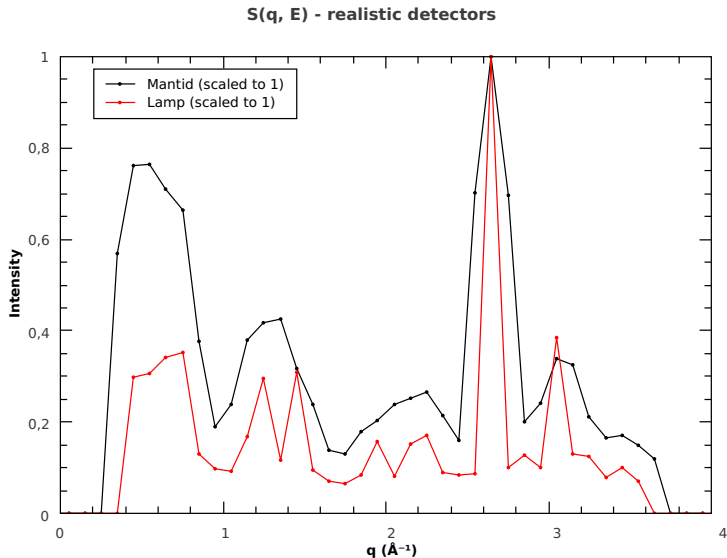- algorithms
- binning
- instrument description
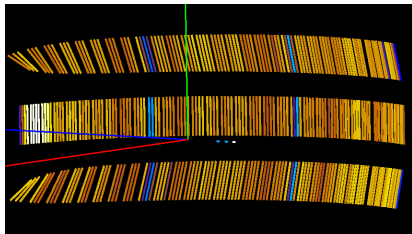- . . .

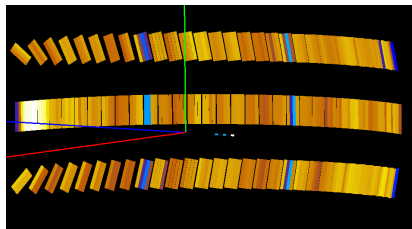# Example: from raw data to $S(\phi, E)$

Example: `SofQWNormalizedPolygon`

S(q, E) - point detectors

Legend:
- Mantid (scaled to 1)
- Lamp (scaled to 1)

Y-axis: Intensity
X-axis: q (Å^{-1})

Example: `SofQWNormalizedPolygon`

S(q, E) - realistic detectors

Legend:
- Mantid (scaled to 1)
- Lamp (scaled to 1)

y-axis: **Intensity**
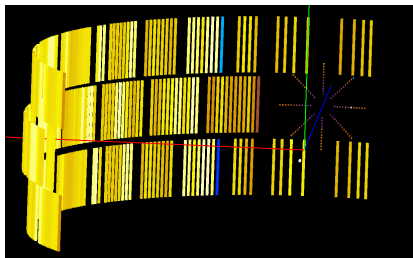
x-axis: **q (Å⁻¹)**

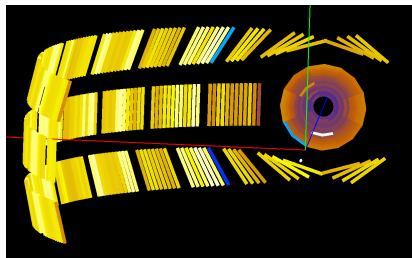# Improving IDFs: IN6

May 2016

current

- IDFs generated by python scripts
- Old instruments — no accurate blueprints available

Improving IDFs: IN4

May 2016

- Needs more work

current

TODO: Data reduction workflow

- ▶ Finalize the workflow with instrument scientists
  https://github.com/mantidproject/documents/
  blob/master/Project-Management/ILL/TOF_and_
  BS/Mantid_workflow_proposal.md
- ▶ Open questions include:
  - ▶ Likely to be based on `DGSReduction` or on upcoming MLZ interface
  - ▶ Which readily available algorithms suit us?
  - ▶ How to deal with heterogeneous detectors?
  - ▶ . . .

Outlook

- Finalize IDFs
- Finalize data reduction workflow
- IN5
  - $\sim 10^5$ detector pixels
- BRISP

IN16B Reduction with Mantid

STATUS REPORT

Gagik Vardanyan and Verena Reimund

12.07.16 Mantid Review Meeting

# IndirectILLReduction

❑ Reduces raw data from IN16B instrument at ILL

❑ Some implementation was already in place (Spencer & Co.)

❑ Refinements needed to fit the new requirements

❑ Started with Quasi-elastic mode (QENS)

❑ Elastic and Inelastic Fixed Window Scans to follow (E/I FWS)

Unmirroring

❑ Raw data has 2 wings (Doppler accelerating and decelerating)
❑ They need to be split AND/OR summed in a smart way

❑ Need to shift peaks

❑ According to vanadium run

❑ Detector wise

❑ Need to provide 8 options
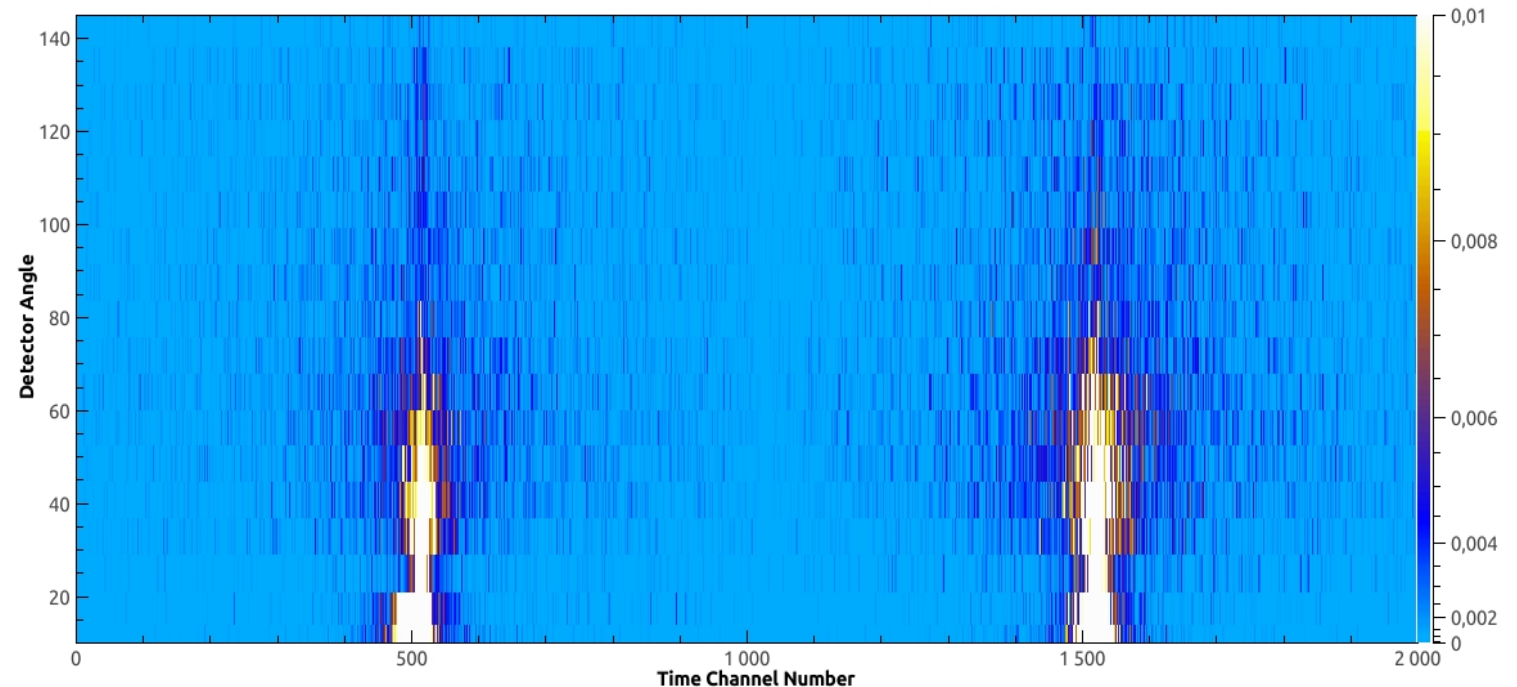
Comparisons with LAMP

❑ Compared workspaces in LAMP and Mantid after each step of reduction workflow for a number of runs

❑ Nearly identical just after loading

❑ Small differences arise later on

❑ Sources are identified

   ❑ E.g. slightly different fitted peak positions in x-axis conversion
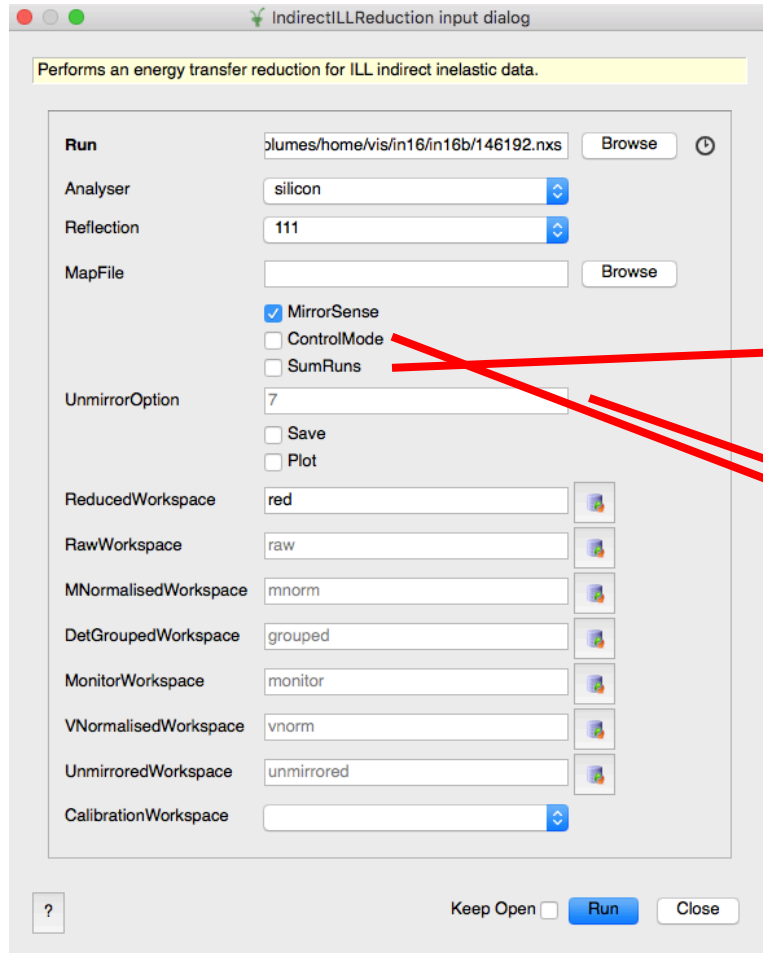
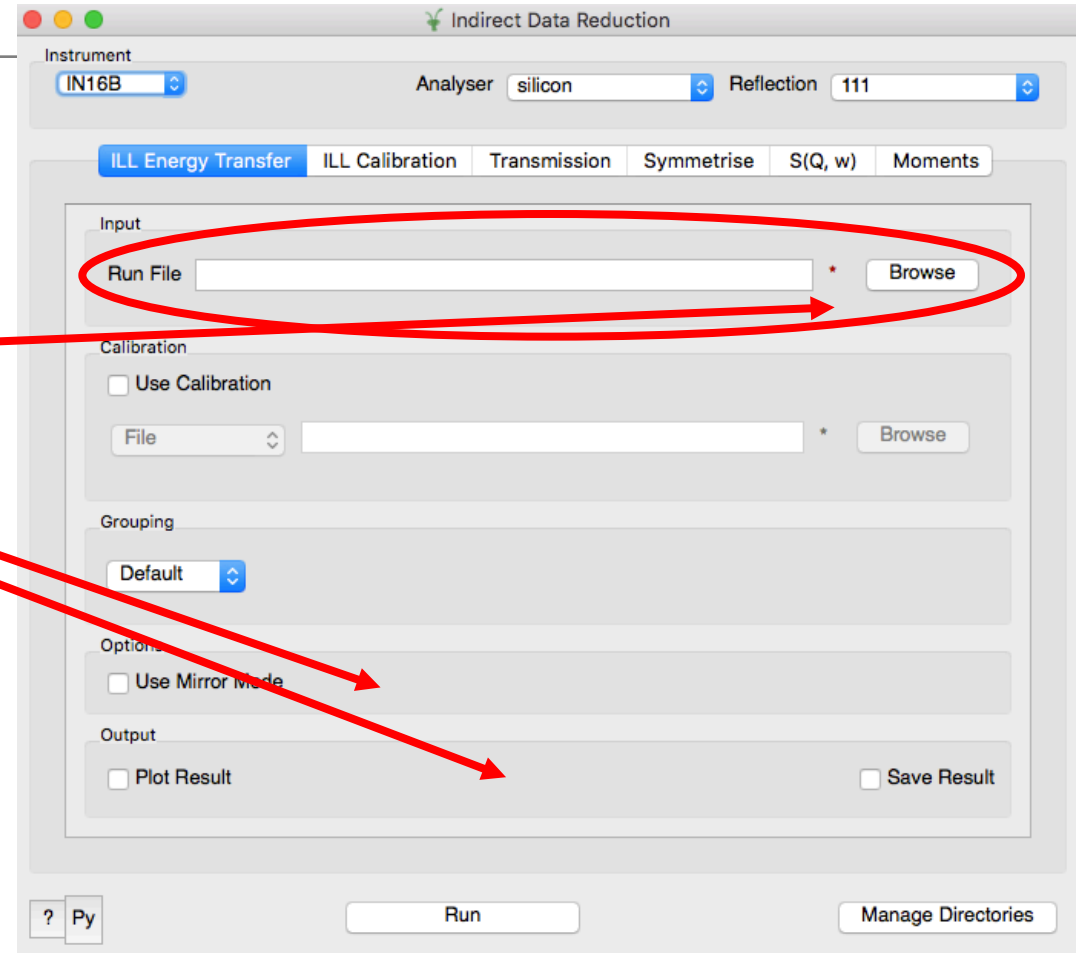❑ The goal is to benchmark Mantid with LAMP
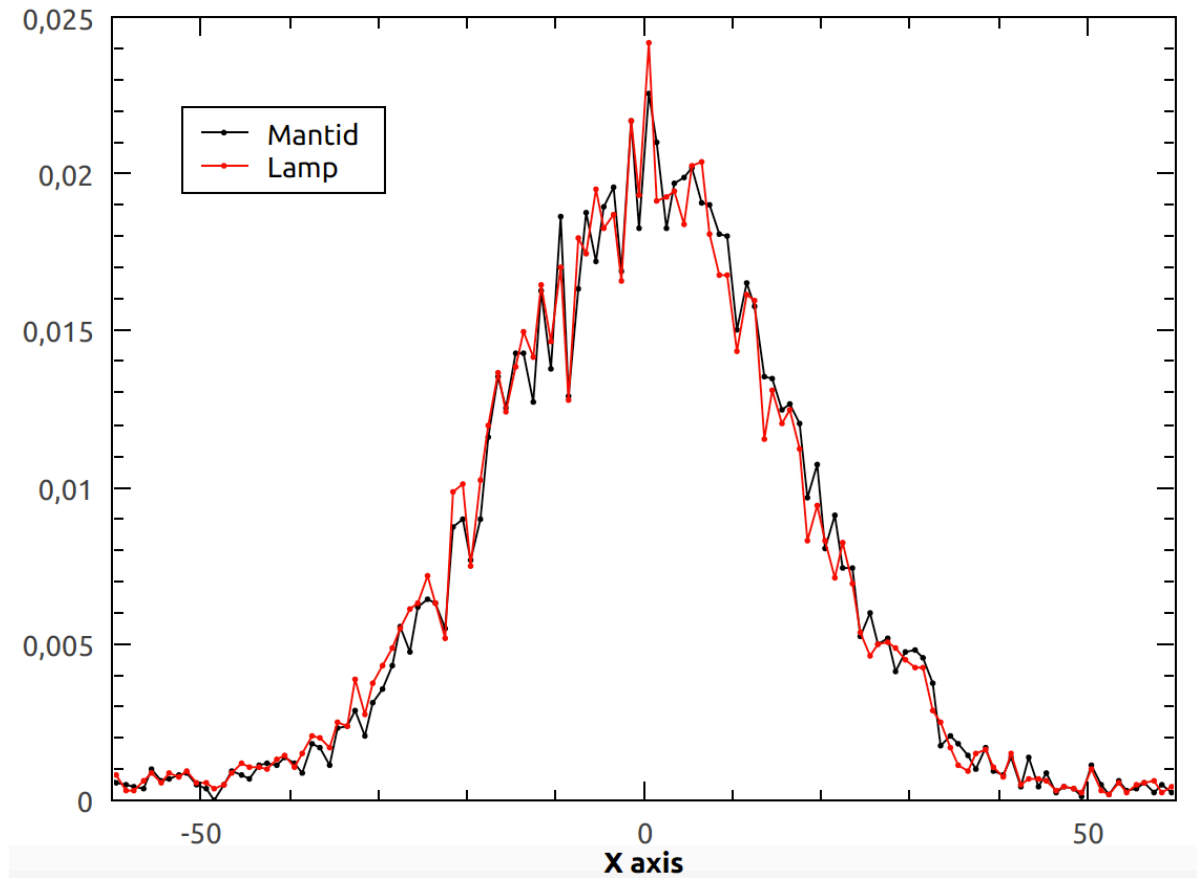
Single Detectors Treatment

127500_silicon_111_left
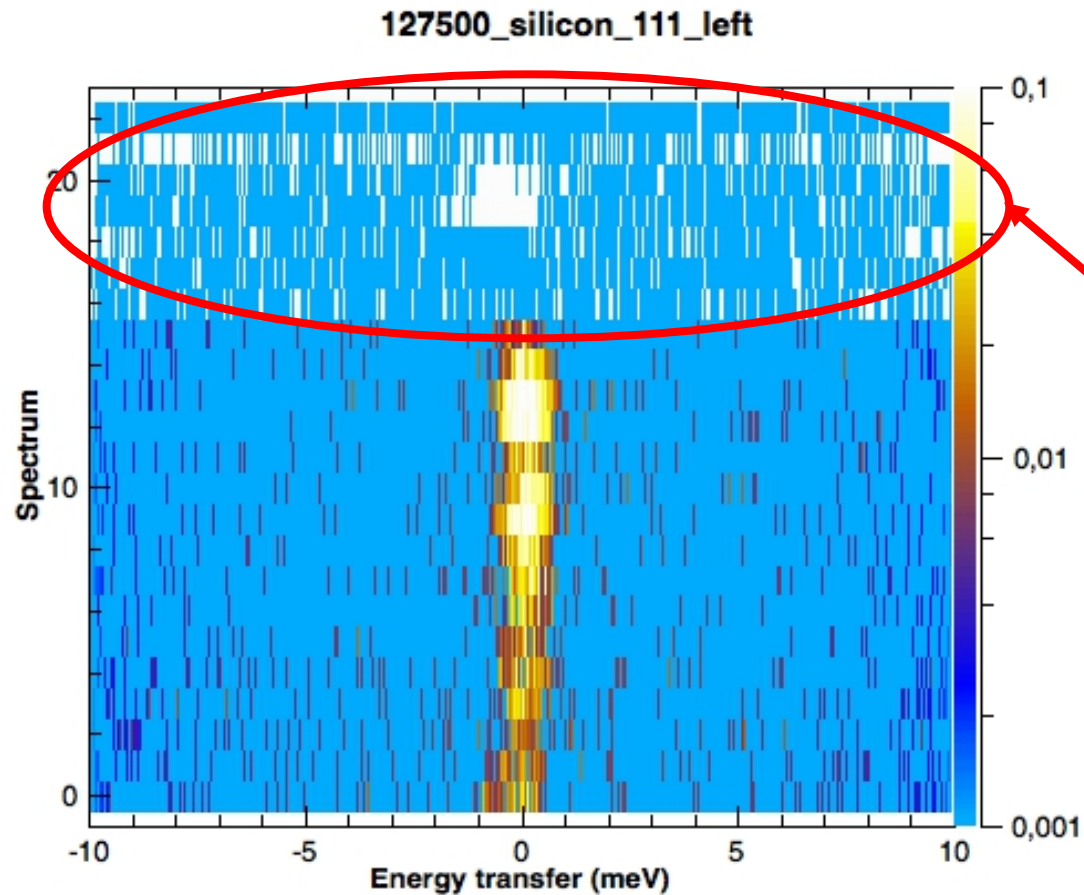
- ❑ There are 8 slots in nexus files
- ❑ But only few are enabled
- ❑ Adjusted the loader

GUI

Auto-generated GUI as is now
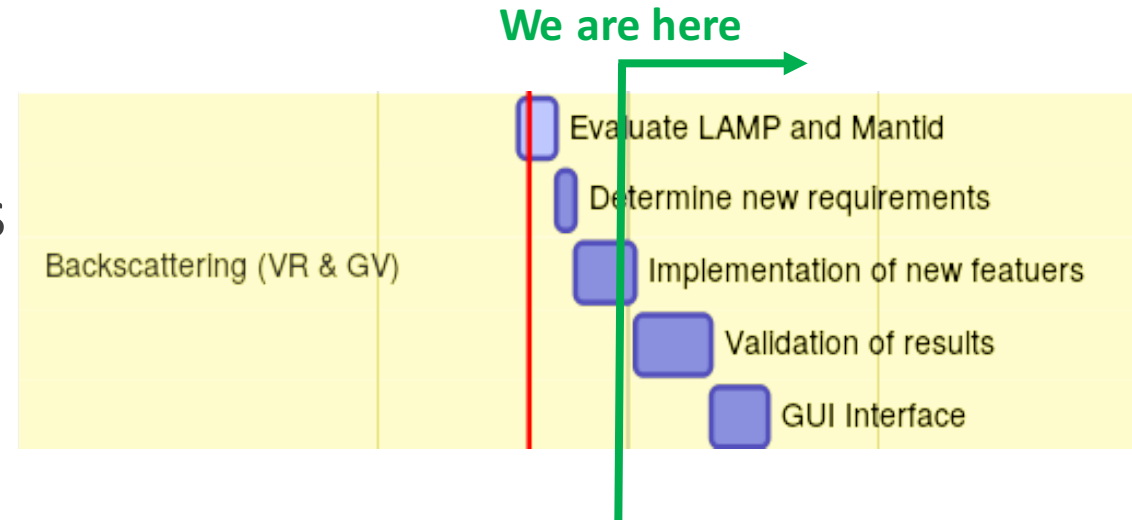
Interfaces -> Indirect Reduction

Issues & PRs so far

#	Description	Status
PR #16620	Renamed entry in nexus file [technical]	Merged
PR #16707	ILL: Load Multiple Files [technical] (there is no prefix)	Merged
Issue #16753	IndirectILLReduction Algorithm Refactoring* - Handle multiple files - Treatment of active single detectors in the LoadILLIndirect - Unmirror options - Control mode	In progress
Issue #16754	IndirectILLReduction GUI* - Allow multiple file selection - Add a checkbox for summing of files - Add a checkbox for Control mode - Add a dropdown for unmirror option	In progress (merge with above?)
	ShiftCircular (needed for unmirroring) - A new generic algorithm to perform circular shift of x-axis of the workspace	TBC
	Generalisation of FindEPP (needed for unmirroring) - Remove unneeded x-axis unit validation, update the category	Green light by the author

*These also partially/fully close some of the issues previously reported by Elliot.

Status and Plans

- ❏ Compared LAMP and Mantid

- ❏ Identified sources of differences

- ❏ Identified new requirements

- ❏ Implementing required functionality, GUI

Screenshot from project gantt-chart

We are here

Backscattering (VR & GV)

Evaluate LAMP and Mantid

Determine new requirements

Implementation of new featuers

Validation of results

GUI Interface

09.16

https://github.com/mantidproject/documents/blob/master/Project-Management/ILL/Gantt_Chart/bastille_gantt_mermaid.md.png