The ILL Joins the Mantid Project

Dr Ian Bush, Dr Gagik Vardanyan, Mrs Verena Reimund,
Dr Antti Soininen, Dr Miguel Gonzàlez

NoBugs – 18th October 2016

MANTID

INSTITUT MAX VON LAUE - PAUL LANGEVIN

NEUTRONS FOR SOCIETY

Talk Overview

- Mantid and Adoption at the ILL
- Working with the Mantid Team
- Lamp and Mantid for Data Reduction
- Workflows
  - Time-of-Flight Spectroscopy
  - Backscattering
- Future Work

The Mantid Project – Neutron Data Reduction

Science & Technology Facilities Council
ISIS

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MANTID

EUROPEAN
SPALLATION
SOURCE

MLZ
Heinz Maier-Leibnitz Zentrum

PAUL SCHERRER INSTITUT
PSI

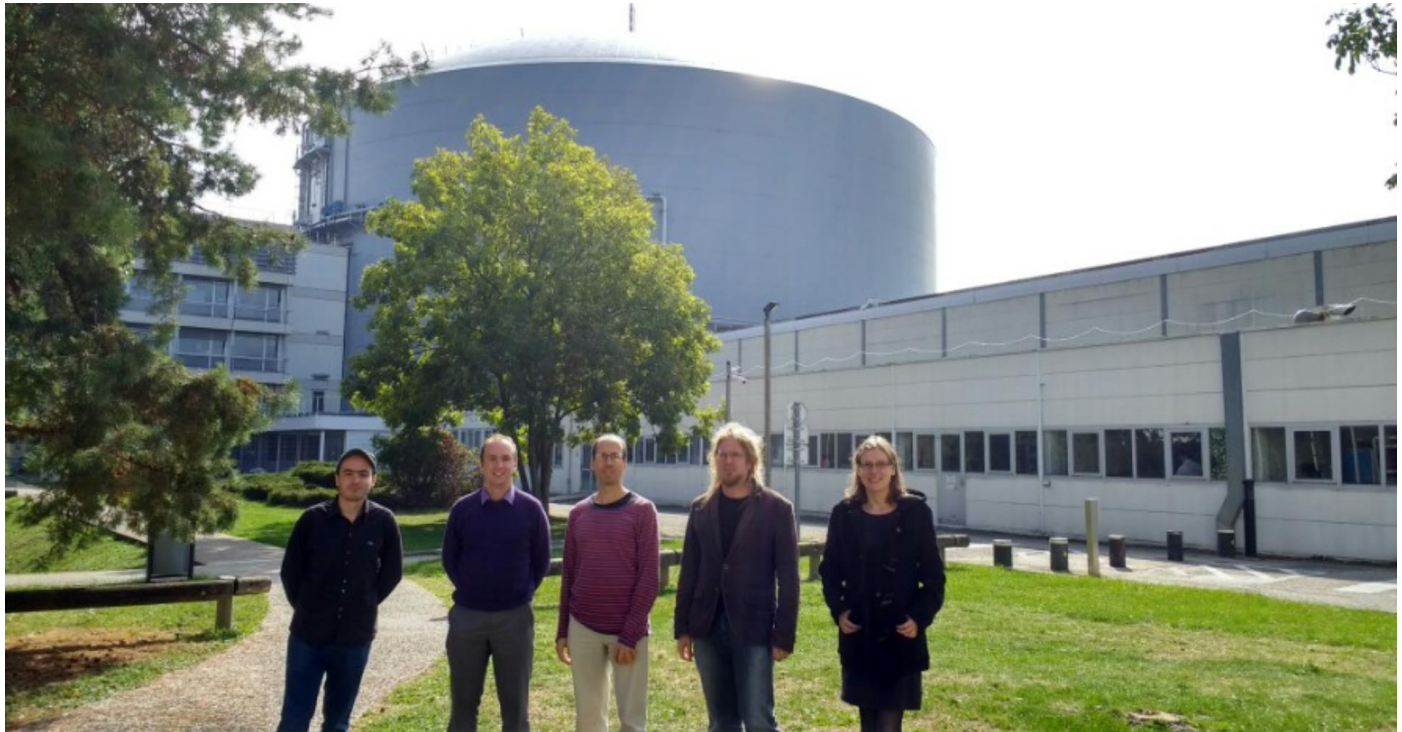
ansto

McStas
n

Tessella

The Bastille Project for Mantid Adoption

- Bastille project, part of ILL's Endurance programme, to support 20 ILL instruments after 3 years, replacing Lamp
- People involved:
  - Antti Soininen, Verena Reimund, Gagik Vardanyan
  - Ian Bush – technical lead for one year – from Tessella
  - Miguel Gonzàlez – scientific lead for the project – from ILL's CS Group



Working with the Mantid Team

GitHub

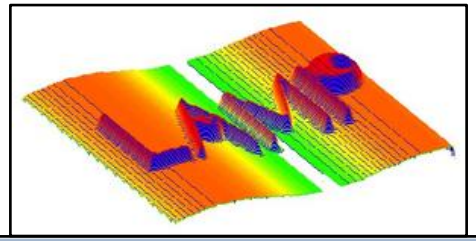
Jenkins

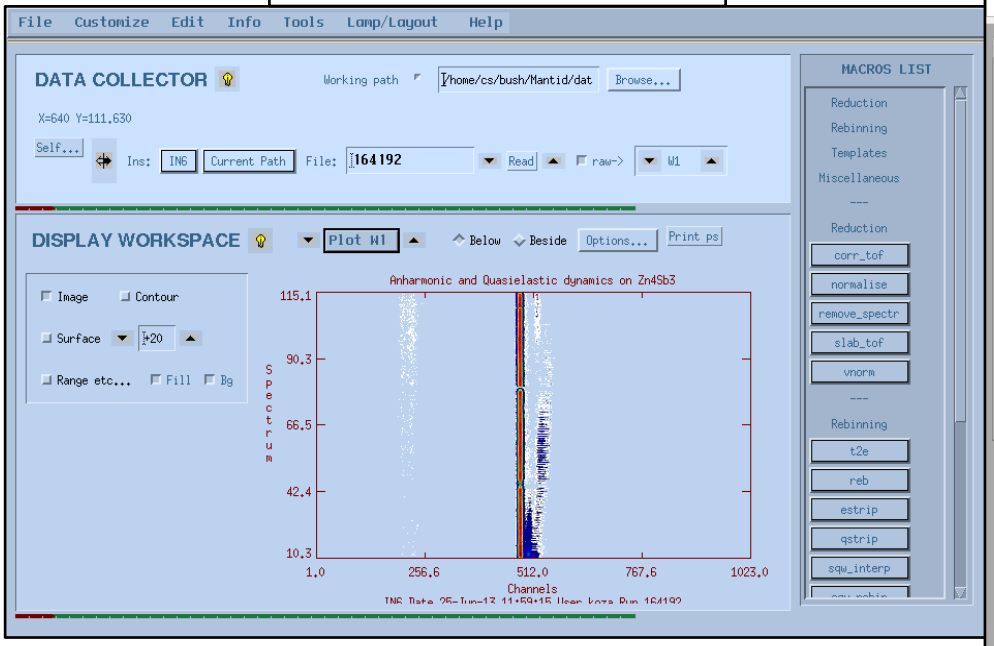
slack

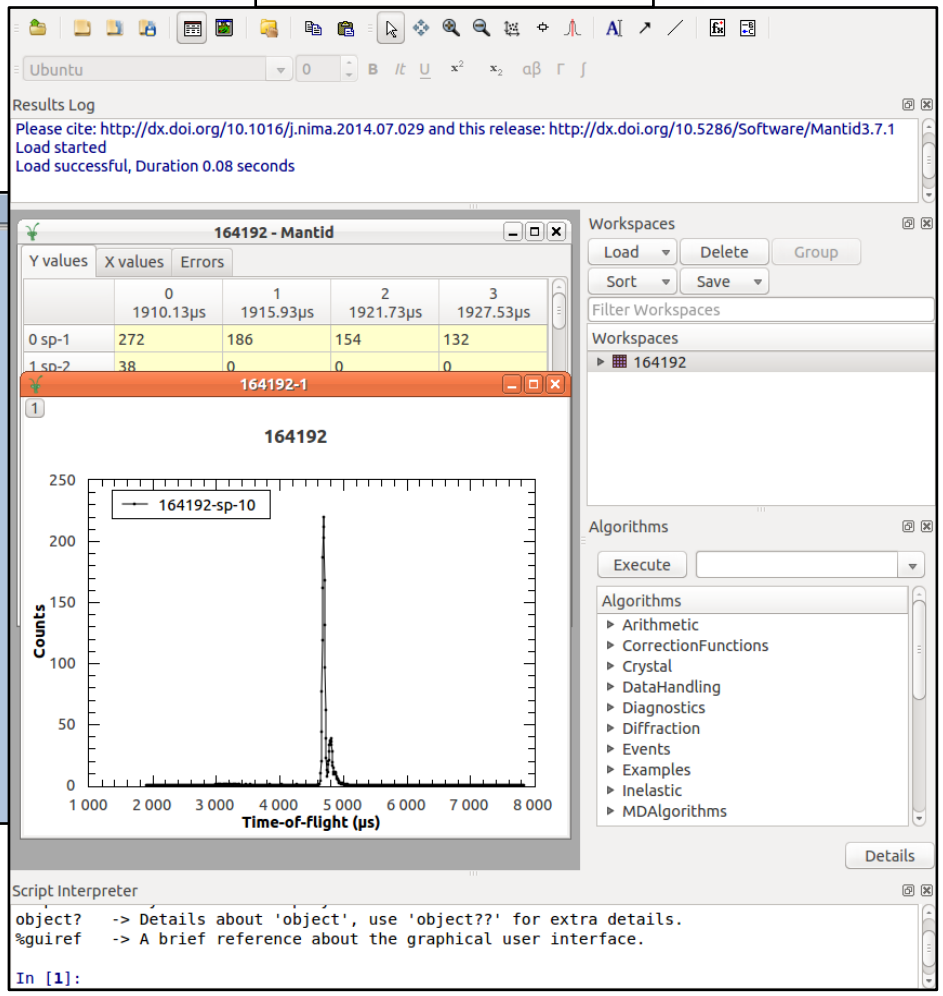
BlueJeans

skype

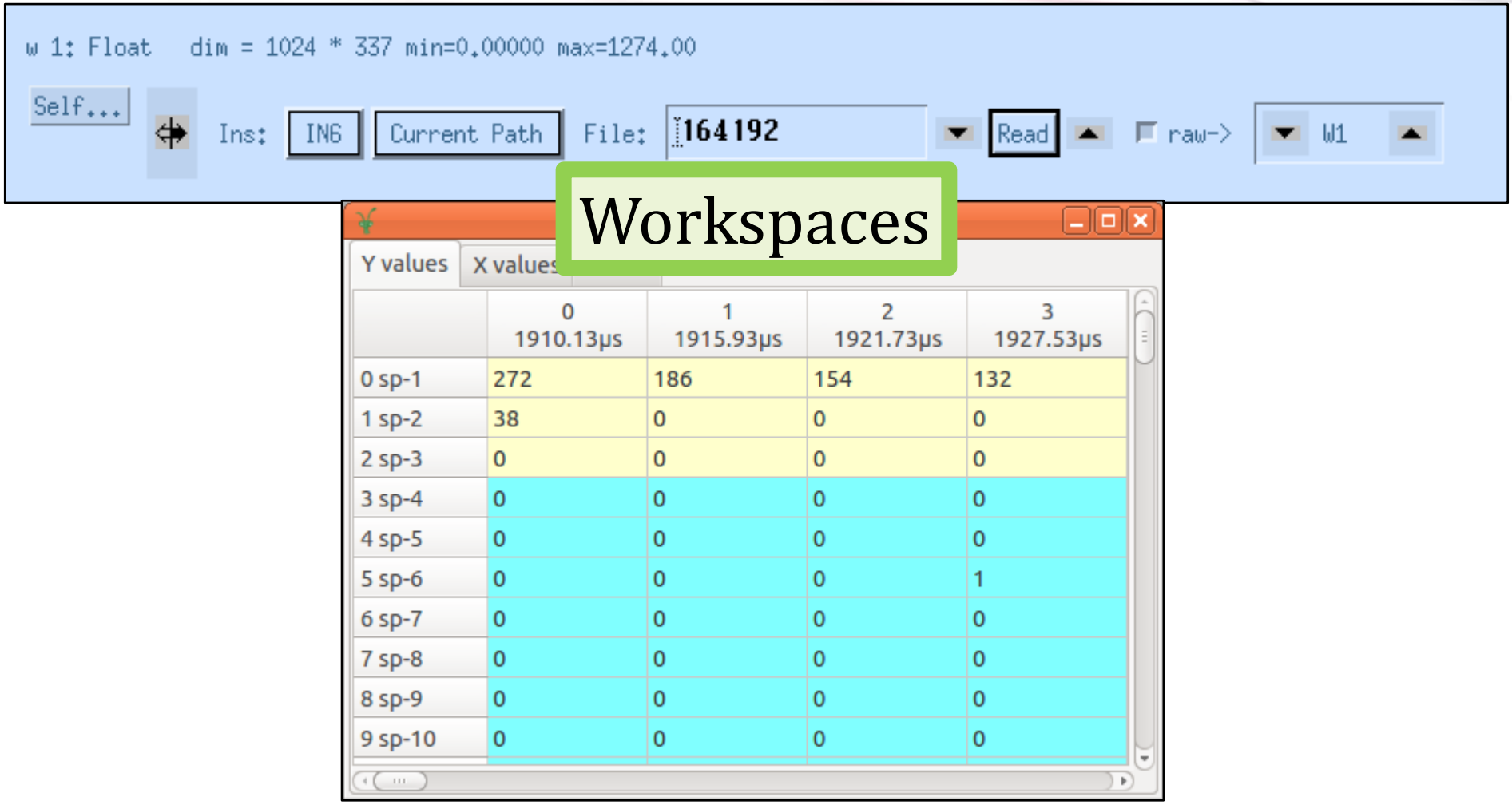
LAMP and Mantid





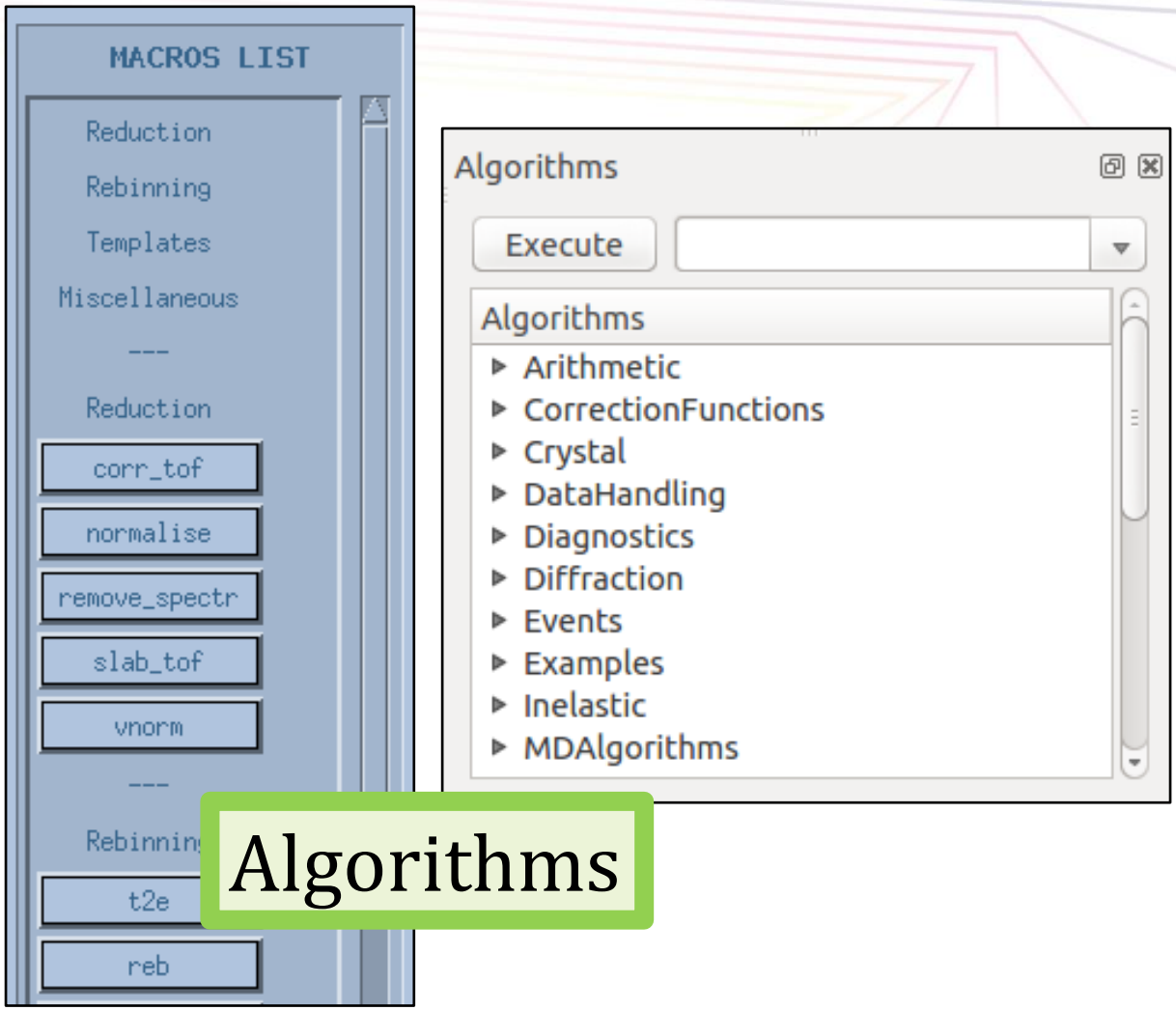


LAMP and Mantid

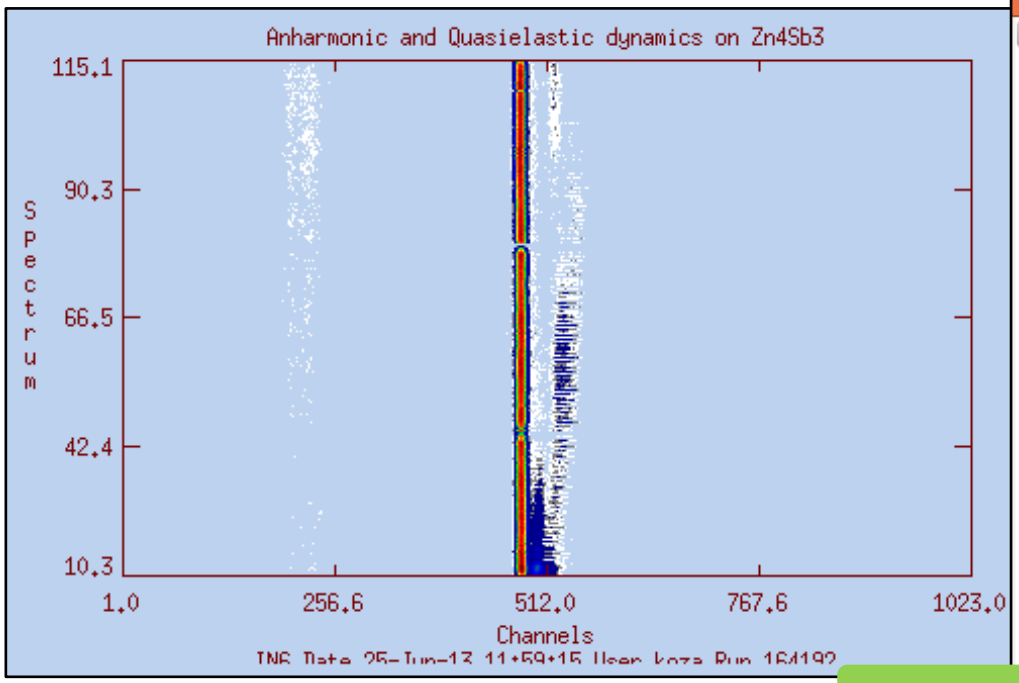


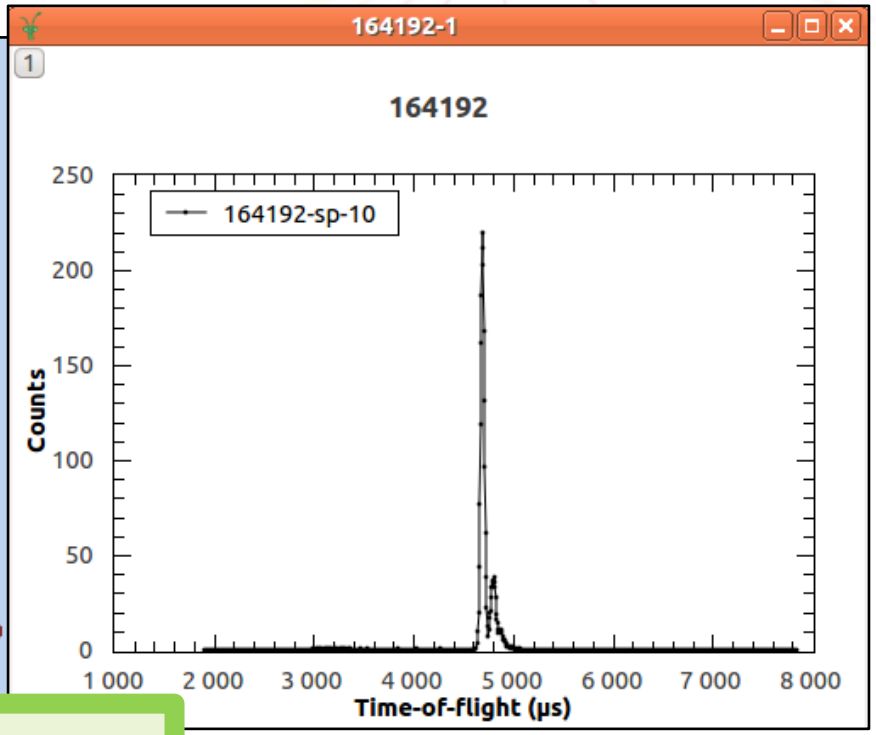
	0 1910.13µs	1 1915.93µs	2 1921.73µs	3 1927.53µs
0 sp-1	272	186	154	132
1 sp-2	38	0	0	0
2 sp-3	0	0	0	0
3 sp-4	0	0	0	0
4 sp-5	0	0	0	0
5 sp-6	0	0	0	1
6 sp-7	0	0	0	0
7 sp-8	0	0	0	0
8 sp-9	0	0	0	0
9 sp-10	0	0	0	0

LAMP and Mantid



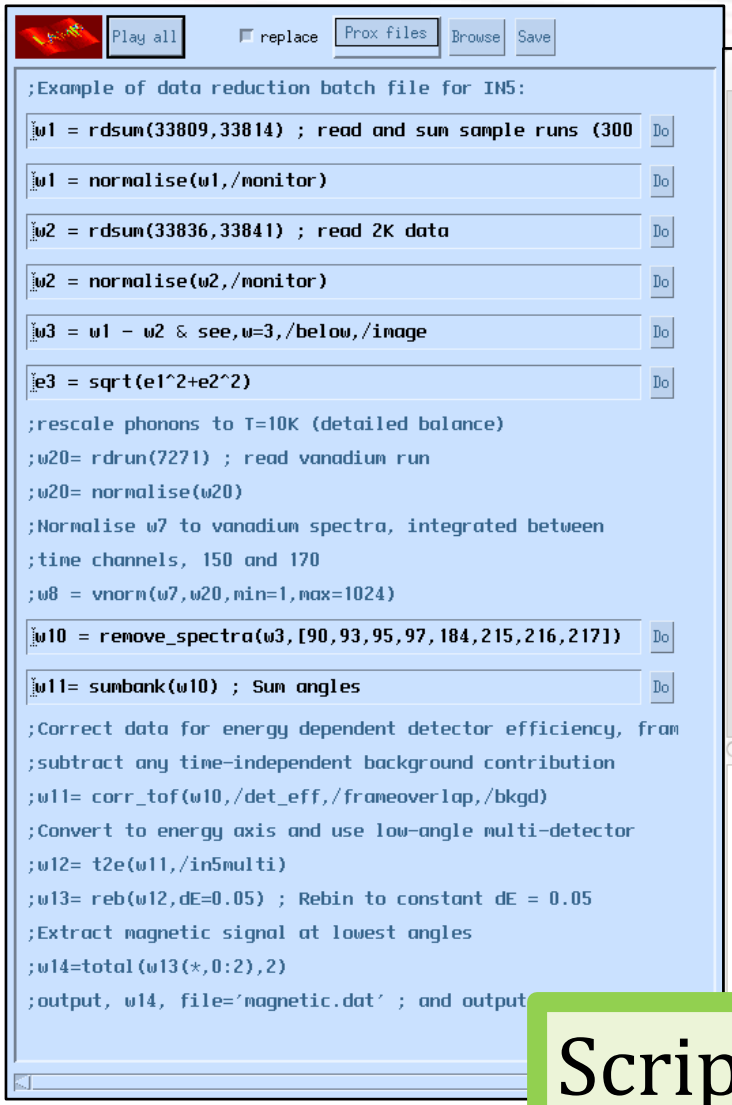
LAMP and Mantid

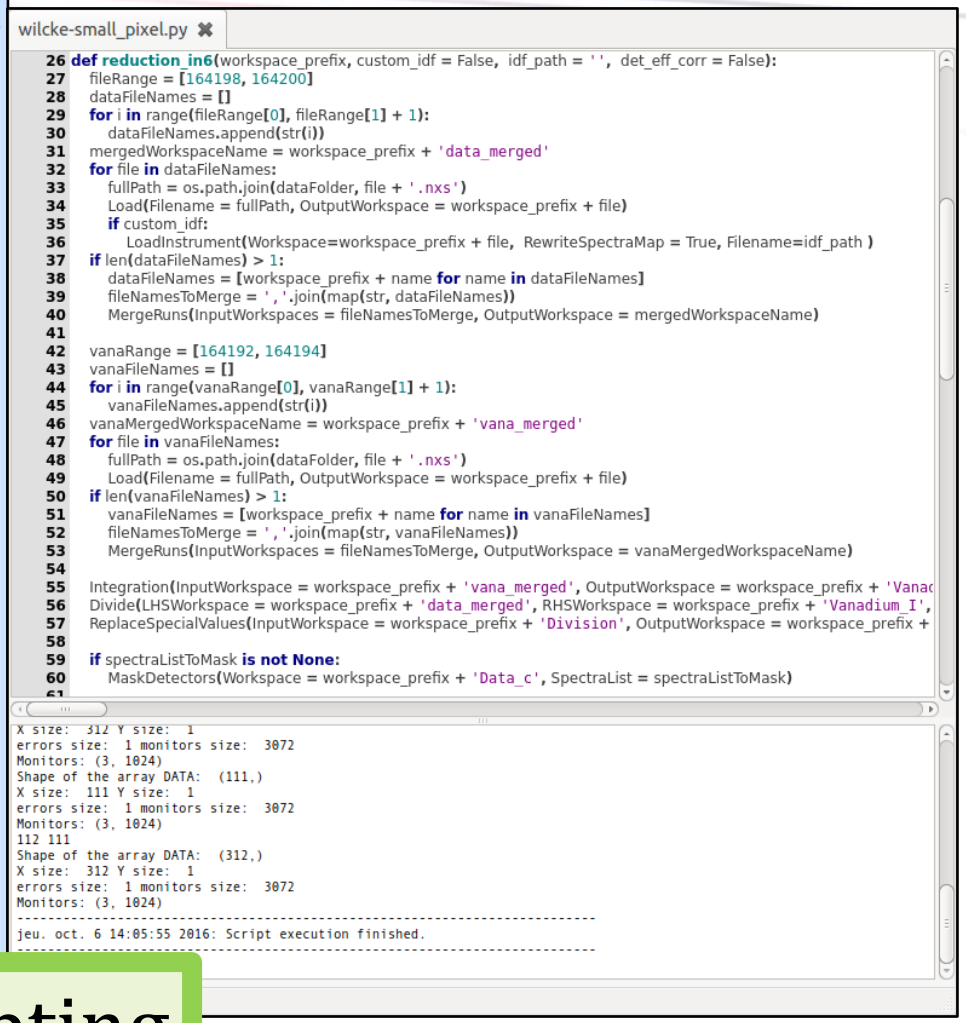




Plotting

LAMP and Mantid



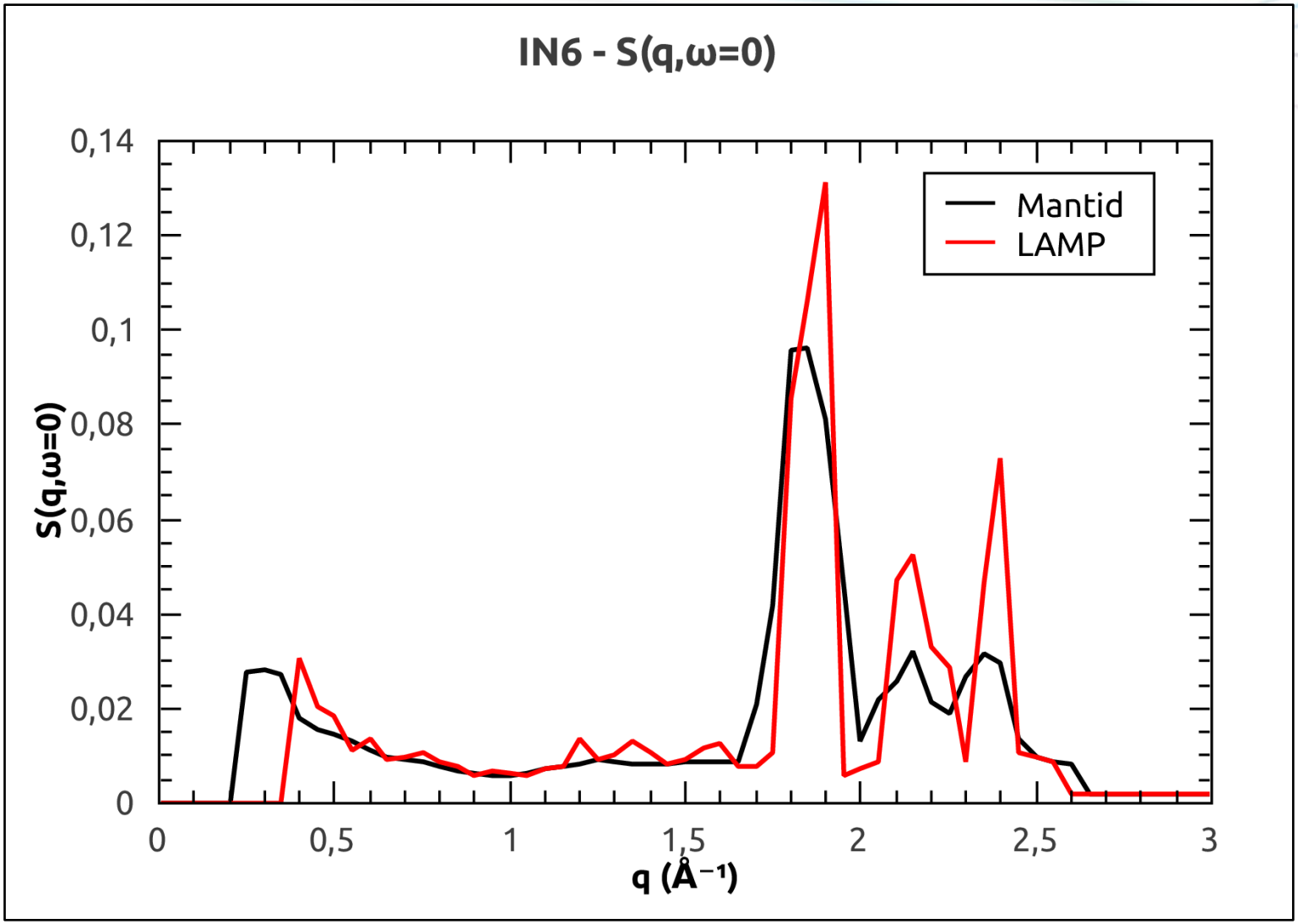


Scripting

ILL Workflows

- Started with Time-of-Flight Spectrometry (IN4/5/6) and Backscattering instruments (IN16B)
- Initial work started by:
  - Ricardo Ferraz-Leal (loaders, instrument definitions, sample scripts)
  - Spencer Howells and Elliot Oram (IN16B workflow)
- Features to support workflows:
  - File loading and merging sample logs
  - Workflow runner
  - Flat background moving window average
  - Incident energy calibration for ToF Instruments

Time-of-Flight Workflow



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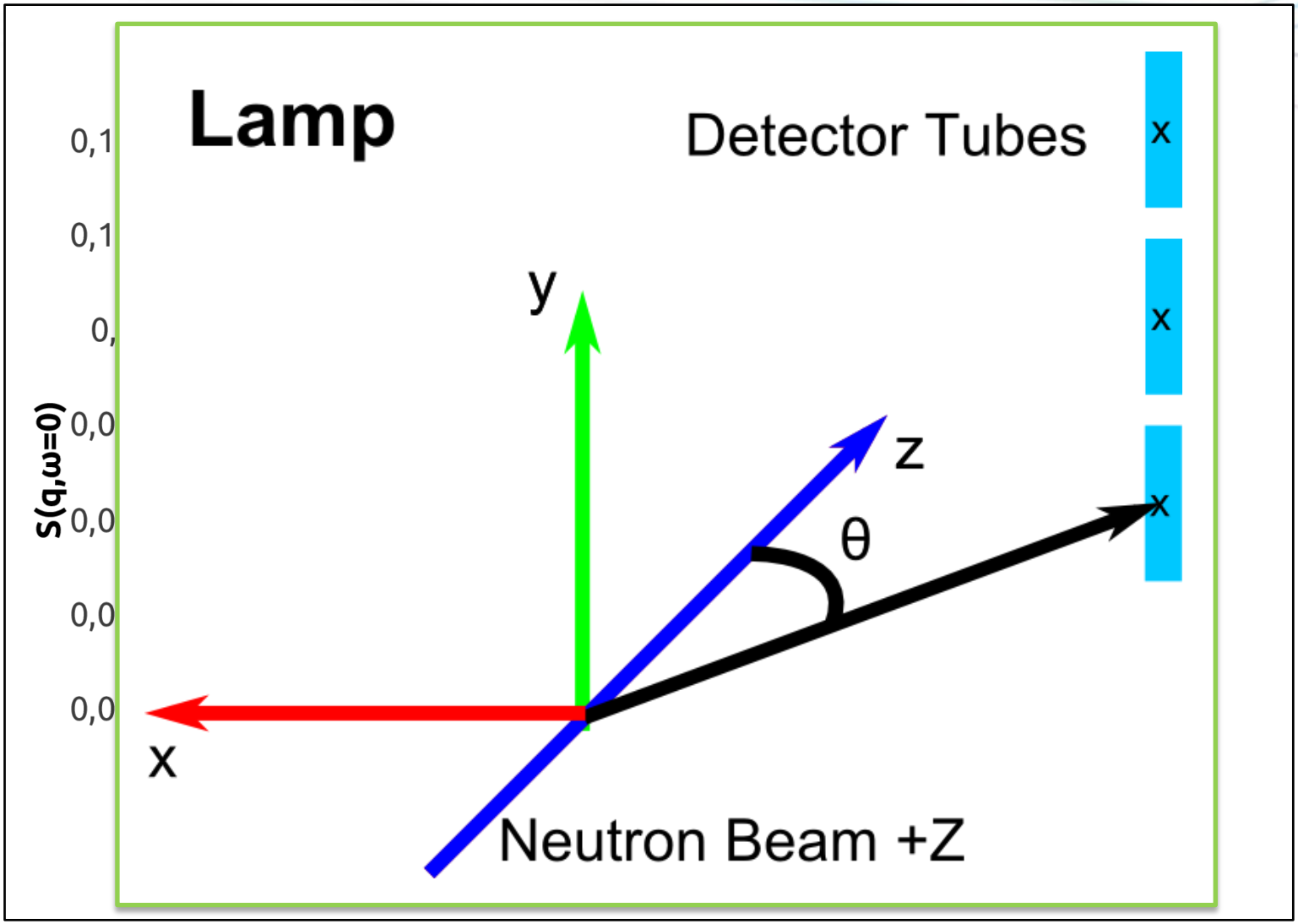

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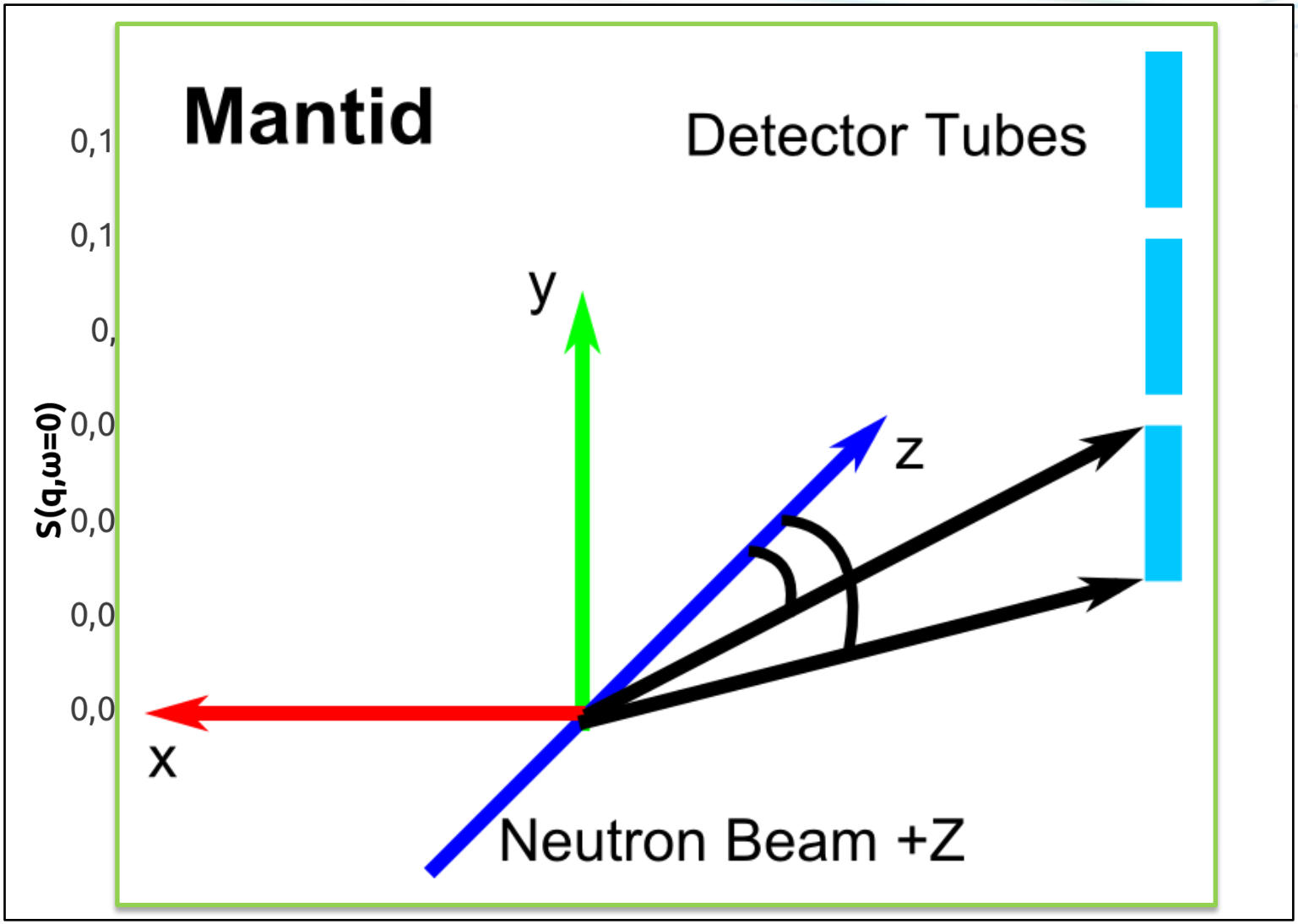
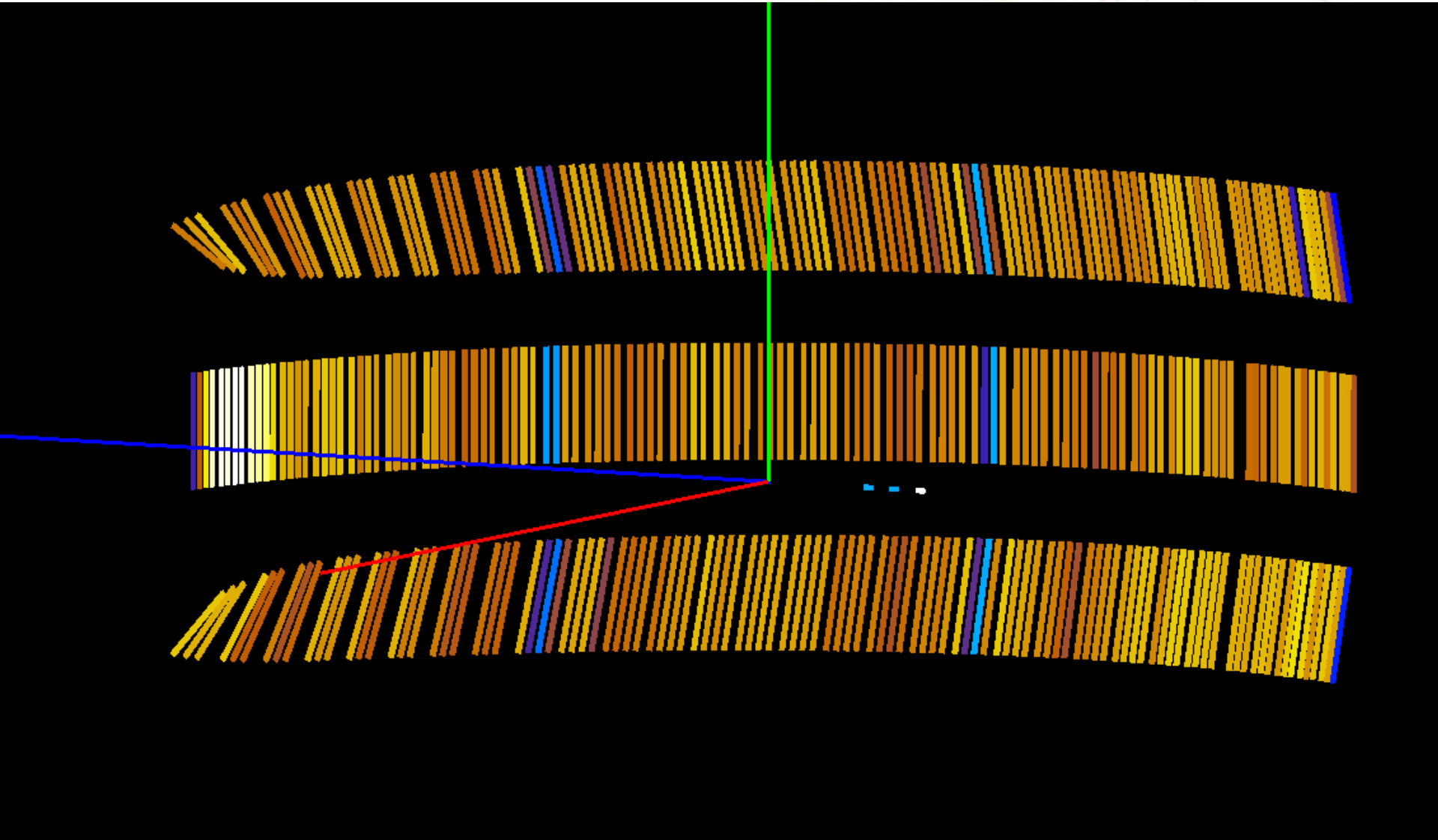


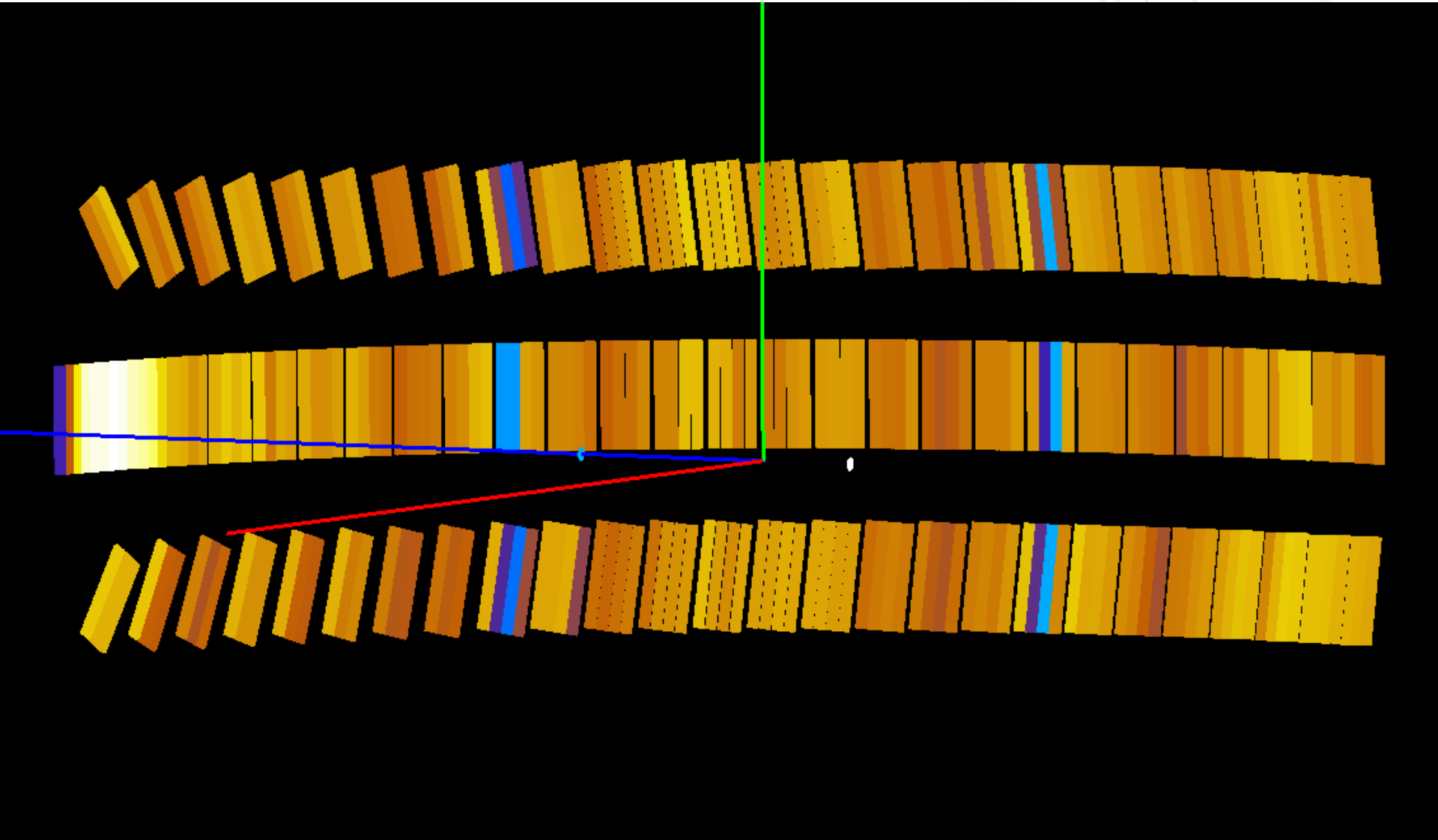
Time-of-Flight Workflow

Instrument Definition – IN6 Original

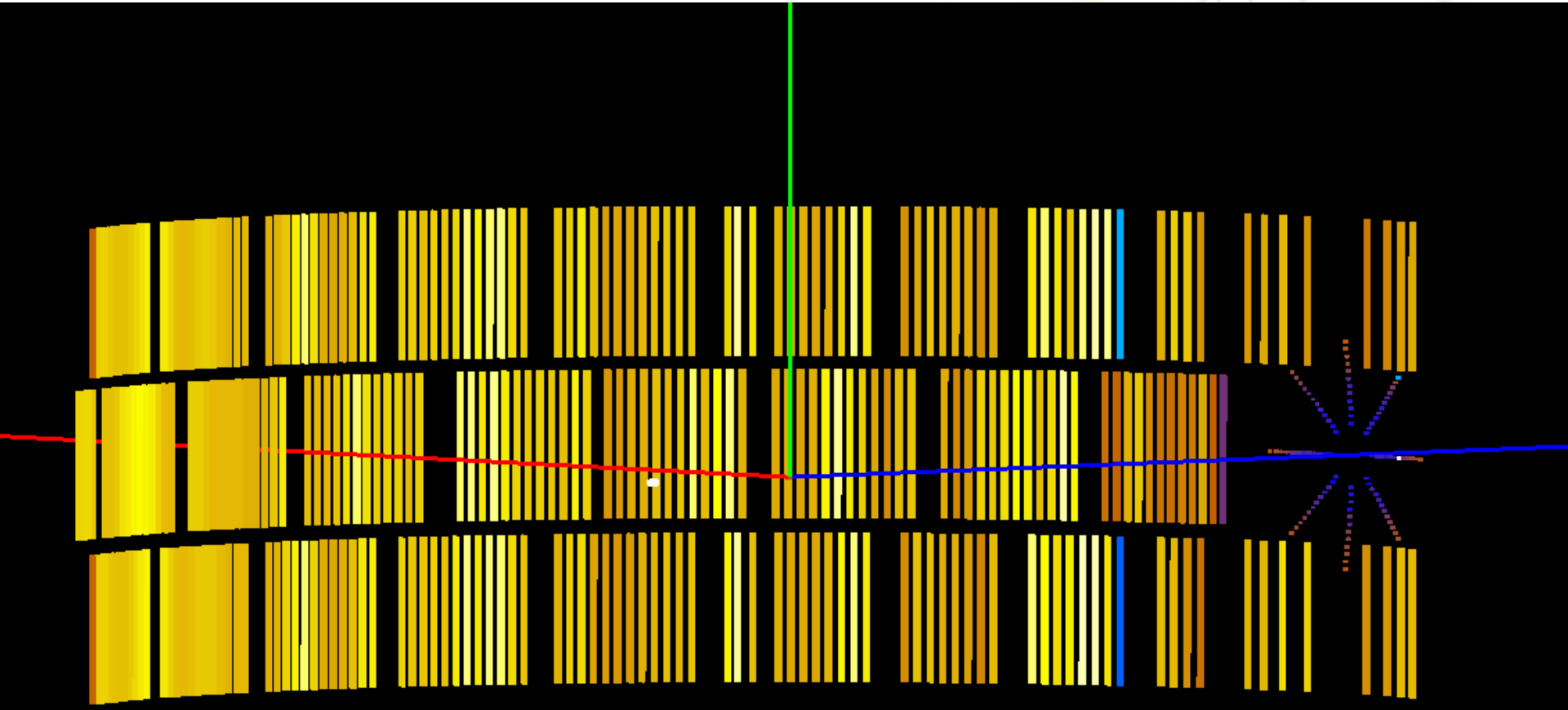


Time-of-Flight Workflow

Instrument Definition – IN6 Updated

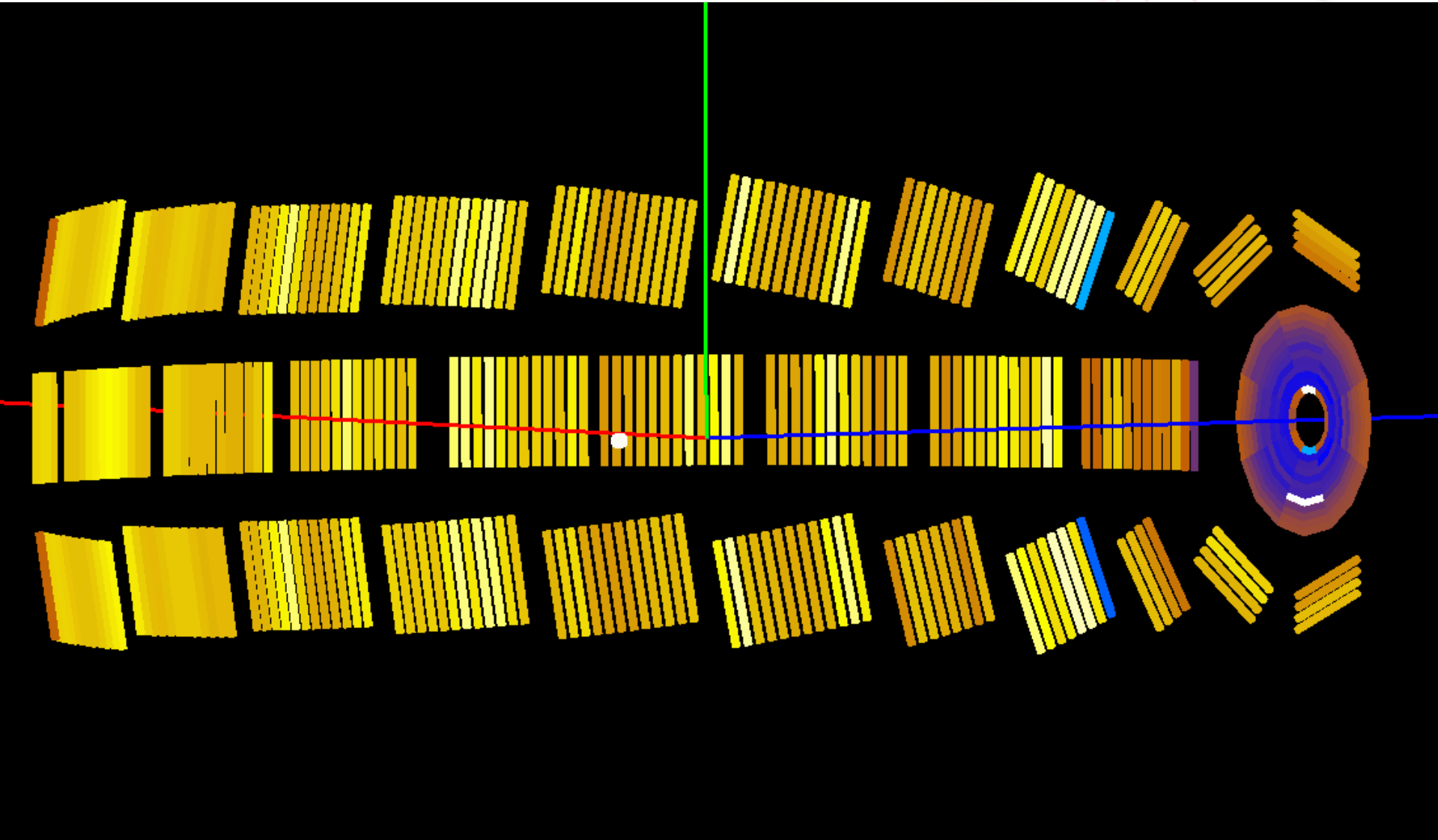


Time-of-Flight Workflow
Instrument Definition – IN4 Original

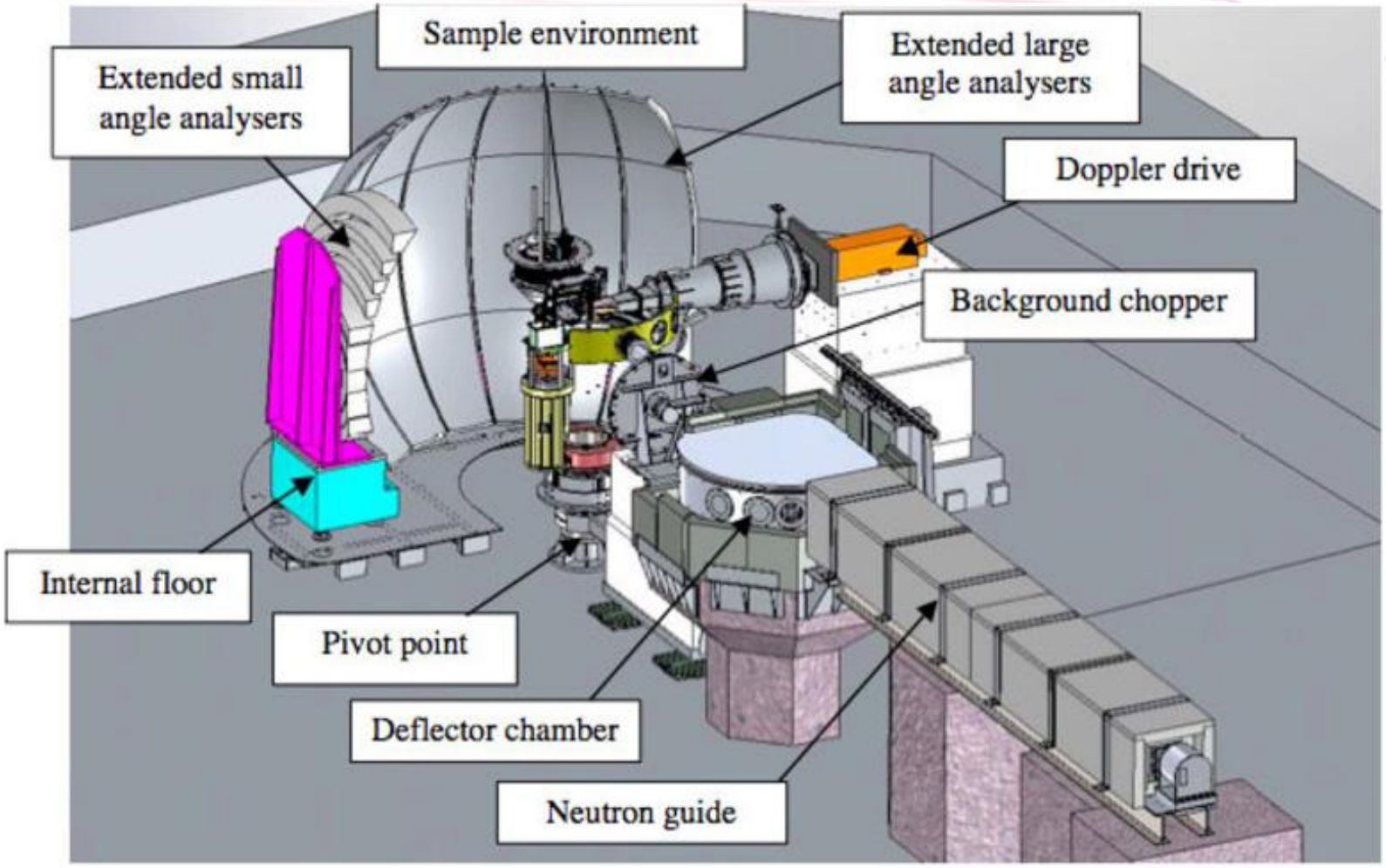


Time-of-Flight Workflow

Instrument Definition – IN4 Updated



Backscattering Workflow – IN16B



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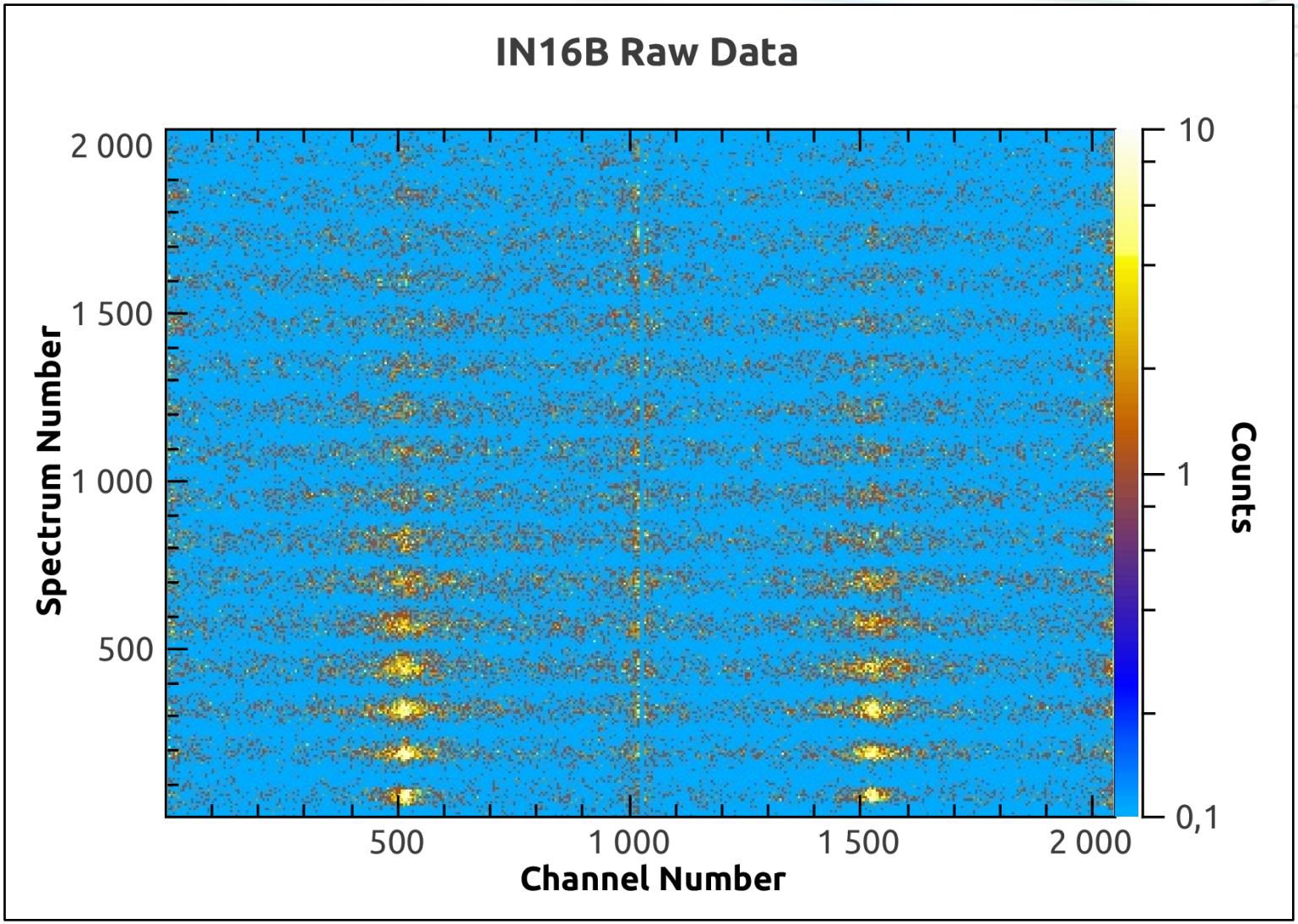
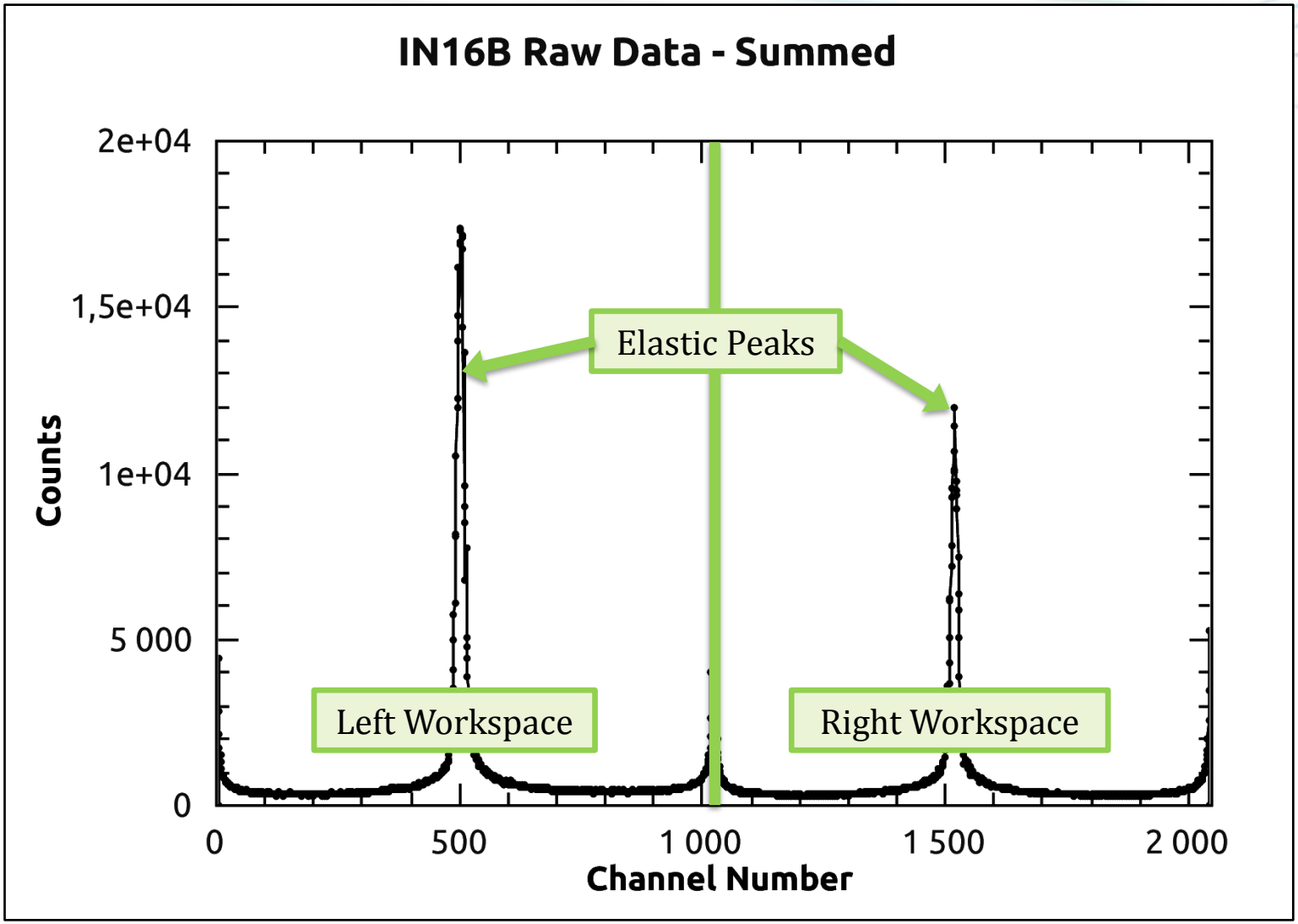
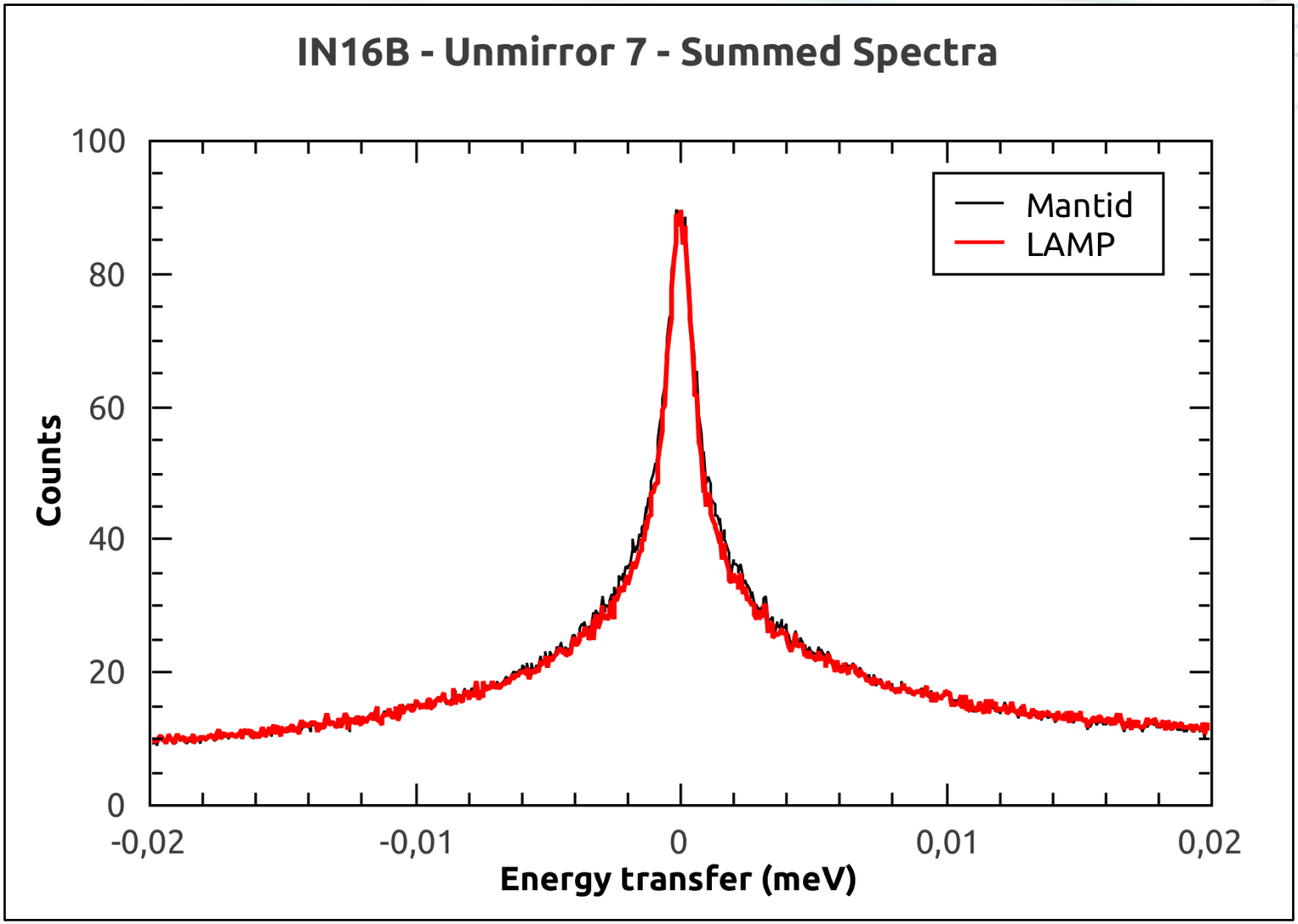


Backscattering Workflow

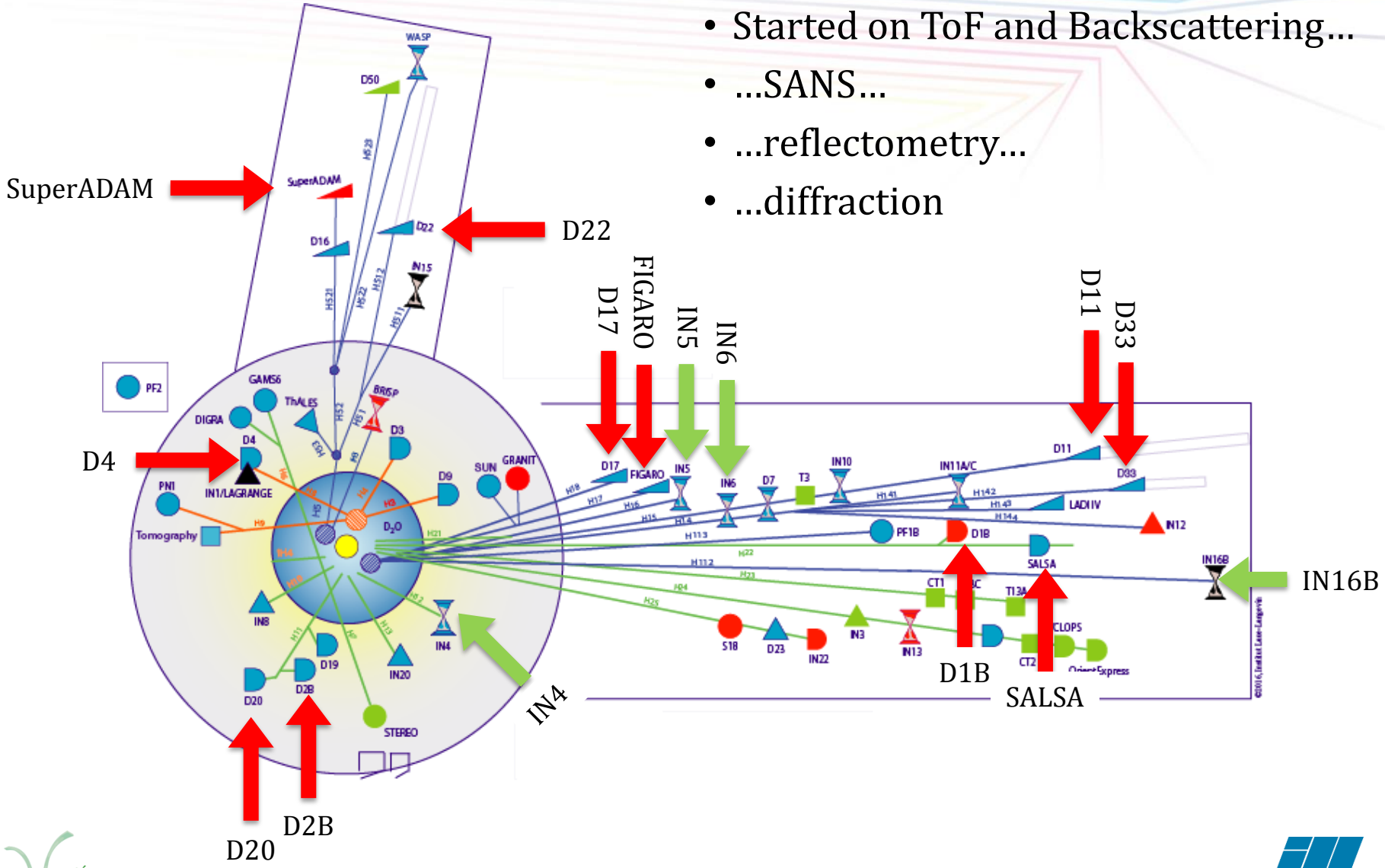


Backscattering Workflow – Lamp and Mantid



Future Work – ILL Instruments

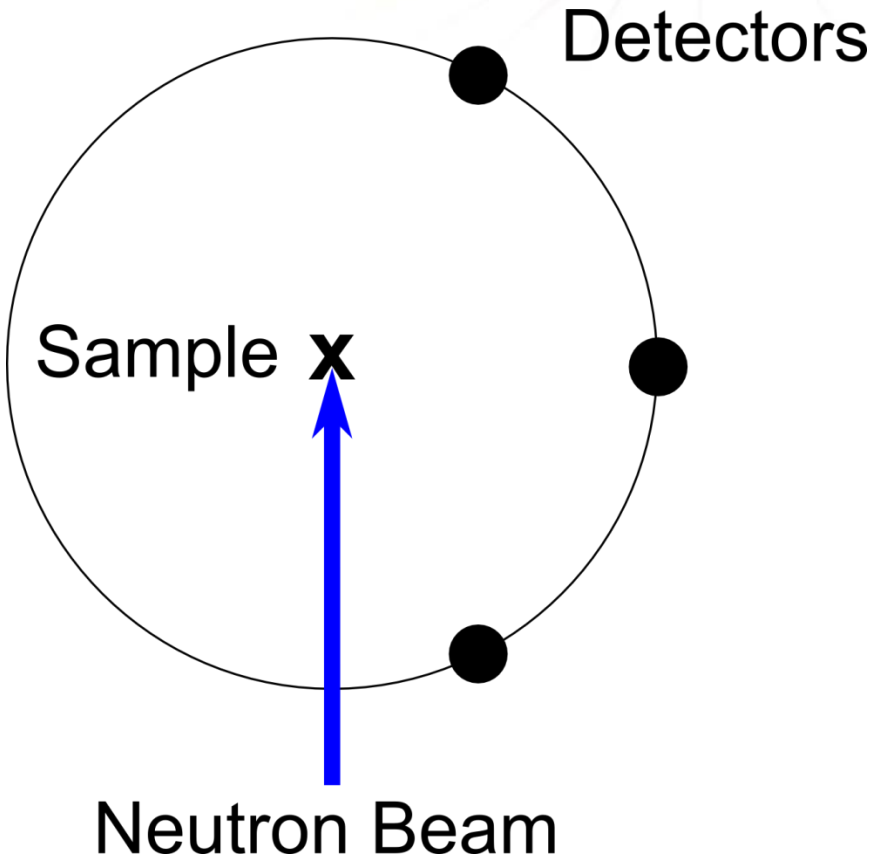
- Started on ToF and Backscattering…
- …SANS…
- …reflectometry…
- …diffraction



Future Work – Scanning Instruments

- Support the instruments at ILL with movable detectors, such as D2B, D4, D7 and D16

D2B – Powder Diffractometer



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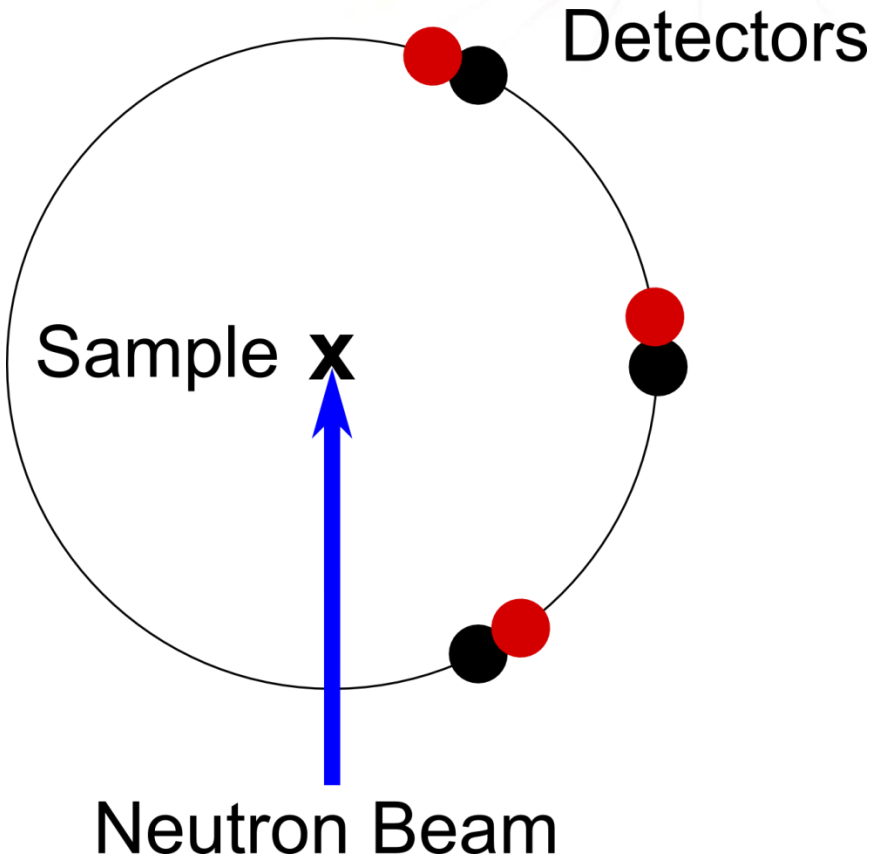

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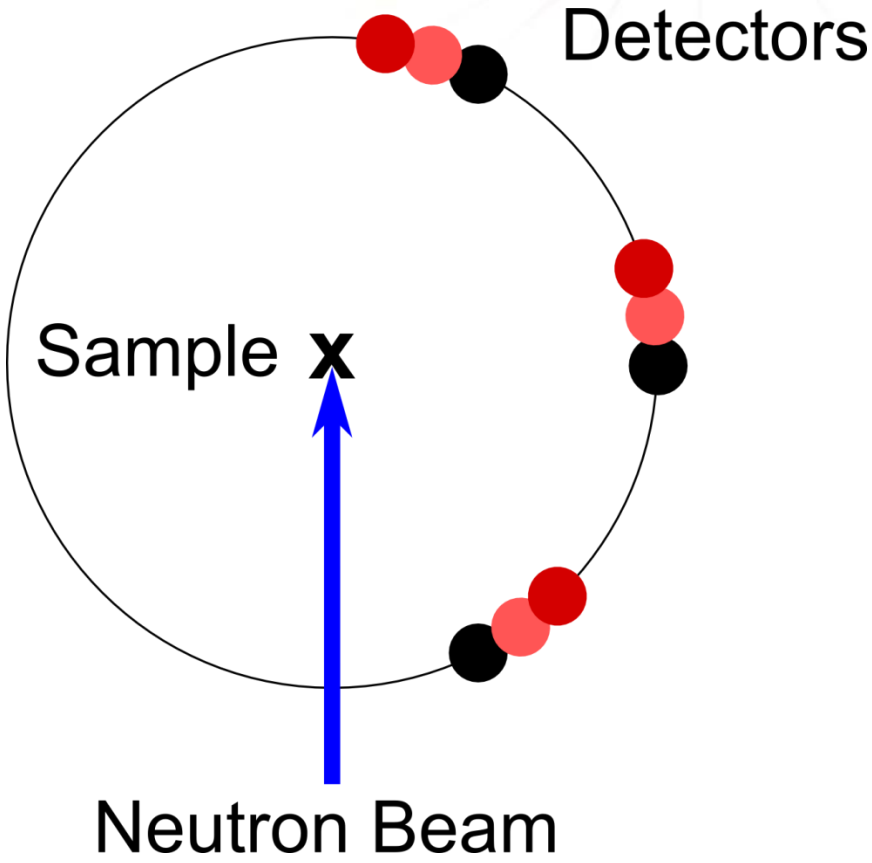

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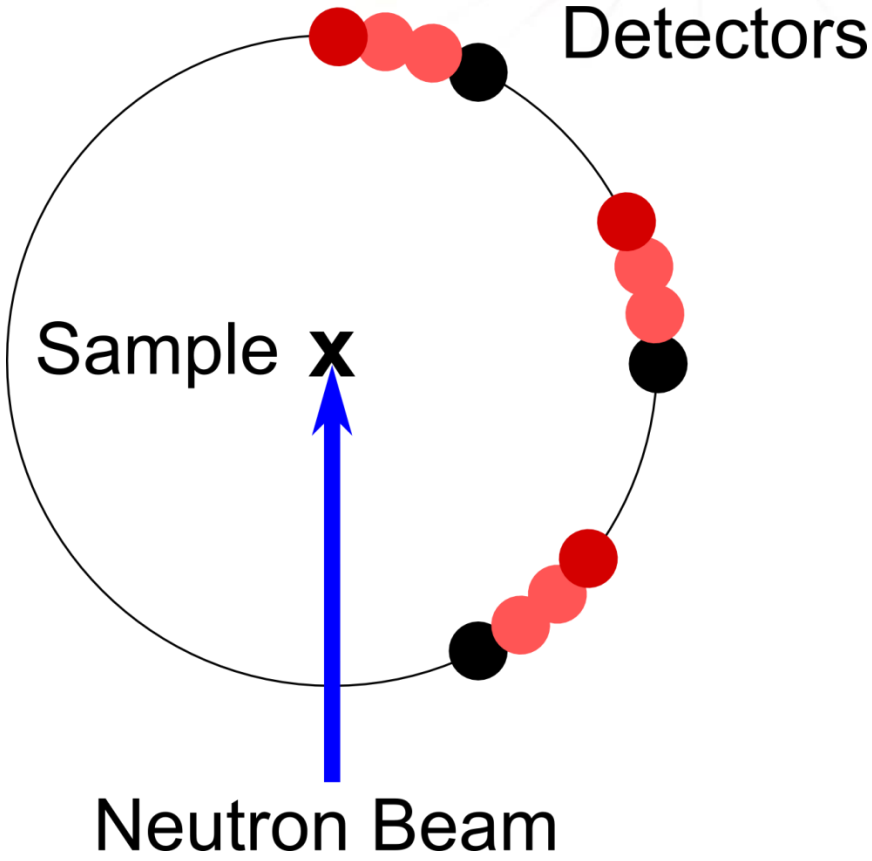

Future Work, Summary and Conclusions

- SINE2020 funding for Mantid on continuous sources
- SINE2020 funding for data analysis work:
  - QENS – GUIs, fitting and analysis in Mantid
  - Simulation – MDANSE, DFT
- Mantid adoption under way at the ILL…
- … but lots still a long way to go

Thanks for listening!