

Powder Diffraction Reduction

20.02.17, ILL

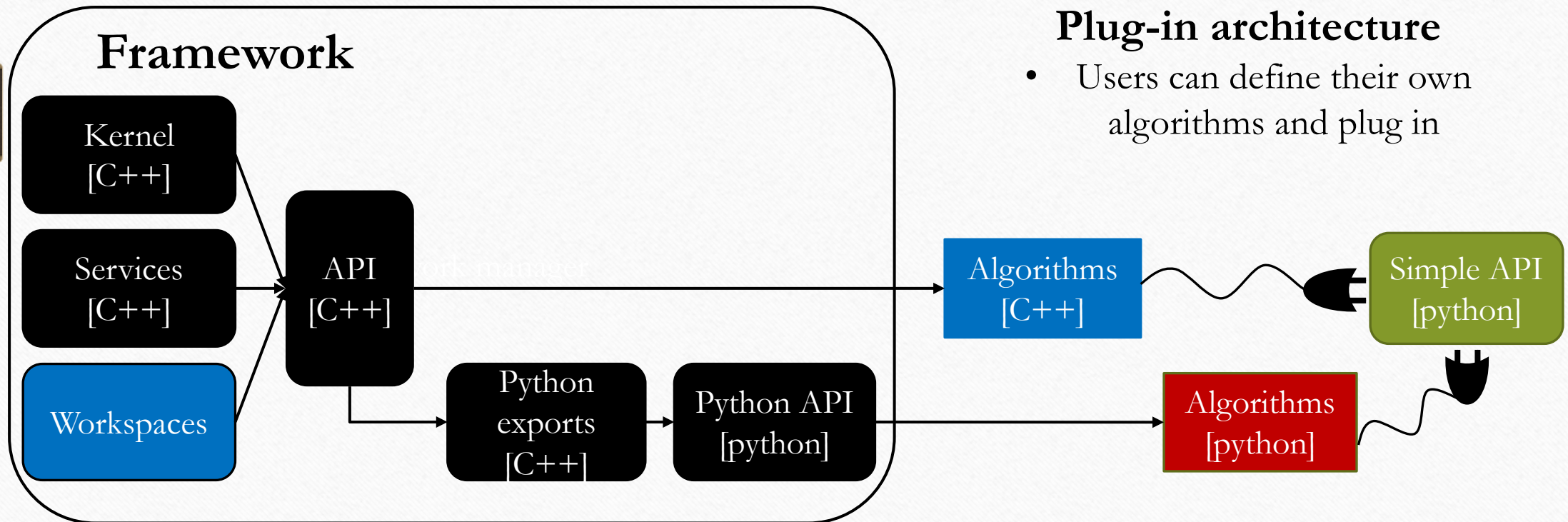
Bastille weekly

Gagik

Outline

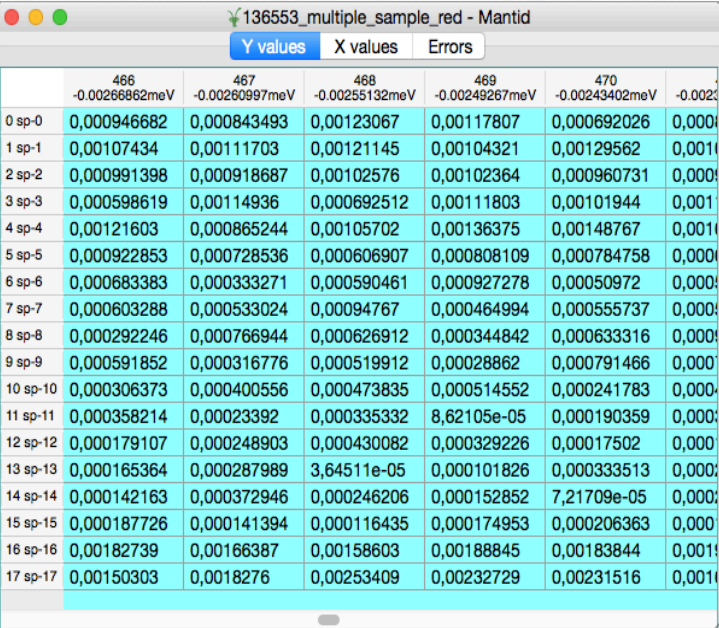
- A (very) short introduction to Mantid
- Reduction workflows in Mantid eco-system
- Instrument definitions for ILL diffractometers
- The new loader for diffraction nexus files

Mantid: the framework, the API, the simpleapi



Workspaces are the 'nouns'

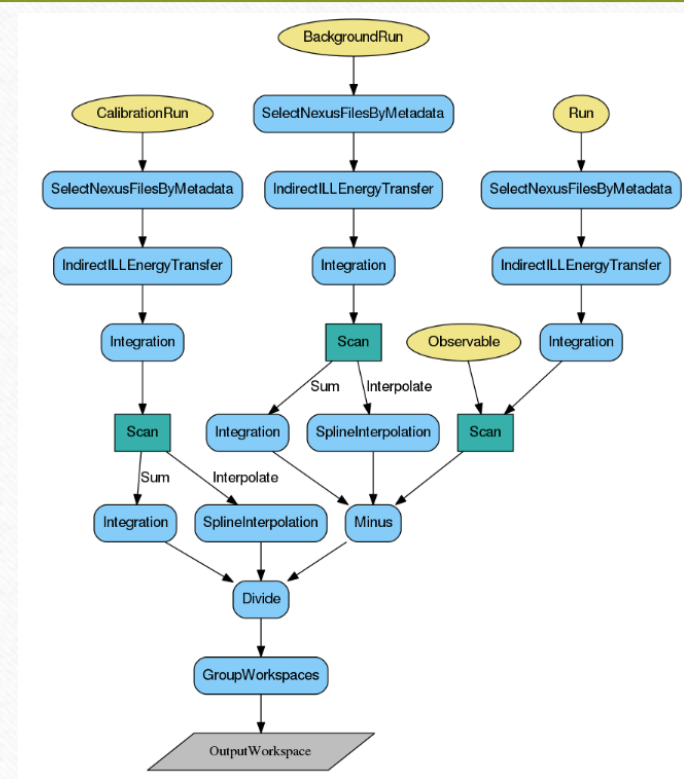
- Workspaces are high-level data structures
 - Holding spectra, histogrammed, event or primitive data
 - Associated metadata
 - Sample logs
 - Algorithm history
 - Virtual instrument geometry – **IDF**
 - A link between instrument components to spectra
- Most common is the **MatrixWorkspace**, which is an array of 1D histograms [linked to the detectors]



	466 -0.00266862meV	467 -0.00260997meV	468 -0.00255132meV	469 -0.00249267meV	470 -0.00243402meV	-0.00237537meV
0 sp-0	0,000946682	0,000843493	0,00123067	0,00117807	0,000692026	0,000633316
1 sp-1	0,00107434	0,00111703	0,00121145	0,00104321	0,00129562	0,00117807
2 sp-2	0,000991398	0,000918687	0,00102576	0,00102364	0,000960731	0,000918687
3 sp-3	0,000598619	0,00114936	0,000692512	0,00111803	0,00101944	0,00101944
4 sp-4	0,00121603	0,000865244	0,00105702	0,00136375	0,00148767	0,00148767
5 sp-5	0,000922853	0,000728536	0,000606907	0,000808109	0,000784758	0,000784758
6 sp-6	0,000683383	0,000333271	0,000590461	0,000927278	0,00050972	0,00050972
7 sp-7	0,000603288	0,000533024	0,00094767	0,000464994	0,000555737	0,000555737
8 sp-8	0,000292246	0,000766944	0,000626912	0,000344842	0,000633316	0,000633316
9 sp-9	0,000591852	0,000316776	0,000519912	0,00028862	0,000791466	0,000791466
10 sp-10	0,000306373	0,000400556	0,000473835	0,000514552	0,000241783	0,000241783
11 sp-11	0,000358214	0,00023392	0,000335332	8,62105e-05	0,000190359	0,000190359
12 sp-12	0,000179107	0,000248903	0,000430082	0,000329226	0,00017502	0,00017502
13 sp-13	0,000165364	0,000287989	3,64511e-05	0,000101826	0,000333513	0,000333513
14 sp-14	0,000142163	0,000372946	0,000246206	0,000152852	7,21709e-05	0,000152852
15 sp-15	0,000187726	0,000141394	0,000116435	0,000174953	0,000206363	0,000206363
16 sp-16	0,00182739	0,00166387	0,00158603	0,00188845	0,00183844	0,00183844
17 sp-17	0,00150303	0,0018276	0,00253409	0,00232729	0,00231516	0,00231516

Algorithms are the 'verbs'

- Algorithms implement high-level data manipulation logic [typically] over workspaces
- Examples can be arithmetic operations, e.g. Integrate, Sum, Transpose, etc..
- **Loaders** [C++] are specialized algorithms, that read data from a file to a workspace
- Algorithms can call other algorithms
- **DataProcessor** [python] algorithms (workflow algorithms) are specialized in calling many other algorithms following some sequence



MantidPlot is the GUI

Log shell

Workspace browser

Workspace matrix view

Plotting window

Instrument view

Ipython shell

Python script editor

Custom interface

Algorithm browser

The screenshot displays the MantidPlot GUI with several windows and panels. Red arrows point from labels on the left to specific components in the GUI:

- Log shell:** Points to the top status bar area.
- Workspace browser:** Points to the 'Workspaces' panel on the left, which shows a list of workspaces including 'sample_red'.
- Workspace matrix view:** Points to the 'Matrix' view of the 'sample_red' workspace, showing a table of data.
- Plotting window:** Points to the '136553_multiple_sample_red' plot window, which displays a peak at 0 energy transfer.
- Instrument view:** Points to the 'Instrument' panel, which shows the 'IN16B' instrument and 'silicon' analyser.
- Ipython shell:** Points to the 'Python Window' at the bottom, which contains a prompt and some text.
- Python script editor:** Points to the 'Python Window' at the bottom, which contains a prompt and some text.
- Custom interface:** Points to the 'Indirect Data Reduction' dialog box, which has tabs for 'ILL Energy Tra...', 'ILL Calibr...', 'Transmis...', 'Symme...', 'S(...)', and 'Mom...'. It includes fields for 'Run File', 'Reduction Type' (QENS, E/I - FWS), 'Detector Grouping' (Default, Choose Range, Choose File), 'Background Subtraction' (Background File, Scaling Factor), and 'Detector Calibration' (Calibration File, Peak Range).
- Algorithm browser:** Points to the 'Algorithms' panel on the right, which lists various algorithms such as 'Arithmetic', 'CorrectionFunctions', 'Crystal', 'DataHandling', 'Diagnostics', 'Diffraction', 'Events', 'Examples', 'Inelastic', 'MDAAlgorithms', 'Muon', 'Optimization', 'Reflectometry', 'SANS', 'SINQ', 'Sample', 'Simulation', 'Transforms', 'Utility', and 'Workflow'.

	Y values	X values	Errors
0 sp-0	0.000946682	0.000843493	0.00123067
1 sp-1	0.00107434	0.00111703	0.00121145
2 sp-2	0.000991398	0.000918687	0.00102576
3 sp-3	0.000598619	0.00114936	0.000692512
4 sp-4	0.00121603	0.000865244	0.00105702
5 sp-5	0.000922853	0.000728536	0.000606907
6 sp-6	0.000683383	0.000333271	0.000590461
7 sp-7	0.000603288	0.000533024	0.00094767
8 sp-8	0.000292246	0.000766944	0.000626912
9 sp-9	0.000591852	0.000316776	0.000519912
10 sp-10	0.000306373	0.000480556	0.000473835

```
object? -> Details about 'object', use 'object??' for extra details.
%gui?ref -> A brief reference about the graphical user interface.
In [1]:
```

Instrument View

Legend:

Z-axis, parallel to incoming beam direction

Y-axis, points to top

X-axis, right handed system

Sample is at 0,0,0

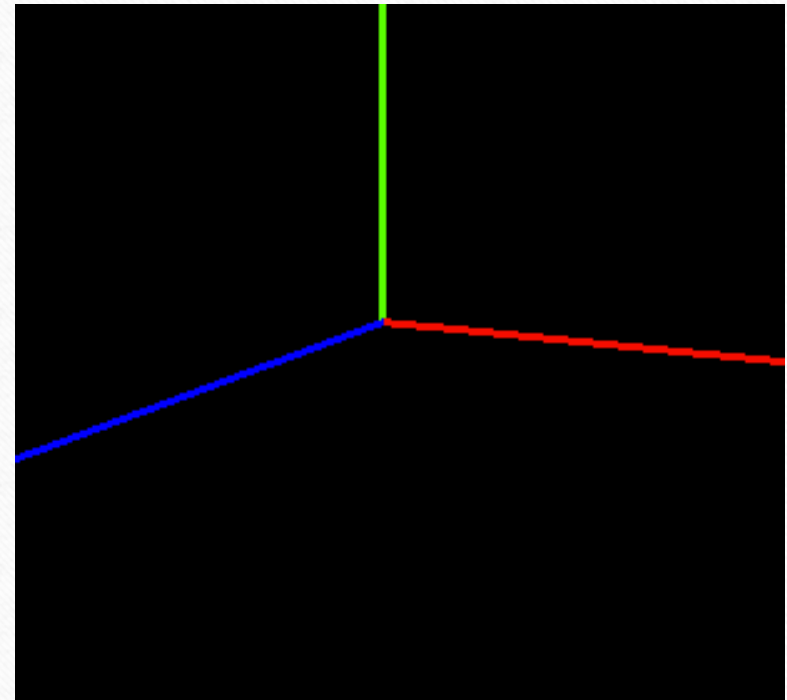
L1 = source to sample

L2 = sample to detector surface

} Critical in TOF mode

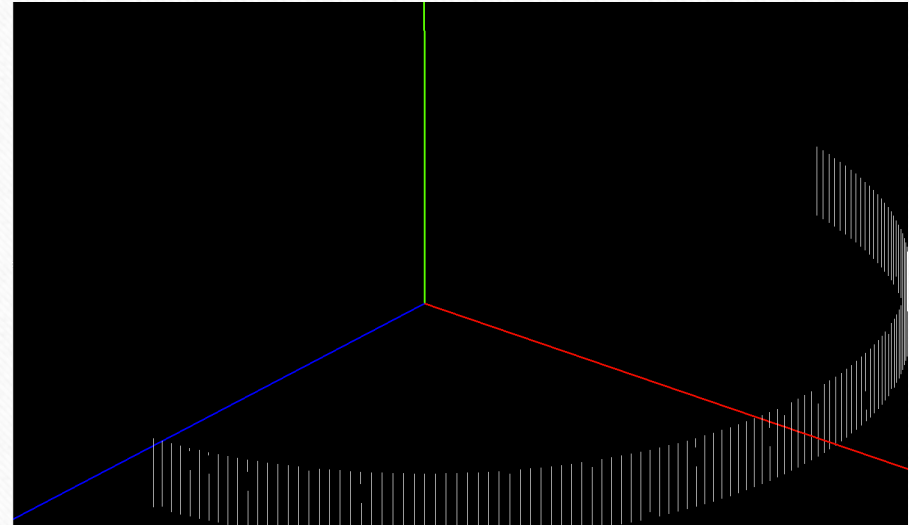
Critical for diffraction is 2θ spacing

- The geometry of the entire ensemble of the detector components is defined statically in IDF file (.xml).
- Can be moved/rotated as needed from the code.



D2B

- Definition existed already
- **Monitor is missing**
- 128 evenly spaced tubes
- $5^\circ < 2\theta < 165^\circ$

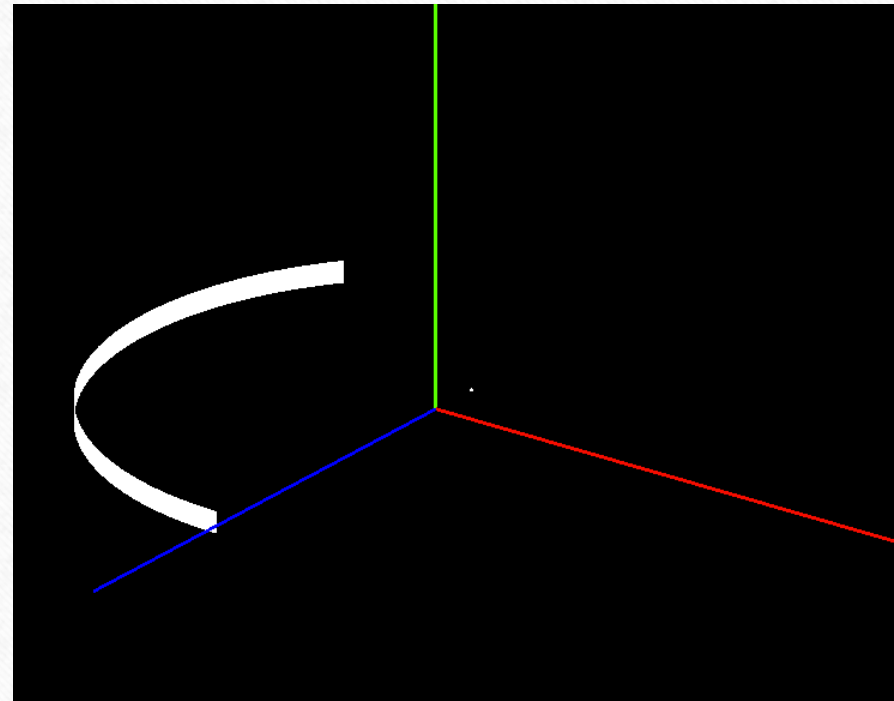


D1B

- $L2 = 1.5\text{m}$
- 1280 cuboid cells with height of 0.1m
- Width is such, that each cell covers $\sim 0.1^\circ$ in 2θ
- Each cell is facing the sample
- $0.8^\circ < 2\theta < 128.8^\circ$

L1 = ?

Monitor = ?

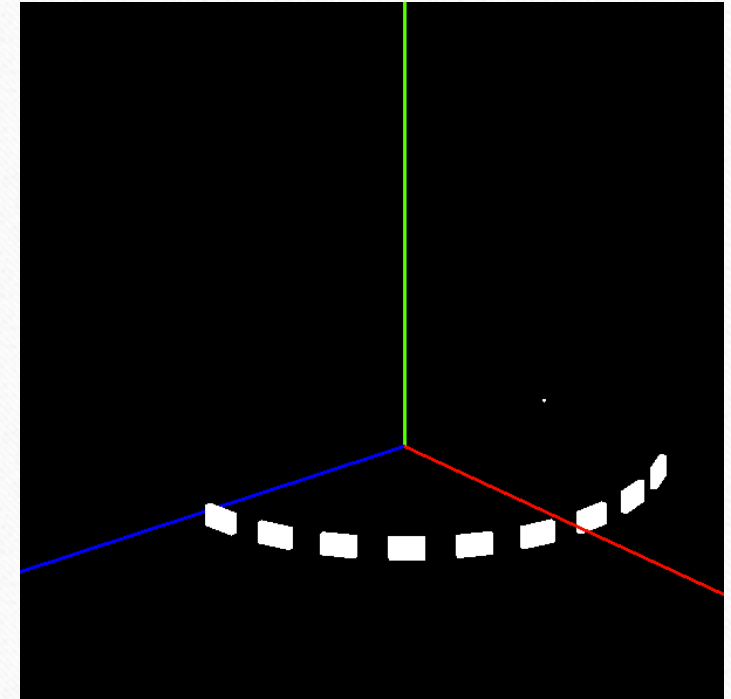


D4

- $L2 = 1.146\text{ m}$
- 9 flat panels in polygonal arrangement, facing the sample
- Each panel covers 8° , gap between two panels is 7°
- Each panel has 64 evenly spaced cuboid cells, $\sim 0.125^\circ$ each
- $1.5^\circ < 2\theta$

L1 = ?

Monitor = ?



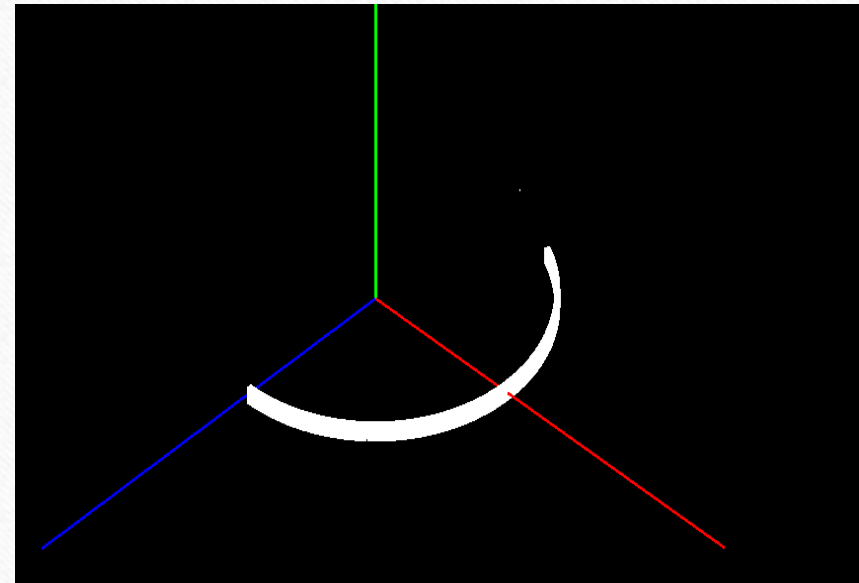
D20

- $L2 = 1.471\text{m}$
- 48 flat panels in polygonal arrangement
- Panels facing the sample
- Each panel has 32 cuboid cells of width 0.002568m
- Each cell covers $\sim 0.1^\circ$
- $0 < 2\theta < 153.6$
- $L1 = 3.2\text{m}$
- Monitor = 2m

The detector cells can be virtually split into 2 or 3 by DAQ.

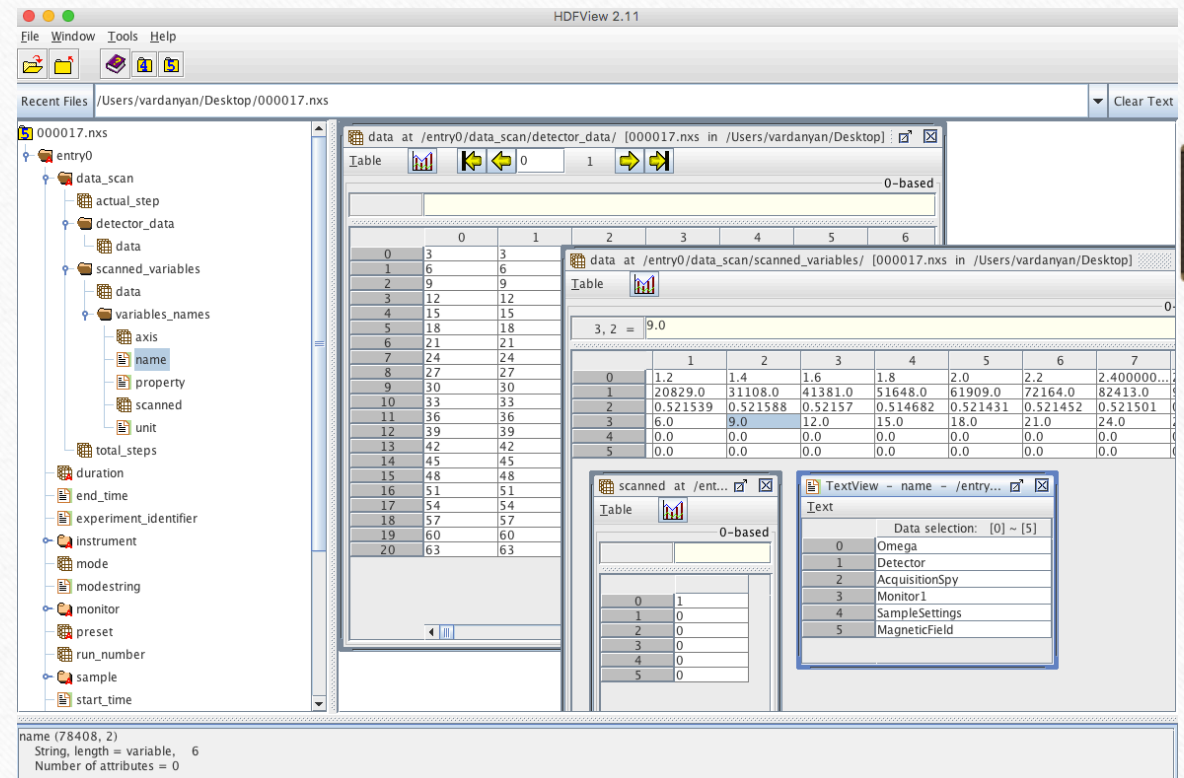
Need to create 3 alternative definitions; D20a, D20b, D20c and load correspondingly.

Does this apply to other instruments as well?



LoadILLDiffraction

- New nexus files produced last week, same format for all diffractometers
- Scanned data stored into one file
- Using some features beyond nexus
- Loader is sketched now
- We are able to read those into Mantid
 - Little technical problem still to sort out concerning the '**NX_class**' attribute



To do

- Finalize and ship the IDFs
- Continue work on the loader
 - Implement the scanning of the detector (Ian)
 - Sample orientation, and other scans
 - Decide on output format (workspace or workspace group?, axes, units)
- When the loader matures, meet to discuss in detail the reduction flow (powder diffraction first)