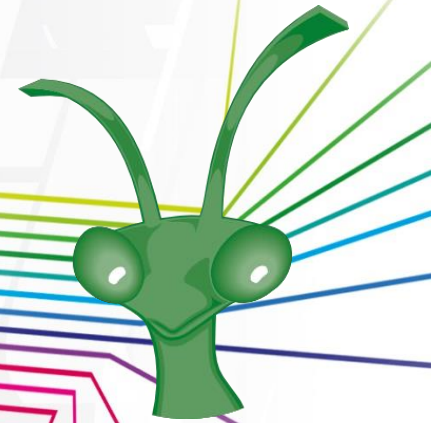




The ILL Joins the Mantid Project

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

NoBugs – 18th October 2016



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



NEUTRONS
FOR SOCIETY

mantid



EUROPEAN
SPALLATION
SOURCE



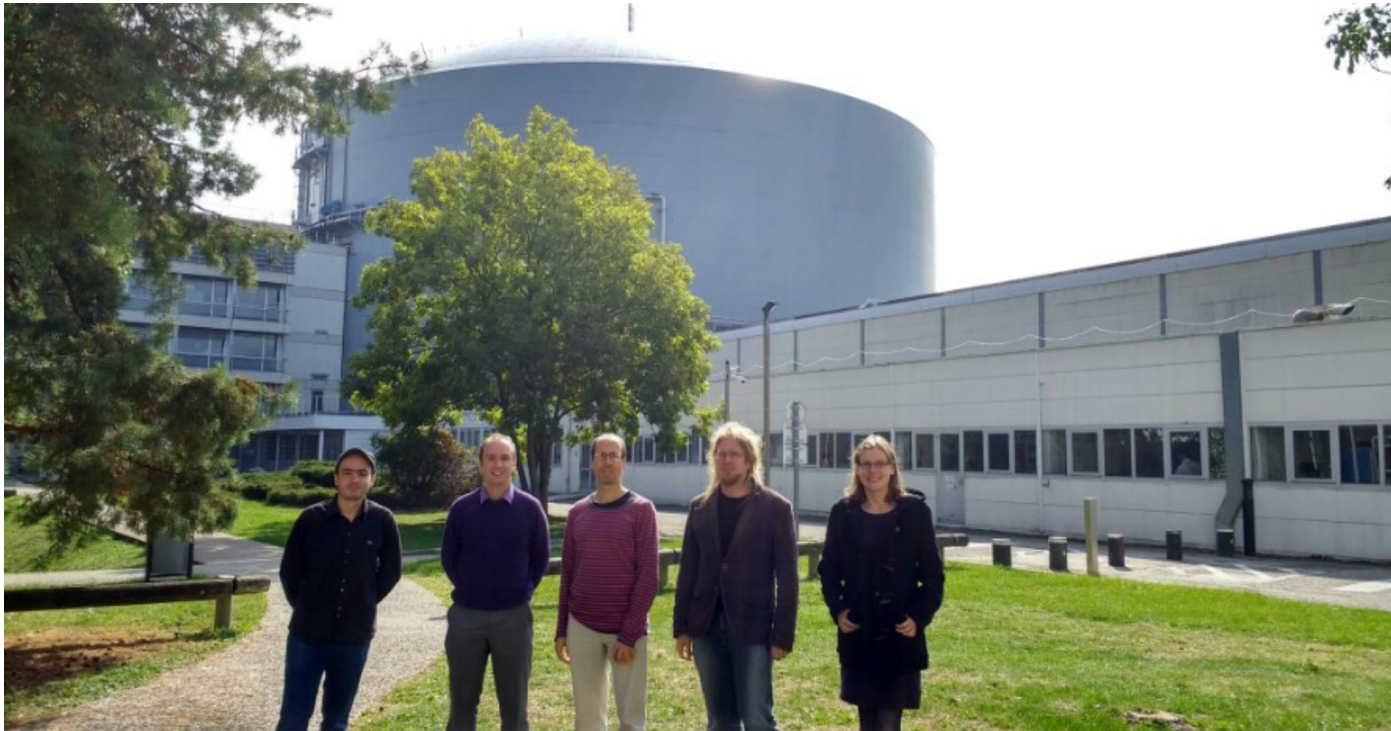
INSTITUT MAX VON LAUE - PAUL LANGEVIN



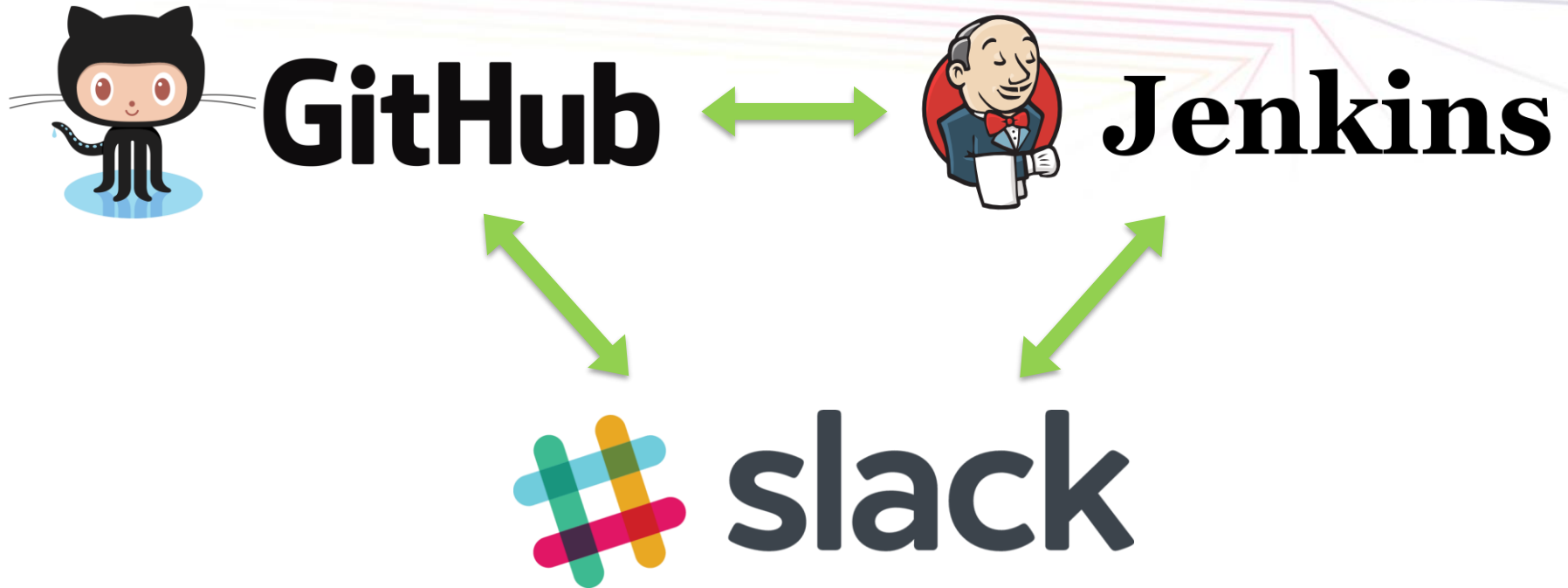
NEUTRONS
FOR SOCIETY

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



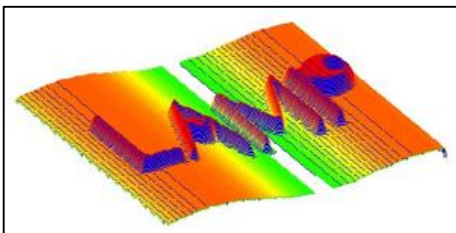
Working with Distributed Partners



BlueJeans

skype™

LAMP and Mantid



File Customize Edit Info Tools Lamp/Layout Help

DATA COLLECTOR Working path

X=640 Y=111,630

Self... File:

DISPLAY WORKSPACE

Image Contour

Surface

Range etc... Fill Bg

Channels

INS Data 25-Jun-12 11:02:16 Scan Name: 164192

MACROS LIST

- Reduction
 -
 -
 -
 -
 -
- Rebinning
 -
 -
 -
 -
 -
 -

Ubuntu 0 B /t U x² x₂ αβ γ f

Results Log

Please cite: <http://dx.doi.org/10.1016/j.nima.2014.07.029> and this release: <http://dx.doi.org/10.5286/Software/Mantid3.7.1>

Load started

Load successful, Duration 0.08 seconds

164192 - Mantid

Y values	X values	Errors	0	1	2	3
			1910.13μs	1915.93μs	1921.73μs	1927.53μs
0 sp-1	272	186	154	132		
1 sp-2	38	0	0	0		

164192-1

164192

Counts

Time-of-flight (μs)

164192-sp-10

Workspaces

Filter Workspaces

Workspaces

- 164192

Algorithms

Algorithms

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction
- Events
- Examples
- Inelastic
- MDAlgorithms

Script Interpreter


object? -> Details about 'object', use 'object??' for extra details.

%quiref -> A brief reference about the graphical user interface.

In [1]:

LAMP and Mantid

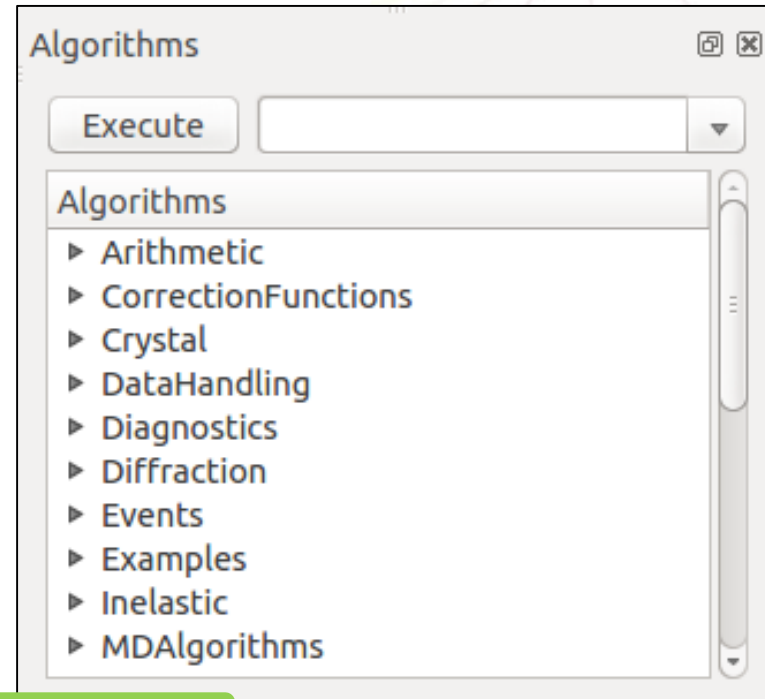
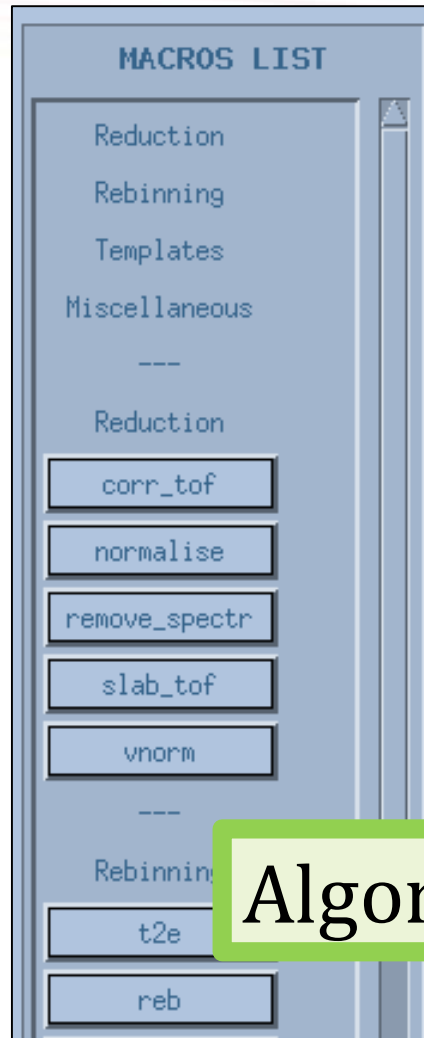
w 1: Float dim = 1024 * 337 min=0,00000 max=1274,00

Self...  Ins: File:

Workspaces

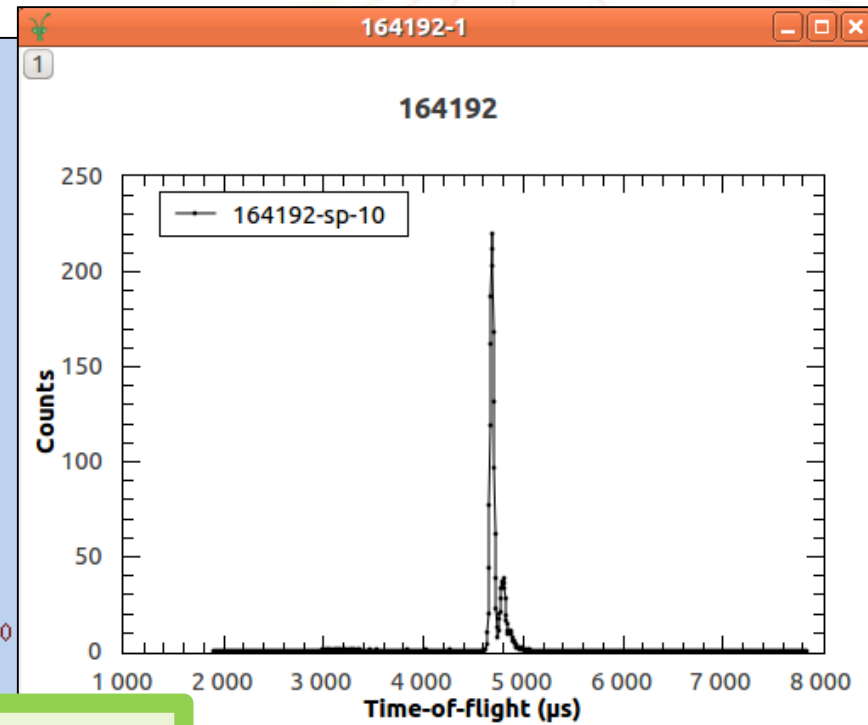
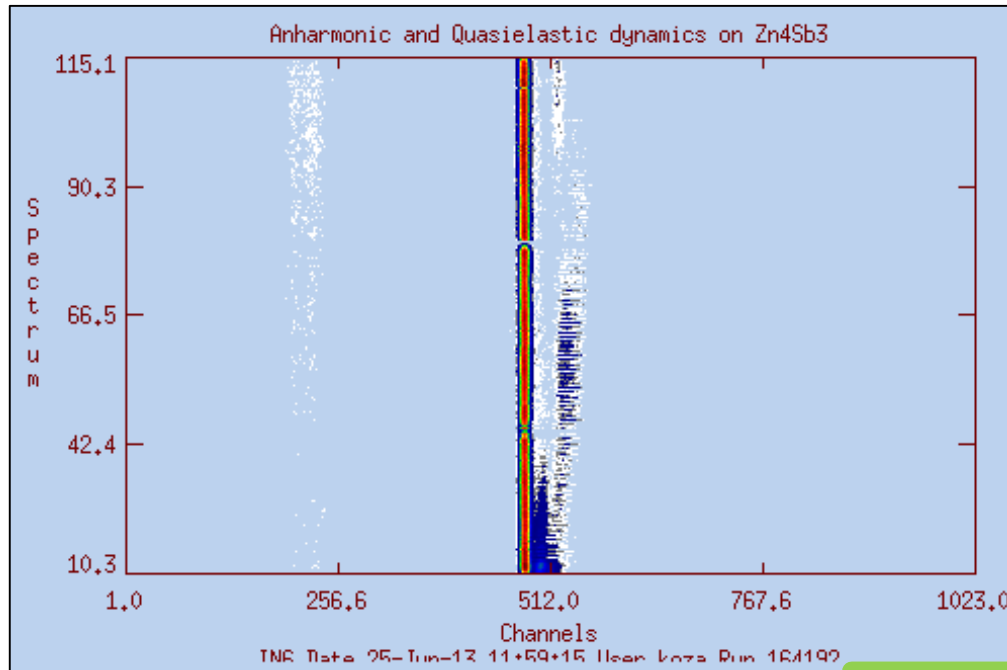
Y values	X values			
	0 1910.13µs	1 1915.93µs	2 1921.73µs	3 1927.53µs
0 sp-1	272	186	154	132
1 sp-2	38	0	0	0
2 sp-3	0	0	0	0
3 sp-4	0	0	0	0
4 sp-5	0	0	0	0
5 sp-6	0	0	0	1
6 sp-7	0	0	0	0
7 sp-8	0	0	0	0
8 sp-9	0	0	0	0
9 sp-10	0	0	0	0

LAMP and Mantid



Algorithms

LAMP and Mantid



Plotting

LAMP and Mantid

```
Play all  replace Prox files Browse Save

;Example of data reduction batch file for IN5:

w1 = rdsun(33809,33814) ; read and sum sample runs (300) Do
w1 = normalise(w1,/monitor) Do
w2 = rdsun(33836,33841) ; read 2K data Do
w2 = normalise(w2,/monitor) Do
w3 = w1 - w2 & see,w=3,/below,/image Do
e3 = sqrt(e1^2+e2^2) Do

;rescale phonons to T=10K (detailed balance)
;w20= rdrun(7271) ; read vanadium run
;w20= normalise(w20)

;Normalise w7 to vanadium spectra, integrated between
;time channels, 150 and 170
;w8 = vnorn(w7,w20,min=1,max=1024)

w10 = remove_spectra(w3, [90,93,95,97,184,215,216,217]) Do
w11= sumbank(w10) ; Sum angles Do

;Correct data for energy dependent detector efficiency, fram
;subtract any time-independent background contribution
;w11= corr_tof(w10,/det_eff,/frameoverlap,/bkgd)
;Convert to energy axis and use low-angle multi-detector
;w12= t2e(w11,/in5multi)
;w13= reb(w12,dE=0.05) ; Rebin to constant dE = 0.05
;Extract magnetic signal at lowest angles
;w14=total(w13(*,0:2),2)
;output, w14, file='magnetic.dat' ; and output
```

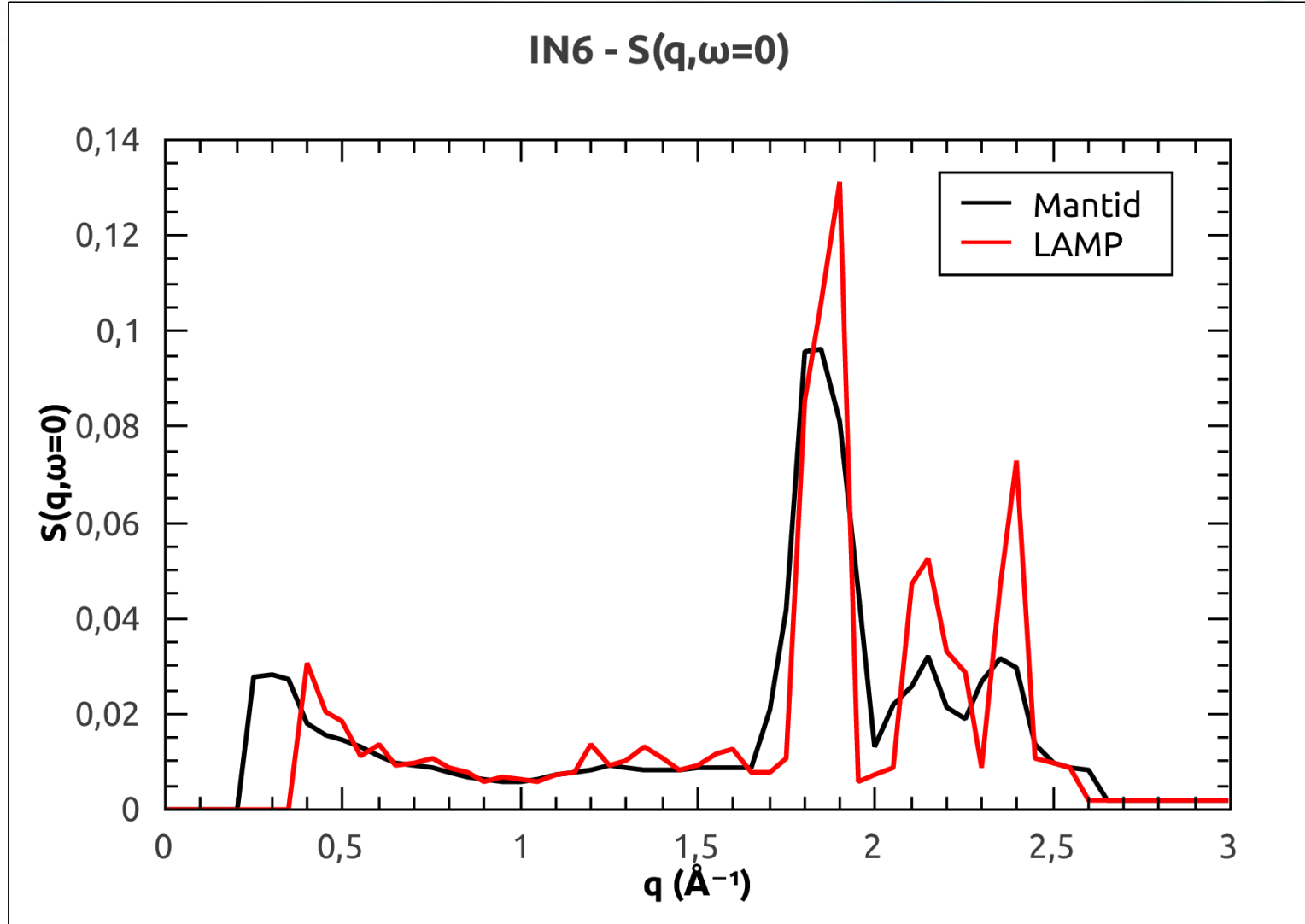
```
wilcke-small_pixel.py x
26 def reduction_in6(workspace_prefix, custom_idf = False, idf_path = '', det_eff_corr = False):
27     fileRange = [164198, 164200]
28     dataFileNames = []
29     for i in range(fileRange[0], fileRange[1] + 1):
30         dataFileNames.append(str(i))
31     mergedWorkspaceName = workspace_prefix + 'data_merged'
32     for file in dataFileNames:
33         fullPath = os.path.join(dataFolder, file + '.nxs')
34         Load(Filename = fullPath, OutputWorkspace = workspace_prefix + file)
35         if custom_idf:
36             LoadInstrument(Workspace=workspace_prefix + file, RewriteSpectraMap = True, Filename=idf_path )
37     if len(dataFileNames) > 1:
38         dataFileNames = [workspace_prefix + name for name in dataFileNames]
39         fileNamesToMerge = ', '.join(map(str, dataFileNames))
40         MergeRuns(InputWorkspaces = fileNamesToMerge, OutputWorkspace = mergedWorkspaceName)
41
42     vanaRange = [164192, 164194]
43     vanaFileNames = []
44     for i in range(vanaRange[0], vanaRange[1] + 1):
45         vanaFileNames.append(str(i))
46     vanaMergedWorkspaceName = workspace_prefix + 'vana_merged'
47     for file in vanaFileNames:
48         fullPath = os.path.join(dataFolder, file + '.nxs')
49         Load(Filename = fullPath, OutputWorkspace = workspace_prefix + file)
50     if len(vanaFileNames) > 1:
51         vanaFileNames = [workspace_prefix + name for name in vanaFileNames]
52         fileNamesToMerge = ', '.join(map(str, vanaFileNames))
53         MergeRuns(InputWorkspaces = fileNamesToMerge, OutputWorkspace = vanaMergedWorkspaceName)
54
55     Integration(InputWorkspace = workspace_prefix + 'vana_merged', OutputWorkspace = workspace_prefix + 'Vanad
56     Divide(LHSWorkspace = workspace_prefix + 'data_merged', RHSWorkspace = workspace_prefix + 'Vanadium_I',
57     ReplaceSpecialValues(InputWorkspace = workspace_prefix + 'Division', OutputWorkspace = workspace_prefix +
58
59     if spectralListToMask is not None:
60         MaskDetectors(Workspace = workspace_prefix + 'Data_c', SpectraList = spectralListToMask)
61
X size: 312 Y size: 1
errors size: 1 monitors size: 3072
Monitors: (3, 1024)
Shape of the array DATA: (111,)
X size: 111 Y size: 1
errors size: 1 monitors size: 3072
Monitors: (3, 1024)
112 111
Shape of the array DATA: (312,)
X size: 312 Y size: 1
errors size: 1 monitors size: 3072
Monitors: (3, 1024)
-----
jeu. oct. 6 14:05:55 2016: Script execution finished.
```

Scripting

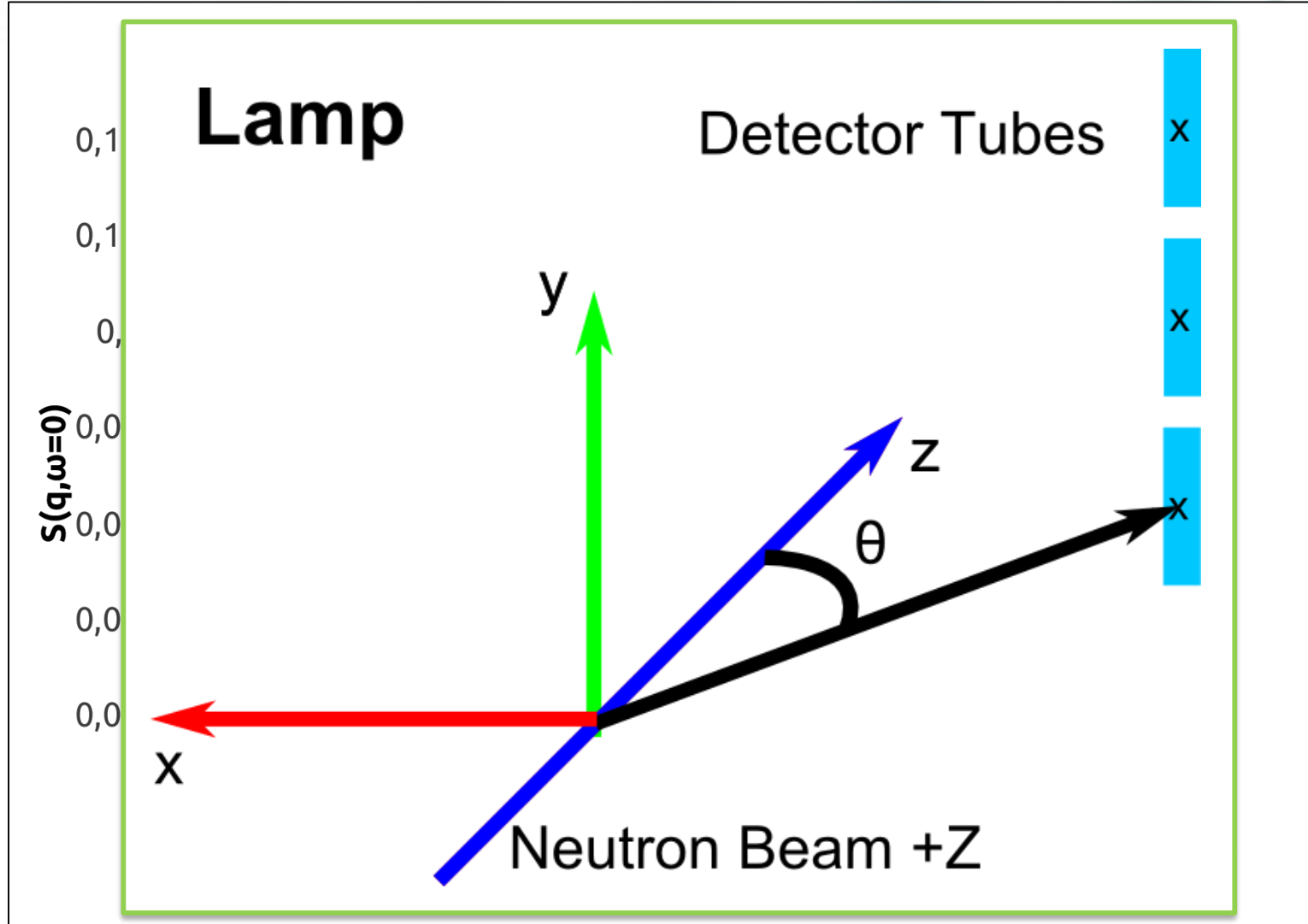
ILL Workflows

- 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
 - Flat background moving window average
 - Incident energy calibration for ToF Instruments

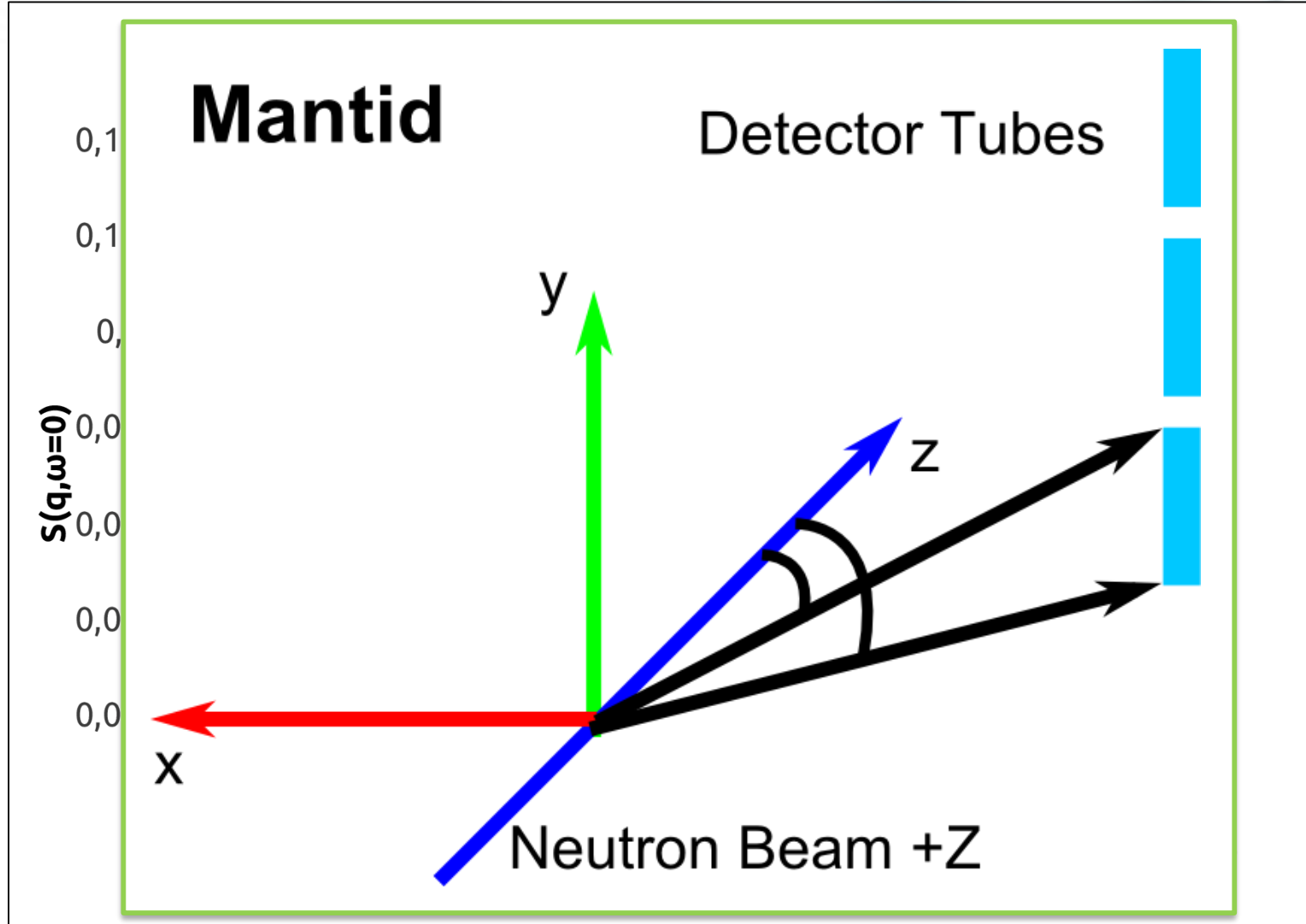
Time-of-Flight Workflow



Time-of-Flight Workflow

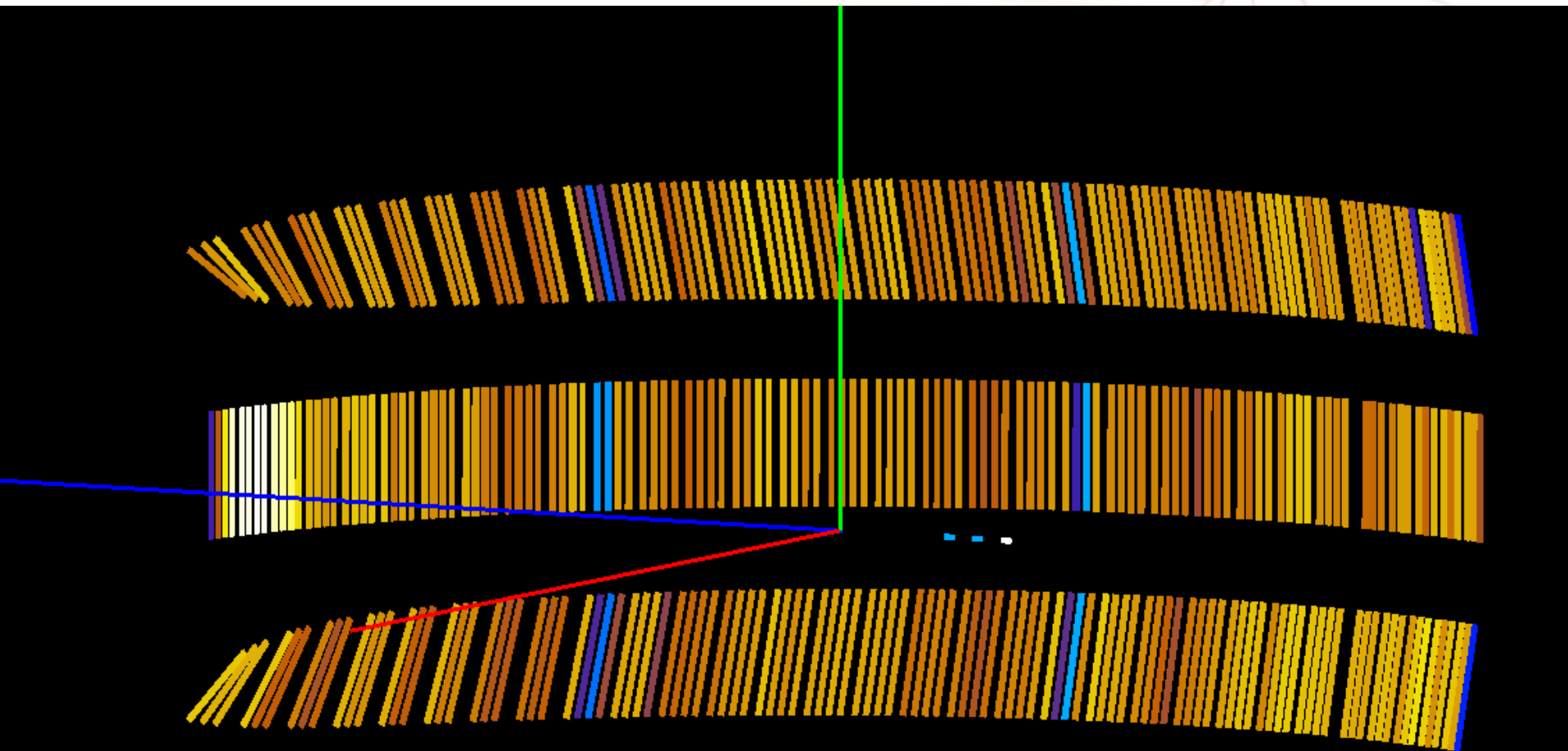


Time-of-Flight Workflow



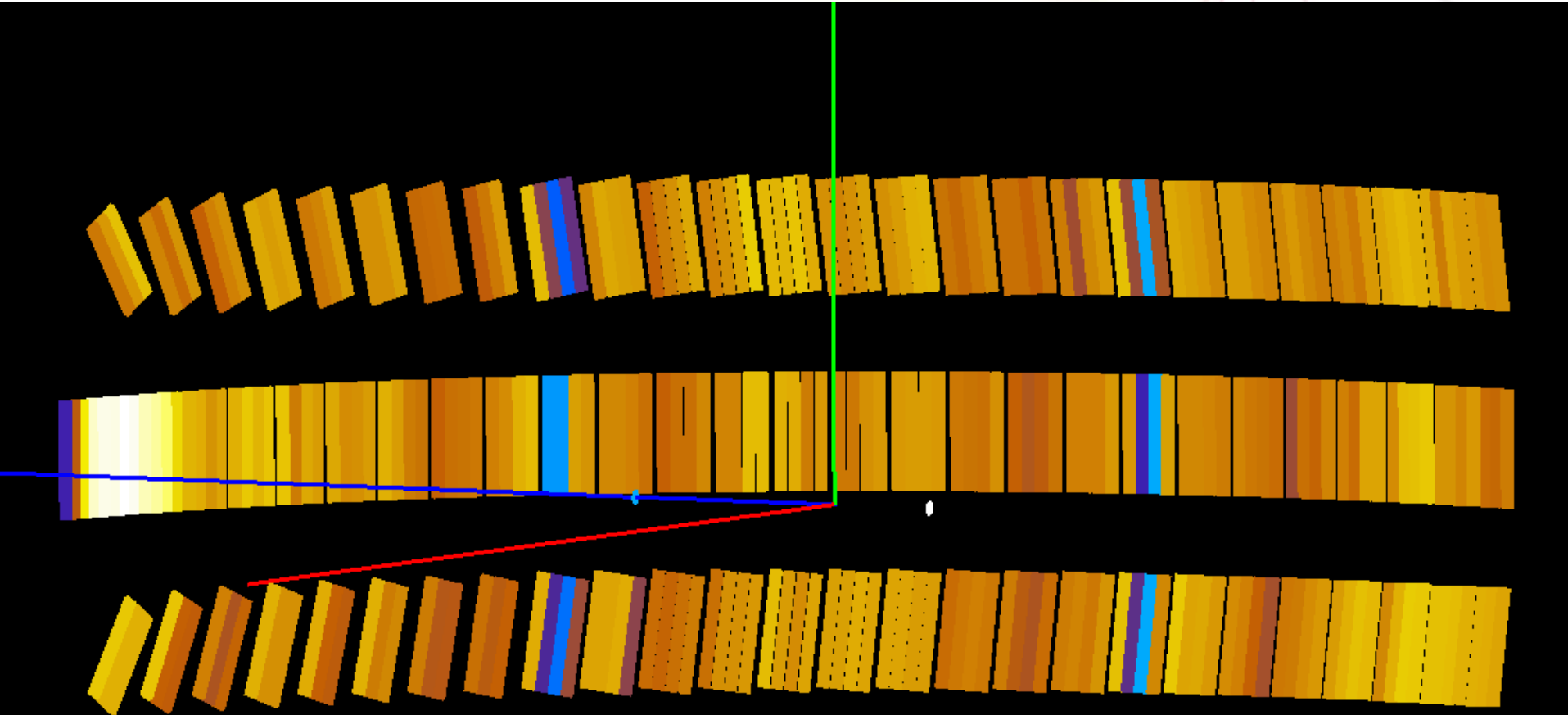
Time-of-Flight Workflow

Instrument Definition - IN6 Original



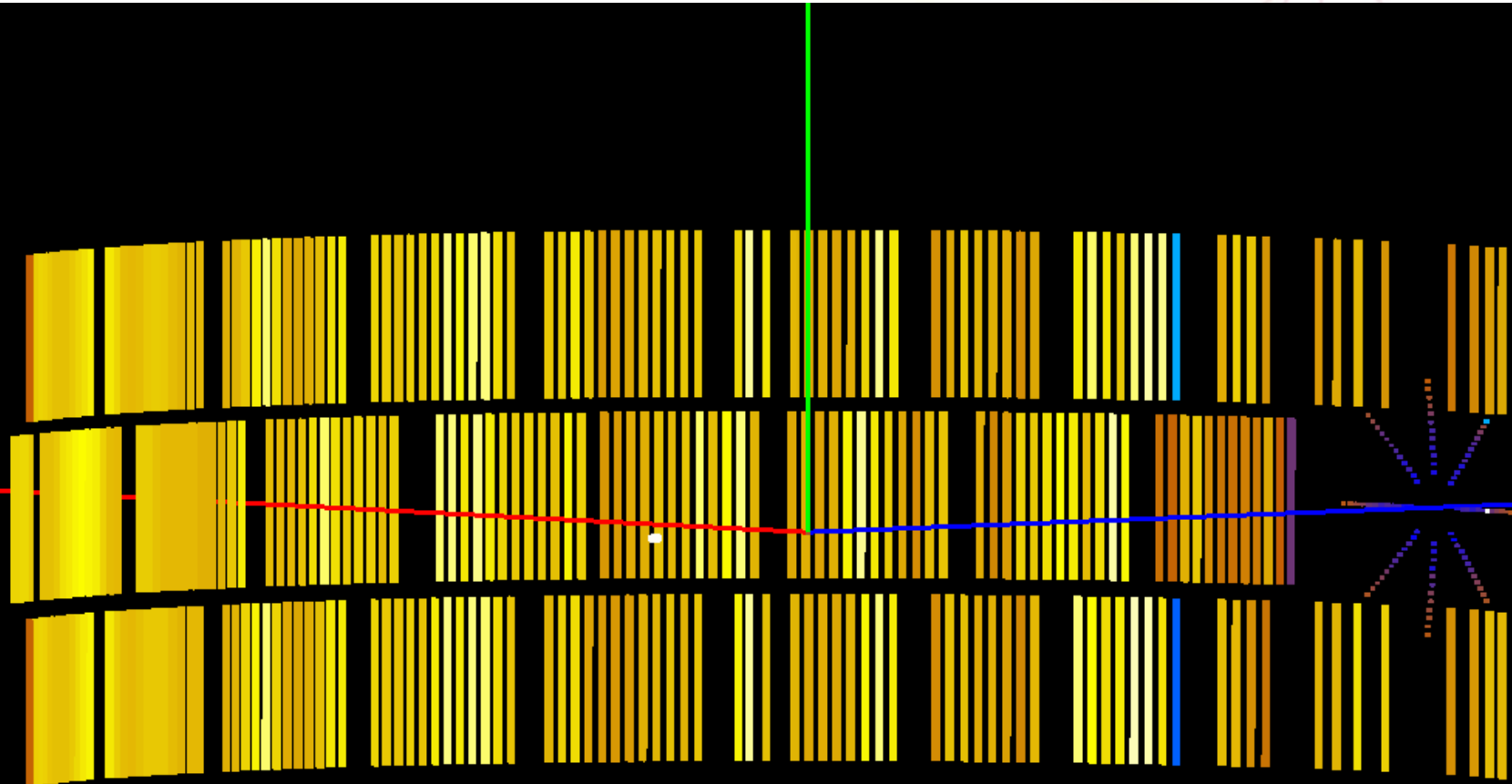
Time-of-Flight Workflow

Instrument Definition - IN6 Updated



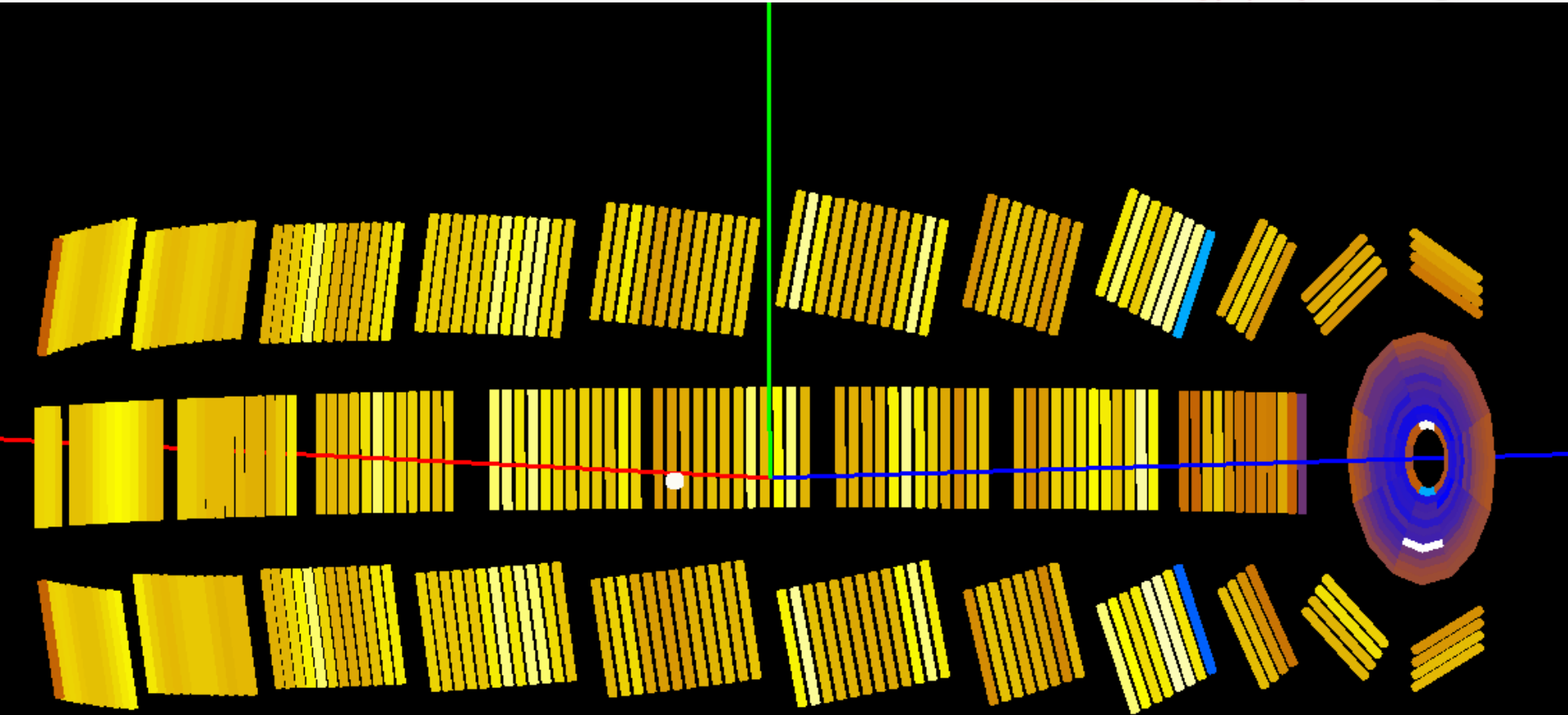
Time-of-Flight Workflow

Instrument Definition - IN4 Original

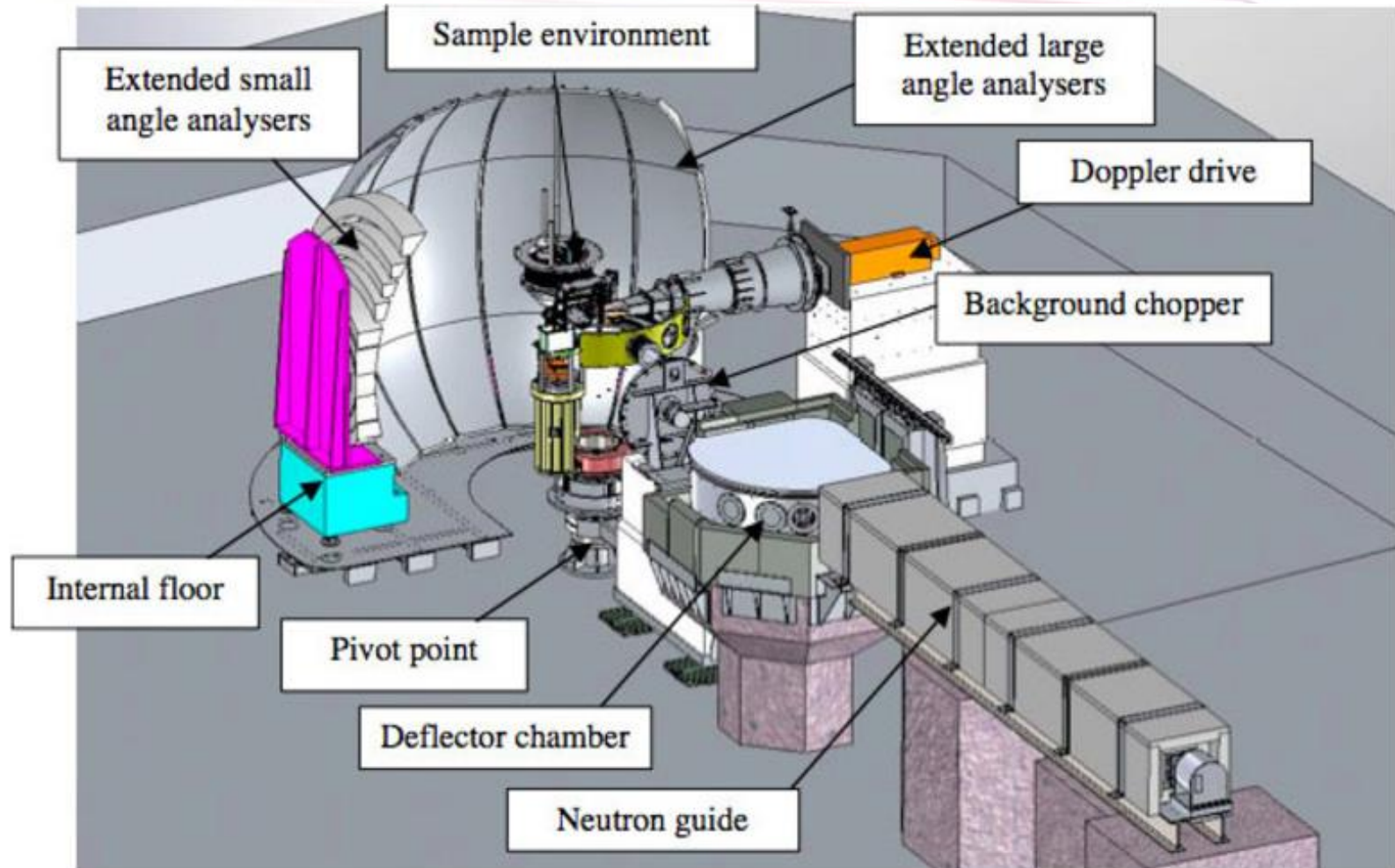


Time-of-Flight Workflow

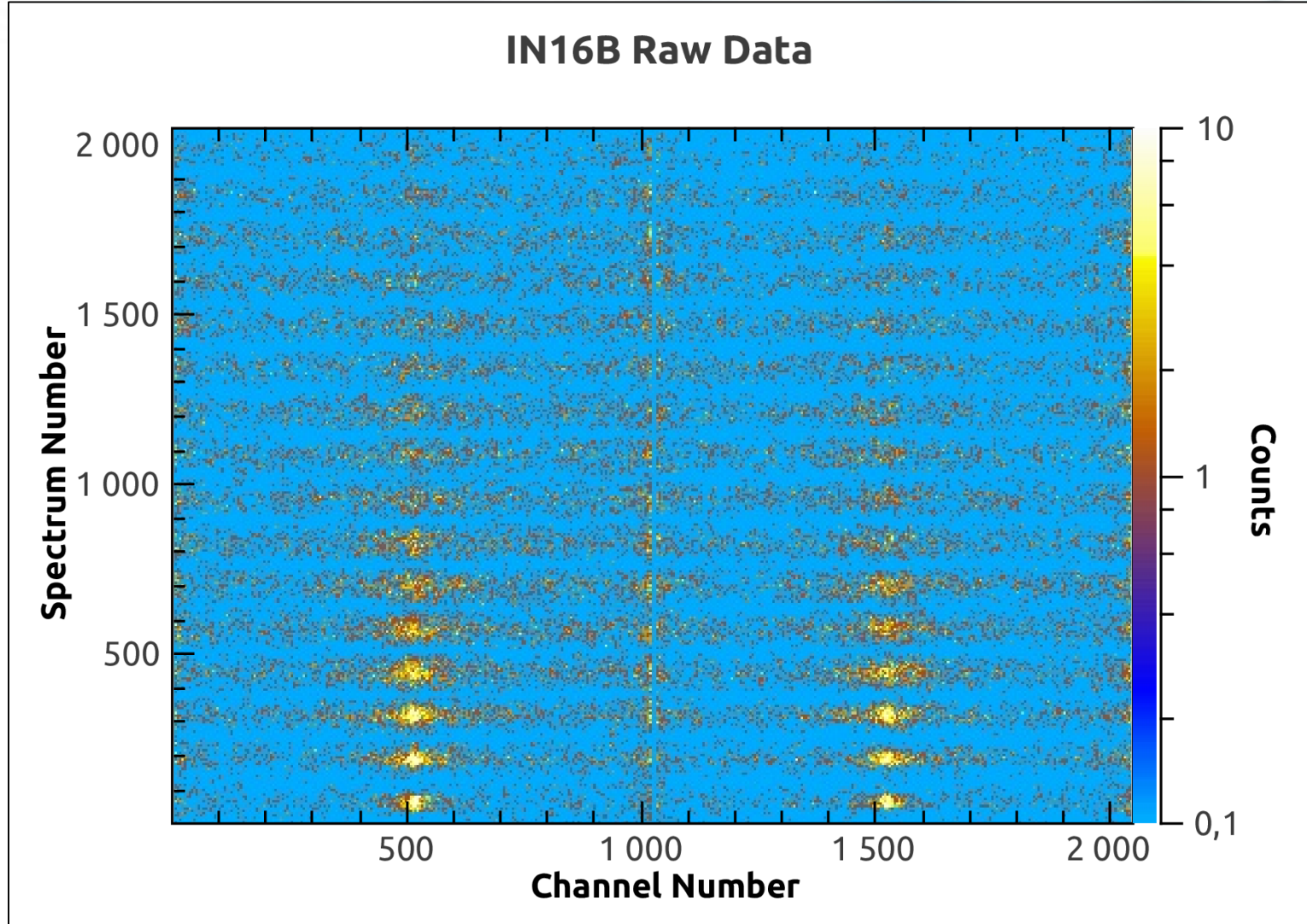
Instrument Definition - IN4 Updated



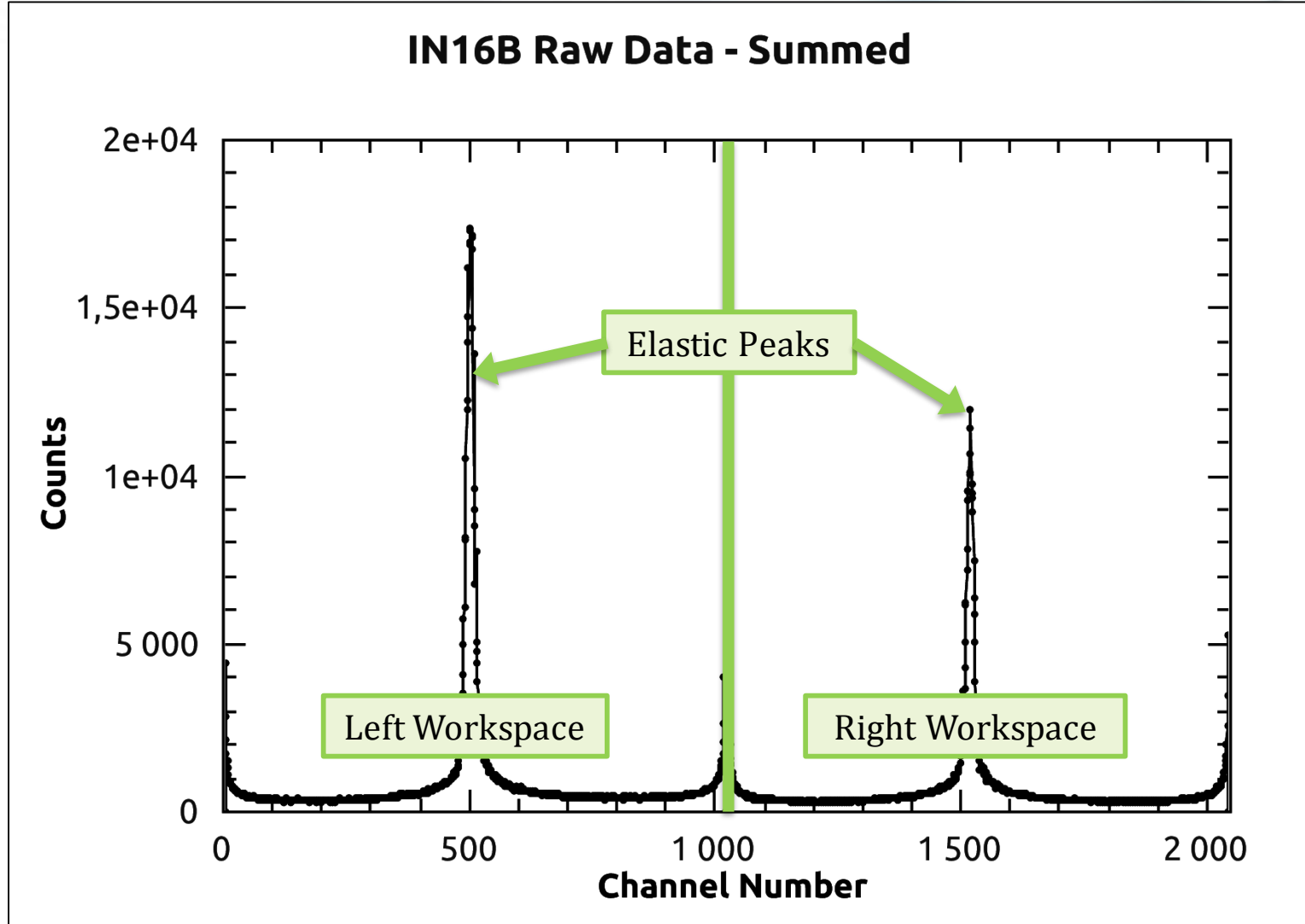
Backscattering Workflow - IN16B



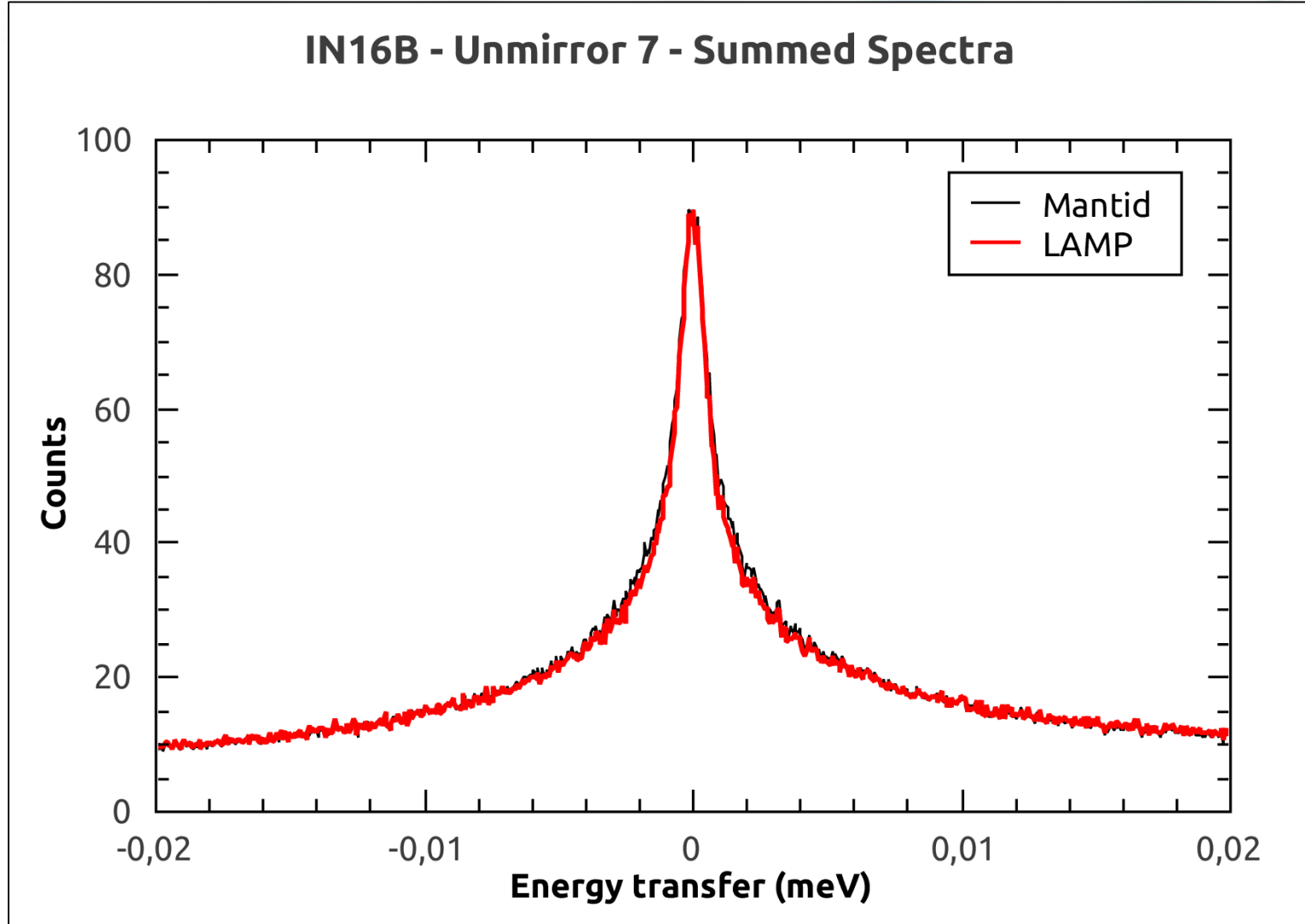
Backscattering Workflow - IN16B



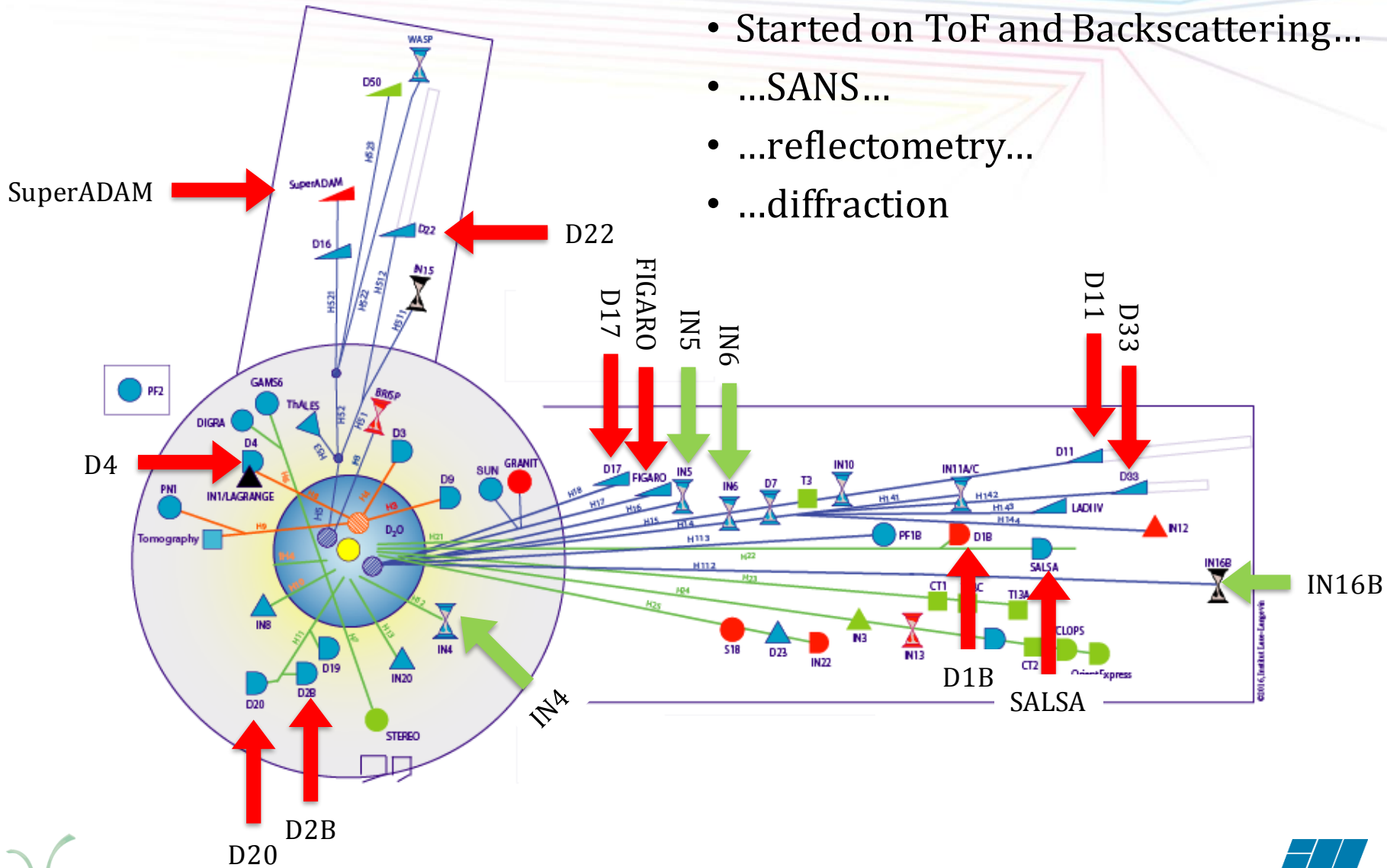
Backscattering Workflow



Backscattering Workflow - Lamp and Mantid



Future Work - ILL Instruments

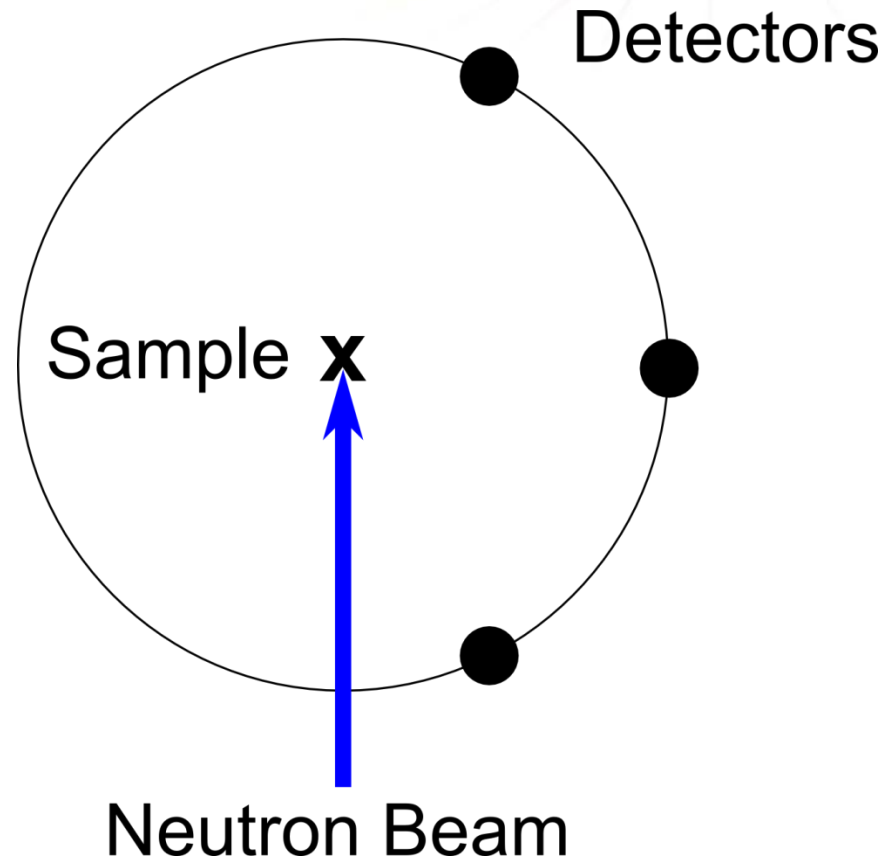


- Started on ToF and Backscattering...
- ...SANS...
- ...reflectometry...
- ...diffraction

Future Work – Scanning Instruments

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

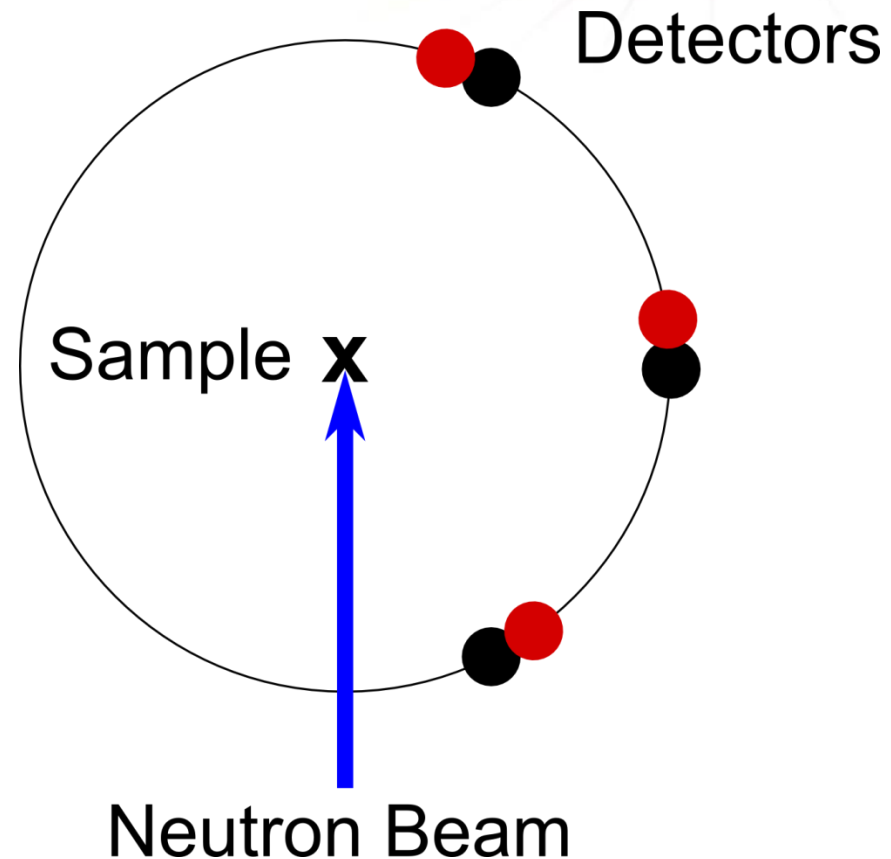
**D2B – Powder
Diffractometer**



Future Work – Scanning Instruments

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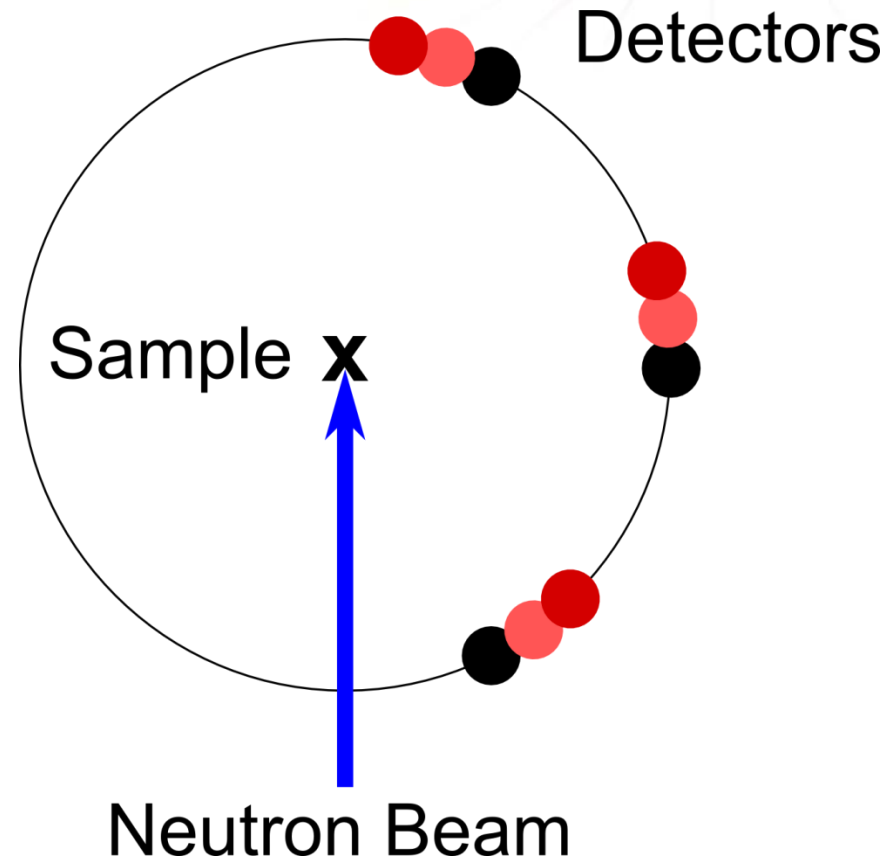
**D2B – Powder
Diffractometer**



Future Work – Scanning Instruments

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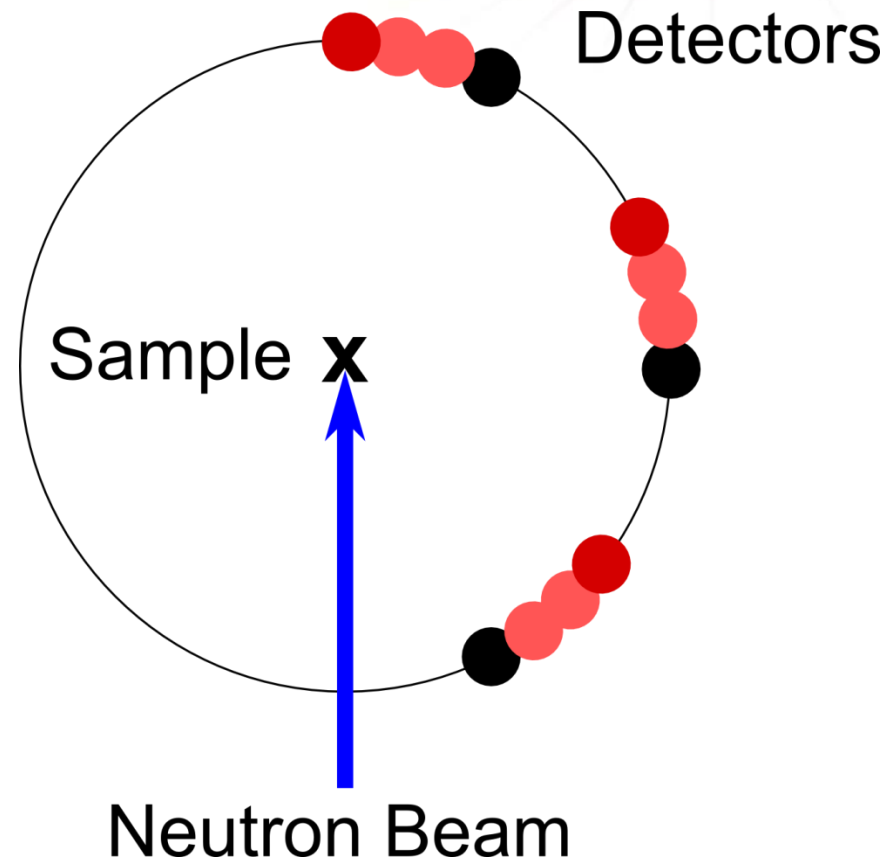
**D2B – Powder
Diffractometer**



Future Work – Scanning Instruments

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

**D2B – Powder
Diffractometer**



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 well under way at the ILL...
- ... but still a long way to go

Thanks for listening!