

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





### **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

























# 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



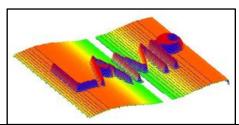


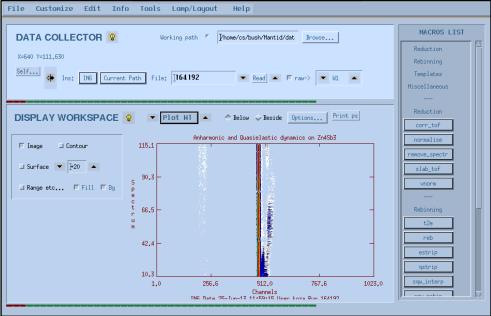
BlueJeans



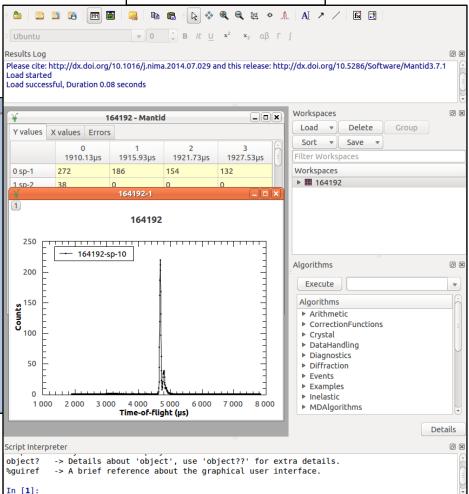


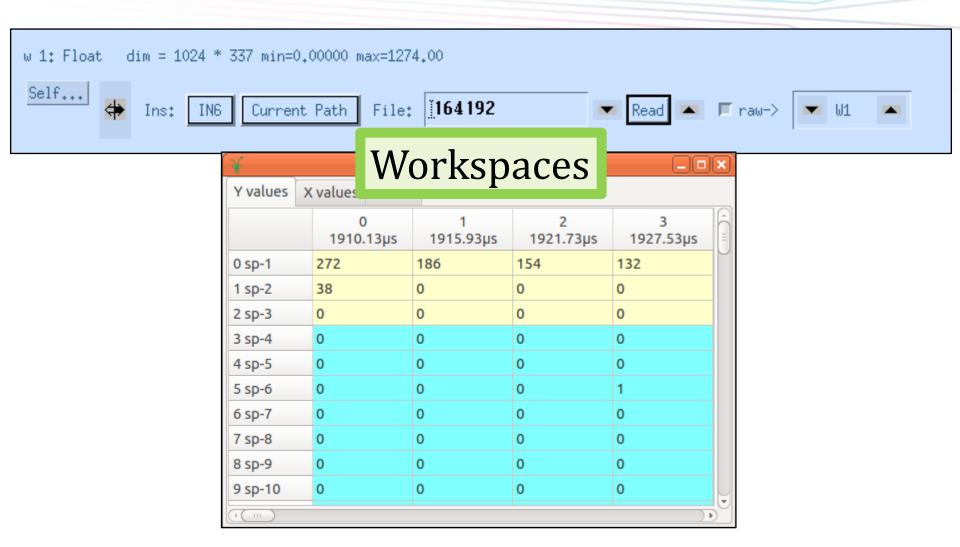






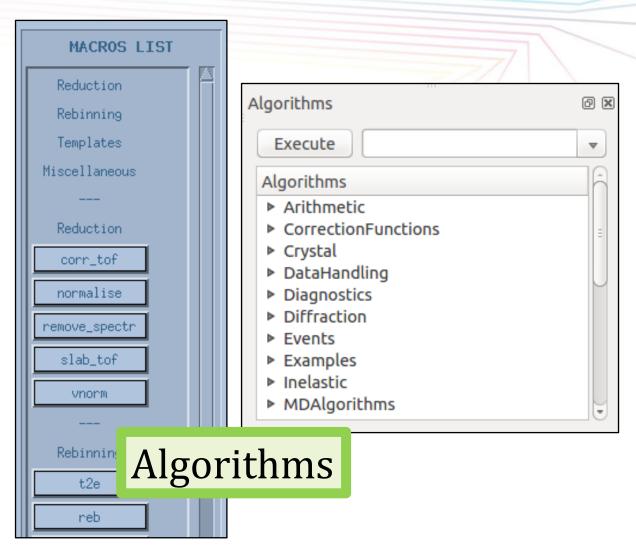






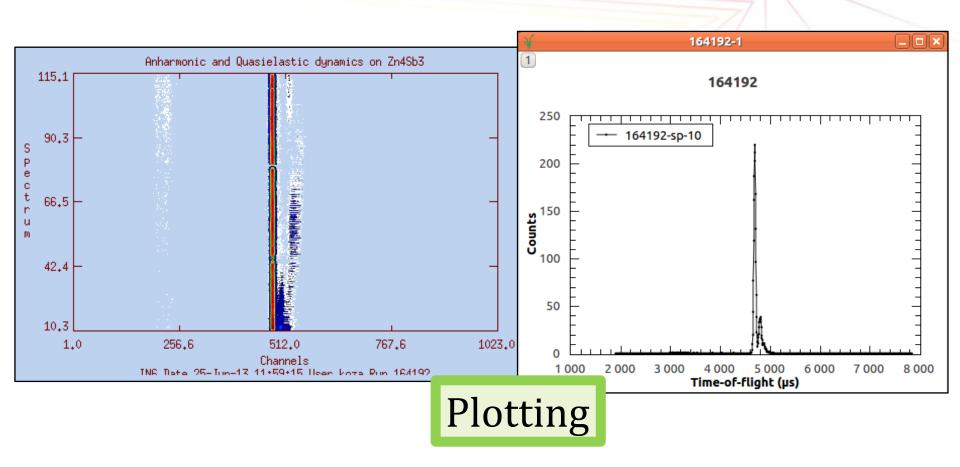
















```
Prox files
         Play all
                       F replace
                                               Browse
                                                                                wilcke-small pixel.pv 💥
:Example of data reduction batch file for IN5:
                                                                                   26 def reduction in6(workspace prefix, custom idf = False, idf path = '', det eff corr = False):
                                                                                       fileRange = [164198, 164200]
₩1 = rdsum(33809,33814) ; read and sum sample runs (300
                                                                                       dataFileNames = []
                                                                                       for i in range(fileRange[0], fileRange[1] + 1):
                                                                                         dataFileNames.append(str(i))
                                                                                  30
w1 = normalise(w1,/monitor)
                                                                                  31
                                                                                       mergedWorkspaceName = workspace prefix + 'data merged'
                                                                                       for file in dataFileNames:
                                                                                  32
                                                                                         fullPath = os.path.join(dataFolder, file + '.nxs')
‰2 = rdsum(33836,33841) ; read 2K data
                                                                                         Load(Filename = fullPath, OutputWorkspace = workspace prefix + file)
                                                                                  34
                                                                                  35
                                                                                         if custom idf:
w2 = normalise(w2,/monitor)
                                                                                  36
                                                                                            LoadInstrument(Workspace=workspace prefix + file, RewriteSpectraMap = True, Filename=idf path)
                                                                                       if len(dataFileNames) > 1:
                                                                                         dataFileNames = [workspace prefix + name for name in dataFileNames]
1ω3 = ω1 − ω2 & see,ω=3,/below,/image
                                                                                         fileNamesToMerge = ', '.join(map(str, dataFileNames))
                                                                                  39
                                                                                         MergeRuns(InputWorkspaces = fileNamesToMerge, OutputWorkspace = mergedWorkspaceName)
                                                                                  40
e^3 = sqrt(e^1^2+e^2^2)
                                                                                   42
                                                                                       vanaRange = [164192, 164194]
                                                                                       vanaFileNames = []
                                                                                   43
rescale phonons to T=10K (detailed balance)
                                                                                       for i in range(vanaRange[0], vanaRange[1] + 1):
                                                                                         vanaFileNames.append(str(i))
                                                                                   45
;w20= rdrun(7271) ; read vanadium run
                                                                                       vanaMergedWorkspaceName = workspace prefix + 'vana merged'
                                                                                       for file in vanaFileNames:
:w20= normalise(w20)
                                                                                         fullPath = os.path.join(dataFolder, file + '.nxs')
                                                                                  49
                                                                                         Load(Filename = fullPath, OutputWorkspace = workspace_prefix + file)
;Normalise w7 to vanadium spectra, integrated between
                                                                                   50
                                                                                       if len(vanaFileNames) > 1:
                                                                                         vanaFileNames = [workspace prefix + name for name in vanaFileNames]
:time channels, 150 and 170
                                                                                  52
                                                                                         fileNamesToMerge = '.'.ioin(map(str. vanaFileNames))
: w8 = vnorm(w7.w20.min=1.max=1024)
                                                                                  53
                                                                                         MergeRuns(InputWorkspaces = fileNamesToMerge, OutputWorkspace = vanaMergedWorkspaceName)
                                                                                  54
                                                                                   55
                                                                                       Integration(InputWorkspace = workspace prefix + 'vana merged', OutputWorkspace = workspace prefix + 'Vana
w10 = remove_spectra(w3,[90,93,95,97,184,215,216,217])
                                                                                       Divide(LHSWorkspace = workspace prefix + 'data merged', RHSWorkspace = workspace prefix + 'Vanadium I',
                                                                                       ReplaceSpecialValues(InputWorkspace = workspace prefix + 'Division', OutputWorkspace = workspace prefix +
                                                                                  57
                                                                                  58
w11= sumbank(w10); Sum angles
                                                                                       if spectraListToMask is not None:
                                                                                  59
                                                                                   60
                                                                                         MaskDetectors(Workspace = workspace prefix + 'Data c', SpectraList = spectraListToMask)
;Correct data for energy dependent detector efficiency, fram
;subtract any time-independent background contribution
                                                                               X size: 312 Y size: 1
                                                                               errors size: 1 monitors size: 3072
;w11= corr tof(w10,/det eff,/frameoverlap,/bkgd)
                                                                               Monitors: (3 1024)
                                                                               Shape of the array DATA: (111,)
;Convert to energy axis and use low-angle multi-detector
                                                                               X size: 111 Y size: 1
                                                                               errors size: 1 monitors size: 3072
;ω12= t2e(ω11,/in5multi)
                                                                               Monitors: (3, 1024)
                                                                               112 111
                                                                               Shape of the array DATA: (312.)
;\omega13= reb(\omega12,dE=0.05); Rebin to constant dE = 0.05
                                                                               X size: 312 Y size: 1
                                                                               errors size: 1 monitors size: 3072
;Extract magnetic signal at lowest angles
                                                                               Monitors: (3, 1024)
; w14 = total(w13(*,0:2),2)
                                                                                jeu. oct. 6 14:05:55 2016: Script execution finished.
;output, w14, file='magnetic.dat'; and output
                                                           Scripting
```



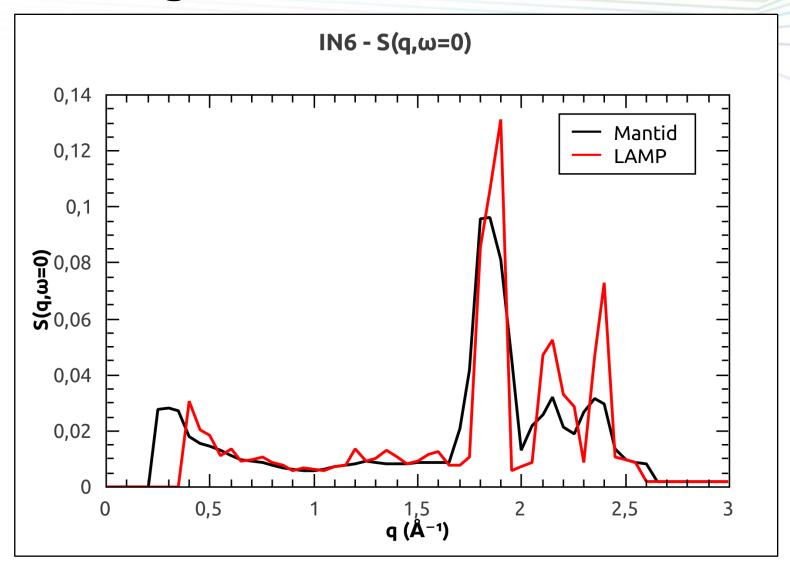


### **ILL Workflows**

- 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



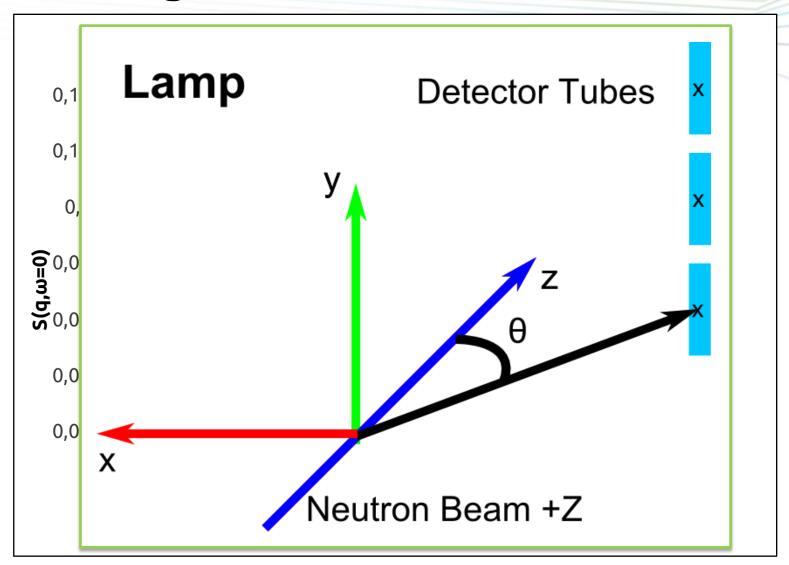
# Time-of-Flight Workflow







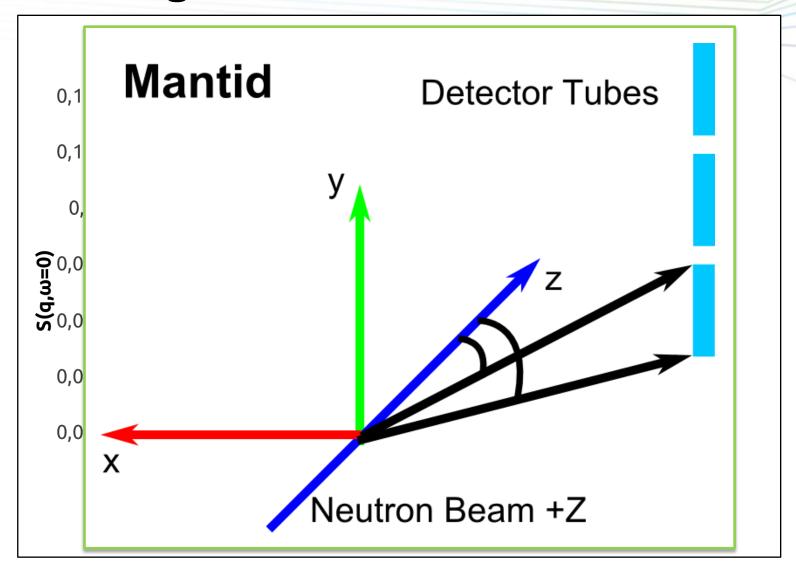
## Time-of-Flight Workflow







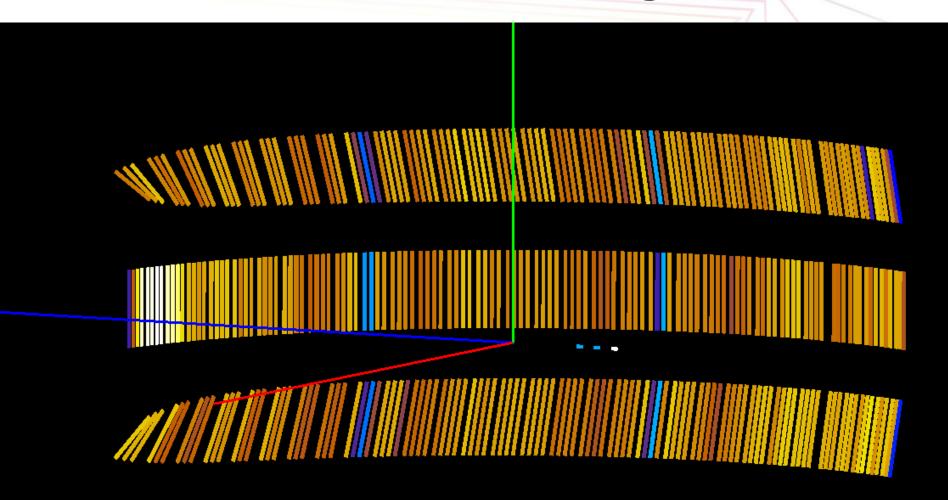
## Time-of-Flight Workflow



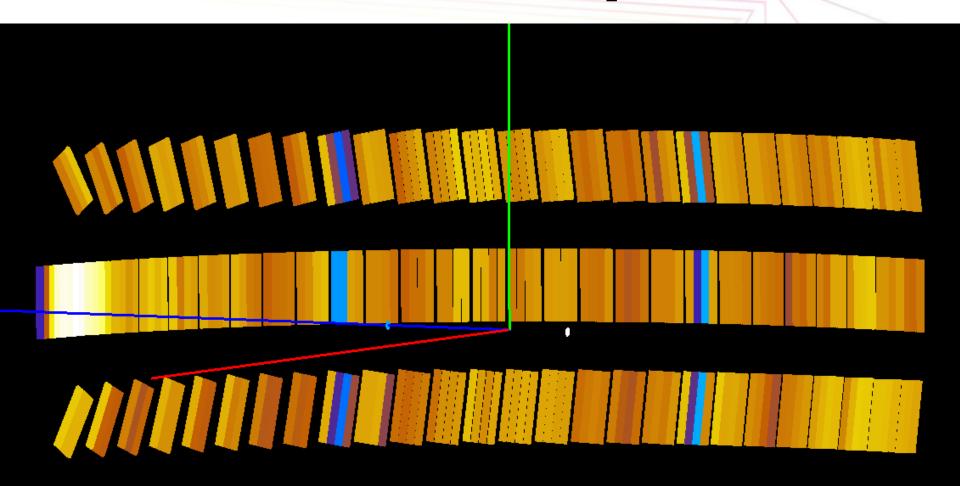




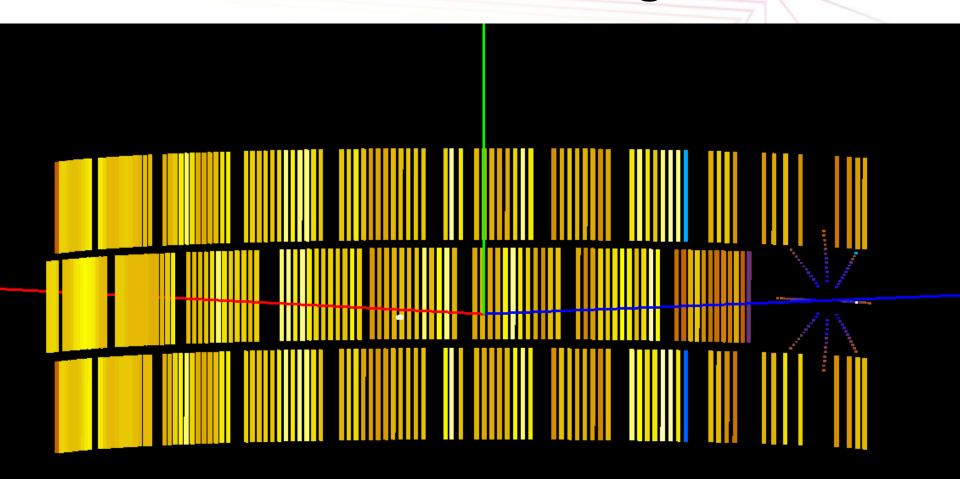
# Time-of-Flight Workflow Instrument Definition – IN6 Original



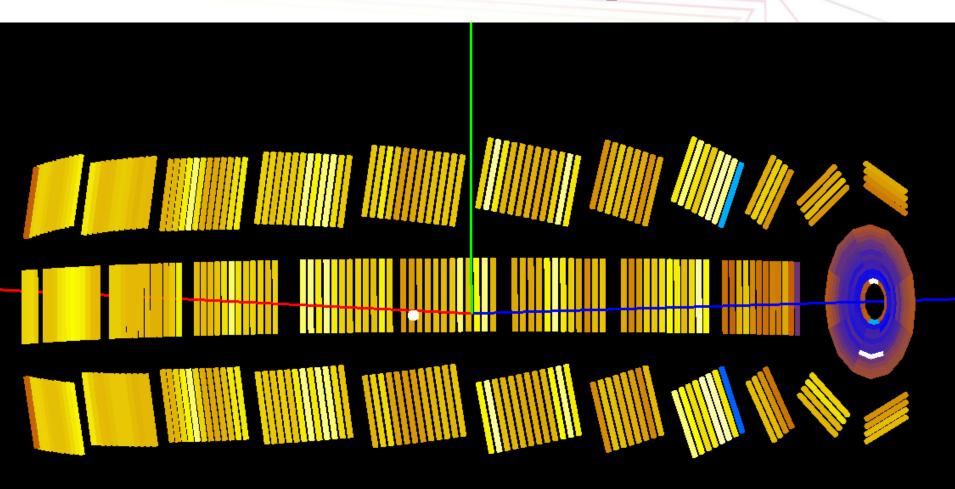
# Time-of-Flight Workflow Instrument Definition – IN6 Updated



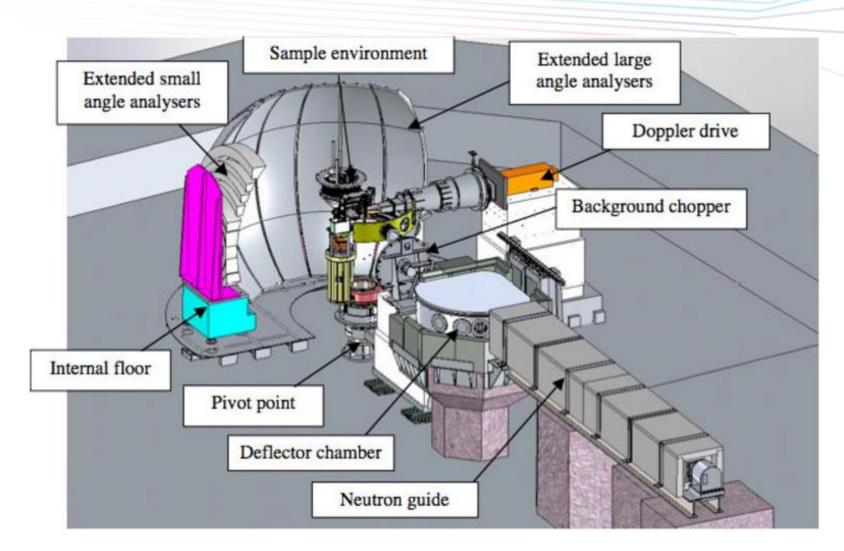
# Time-of-Flight Workflow Instrument Definition – IN4 Original



# Time-of-Flight Workflow Instrument Definition – IN4 Updated



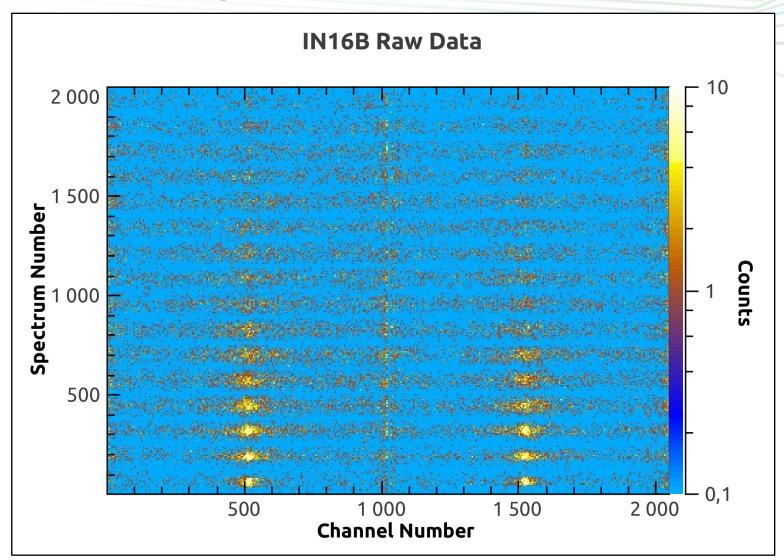
## **Backscattering Workflow - IN16B**







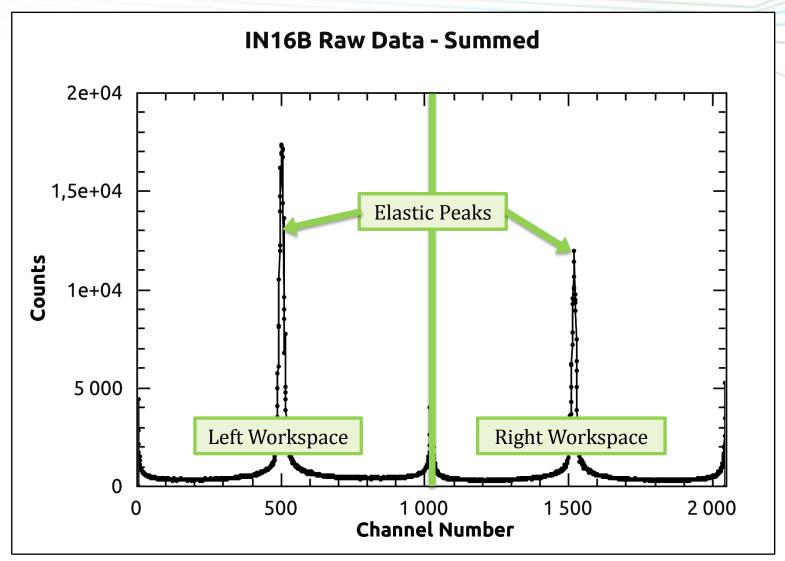
# **Backscattering Workflow - IN16B**







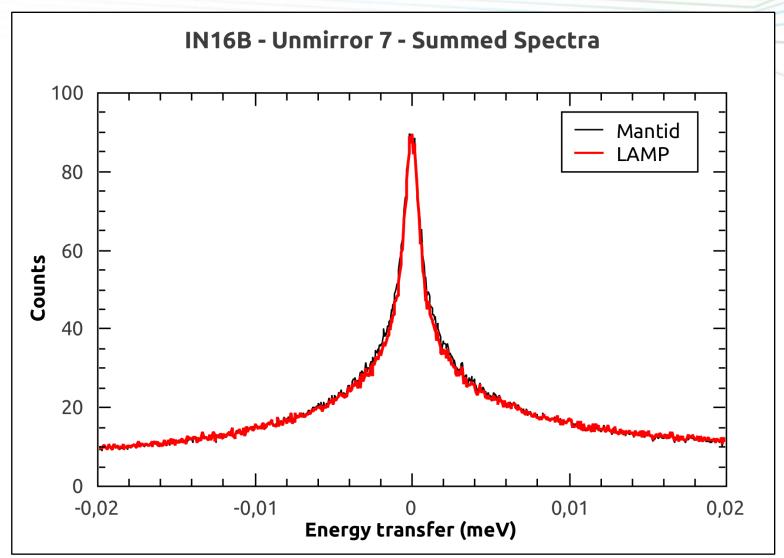
# **Backscattering Workflow**







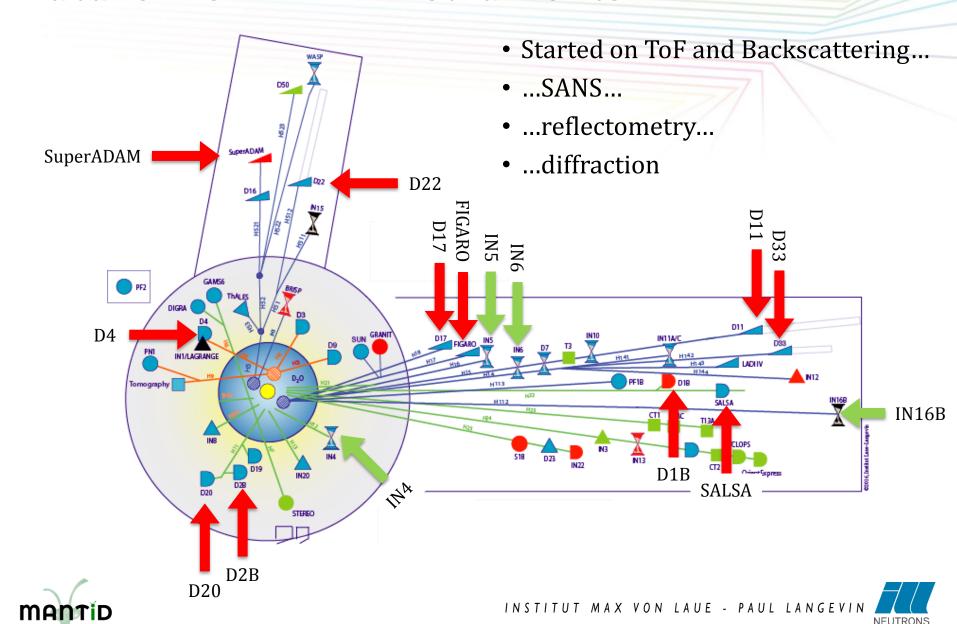
# Backscattering Workflow - Lamp and Mantid



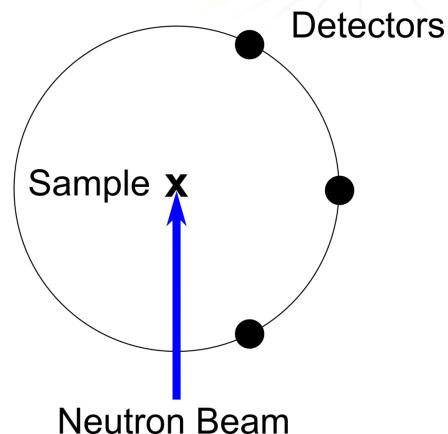




### **Future Work - ILL Instruments**



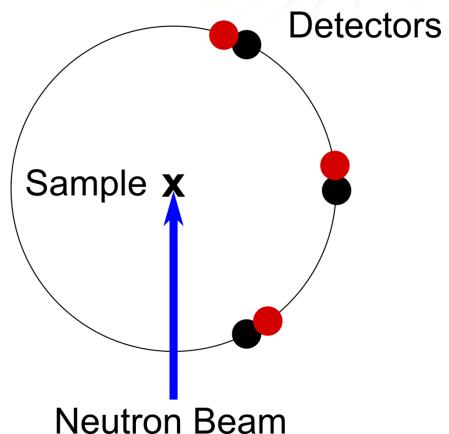
• Support the instruments at ILL with movable detectors, such as D2B, D4, D7 and D16







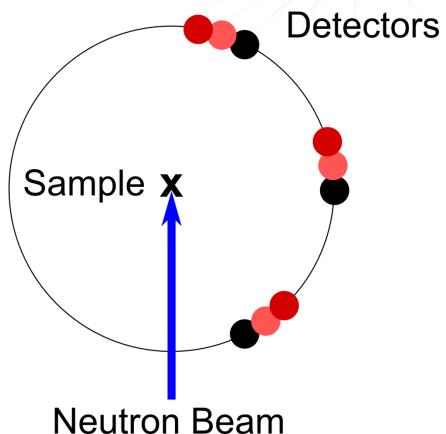
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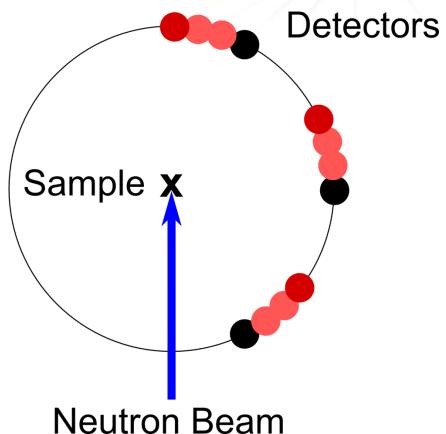
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• Support the instruments at ILL with movable detectors, such as D2B, D4, D7 and D16







## 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!



