Powder Diffraction Reduction

20.02.17, ILL

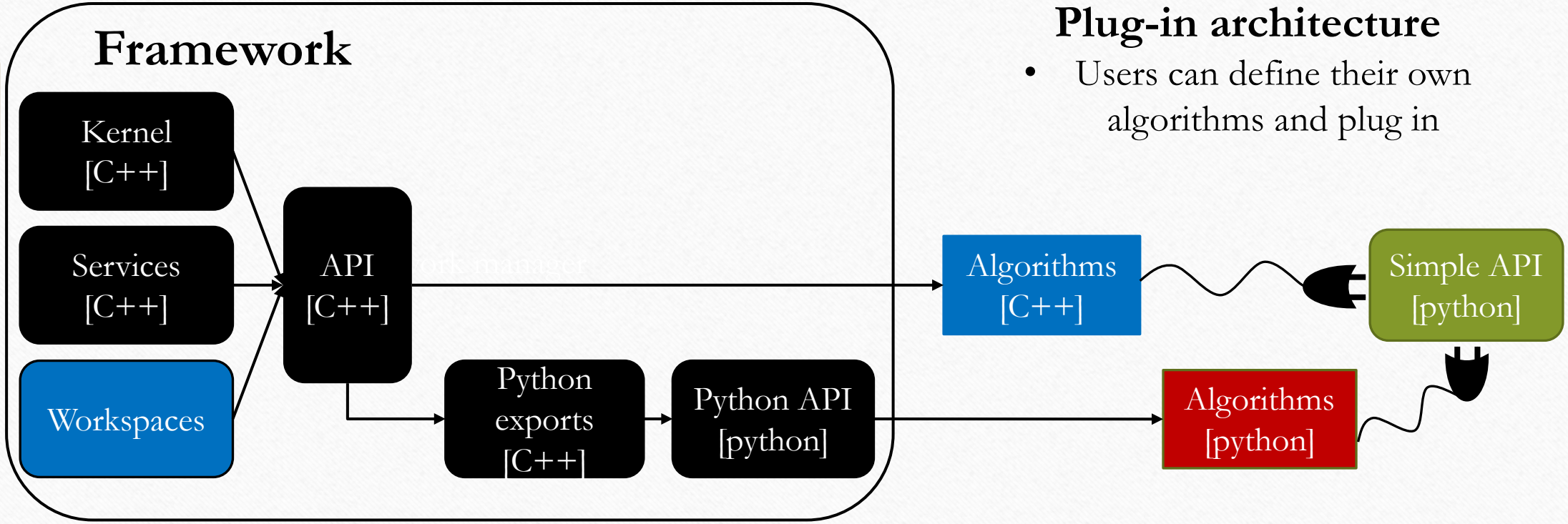
Bastille weekly

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

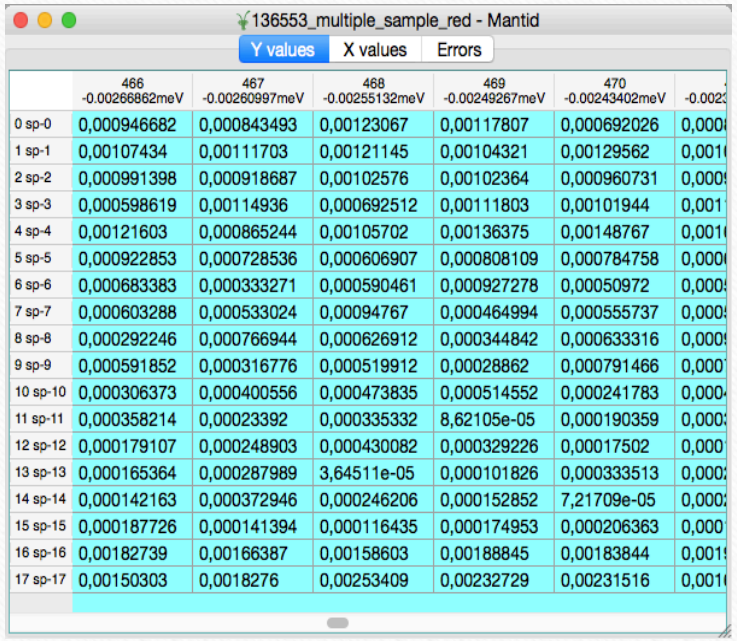


Plug-in architecture

- Users can define their own algorithms and plug in

Workspaces are the 'nouns'

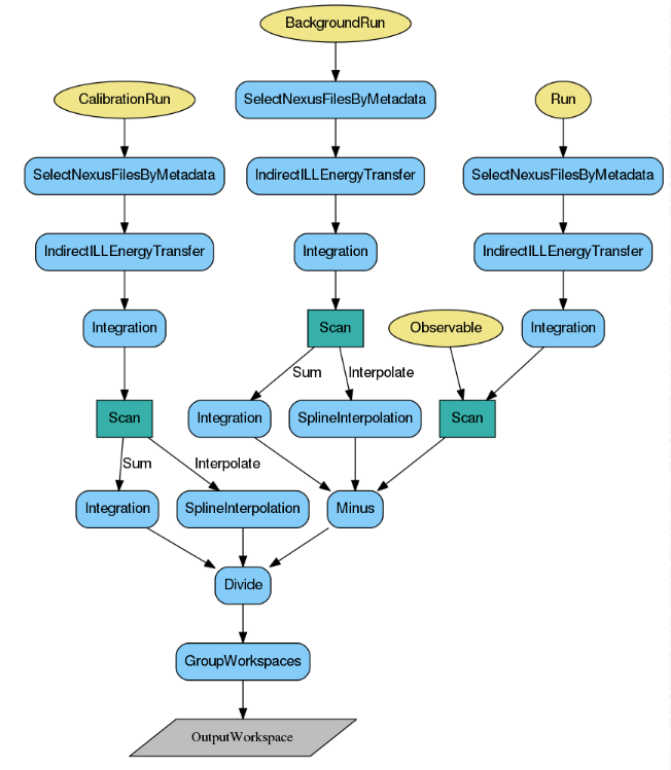
- Workspaces are high-level data structures
  - Holding spectra, histogrammed, event or primitive data
  - Associated metadata
    - Sample logs
    - Algorithm history
  - Virtual instrument geometry – **IDF**
  - A link between instrument components to spectra
- Most common is the **MatrixWorkspace**,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



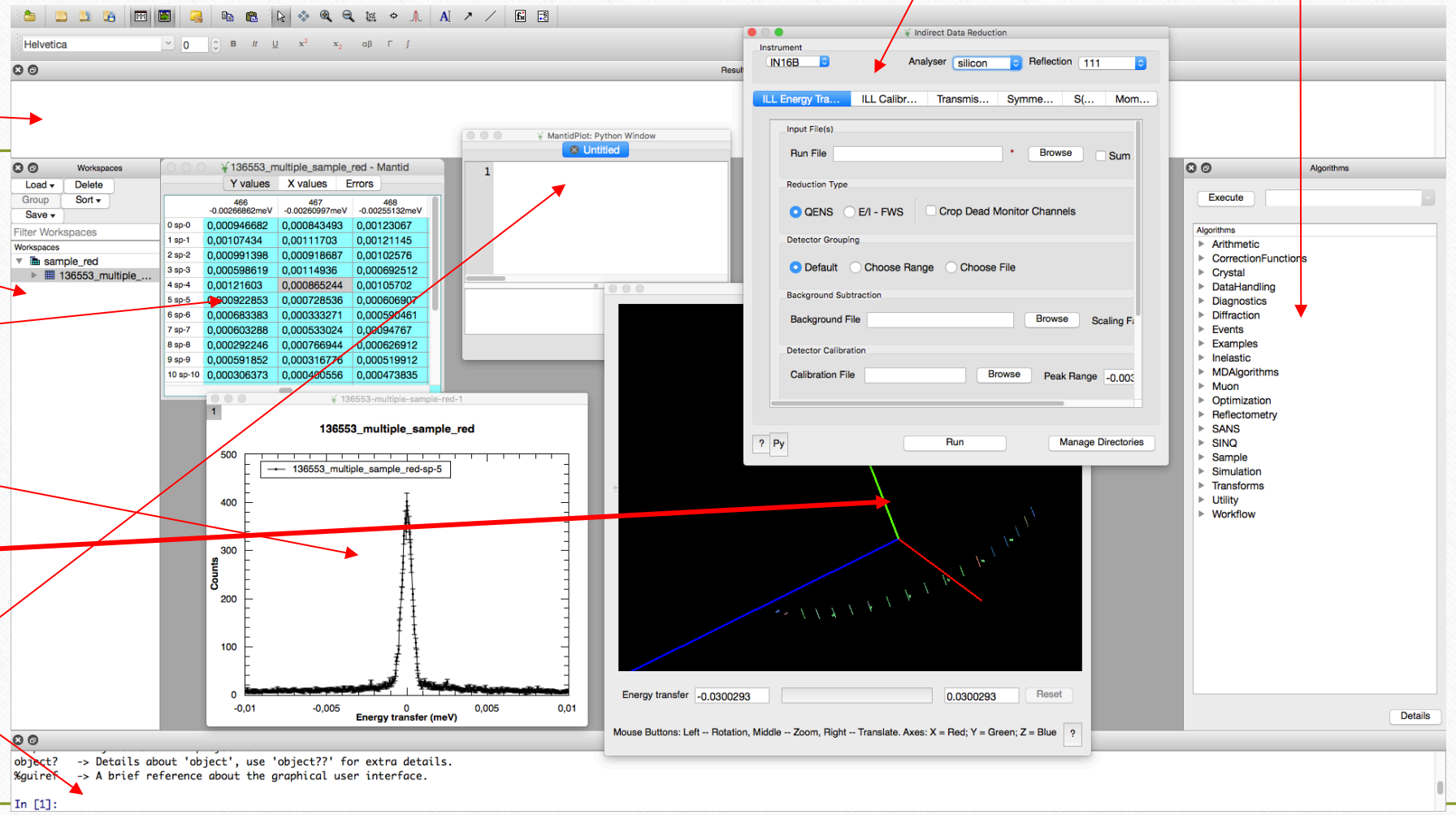
	466 -0.00266862meV	467 -0.00260997meV	468 -0.00255132meV	469 -0.00249267meV	470 -0.00243402meV	-0.0023
0 sp-0	0,000946682	0,000843493	0,00123067	0,00117807	0,000692026	0,000
1 sp-1	0,00107434	0,00111703	0,00121145	0,00104321	0,00129562	0,001
2 sp-2	0,000991398	0,000918687	0,00102576	0,00102364	0,000960731	0,000
3 sp-3	0,000598619	0,00114936	0,000692512	0,00111803	0,00101944	0,001
4 sp-4	0,00121603	0,000865244	0,00105702	0,00136375	0,00148767	0,001
5 sp-5	0,000922853	0,000728536	0,000606907	0,000808109	0,000784758	0,000
6 sp-6	0,000683383	0,000333271	0,000590461	0,000927278	0,00050972	0,000
7 sp-7	0,000603288	0,000533024	0,00094767	0,000464994	0,000555737	0,000
8 sp-8	0,000292246	0,000766944	0,000626912	0,000344842	0,000633316	0,000
9 sp-9	0,000591852	0,000316776	0,000519912	0,00028862	0,000791466	0,000
10 sp-10	0,000306373	0,000400556	0,000473835	0,000514552	0,000241783	0,000
11 sp-11	0,000358214	0,00023392	0,000335332	8,62105e-05	0,000190359	0,000
12 sp-12	0,000179107	0,000248903	0,000430082	0,000329226	0,00017502	0,000
13 sp-13	0,000165364	0,000287989	3,64511e-05	0,000101826	0,000333513	0,000
14 sp-14	0,000142163	0,000372946	0,000246206	0,000152852	7,21709e-05	0,000
15 sp-15	0,000187726	0,000141394	0,000116435	0,000174953	0,000206363	0,000
16 sp-16	0,00182739	0,00166387	0,00158603	0,00188845	0,00183844	0,001
17 sp-17	0,00150303	0,0018276	0,00253409	0,00232729	0,00231516	0,001

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



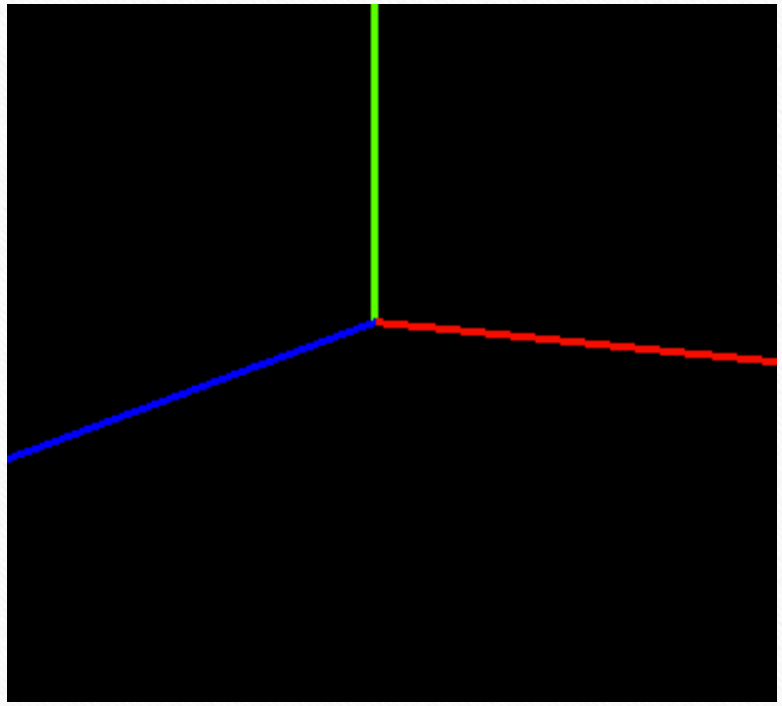
Instrument View

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

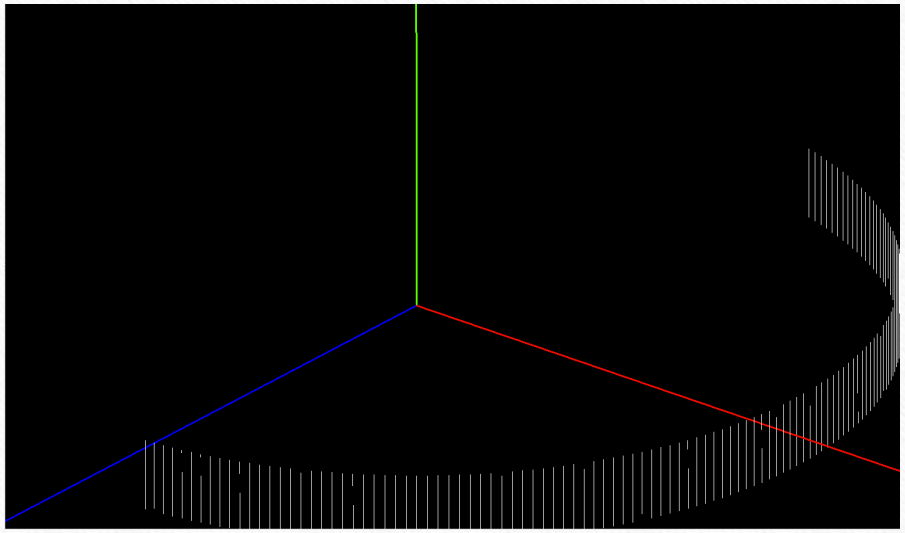
Critical for diffraction is 2θ spacing

- 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

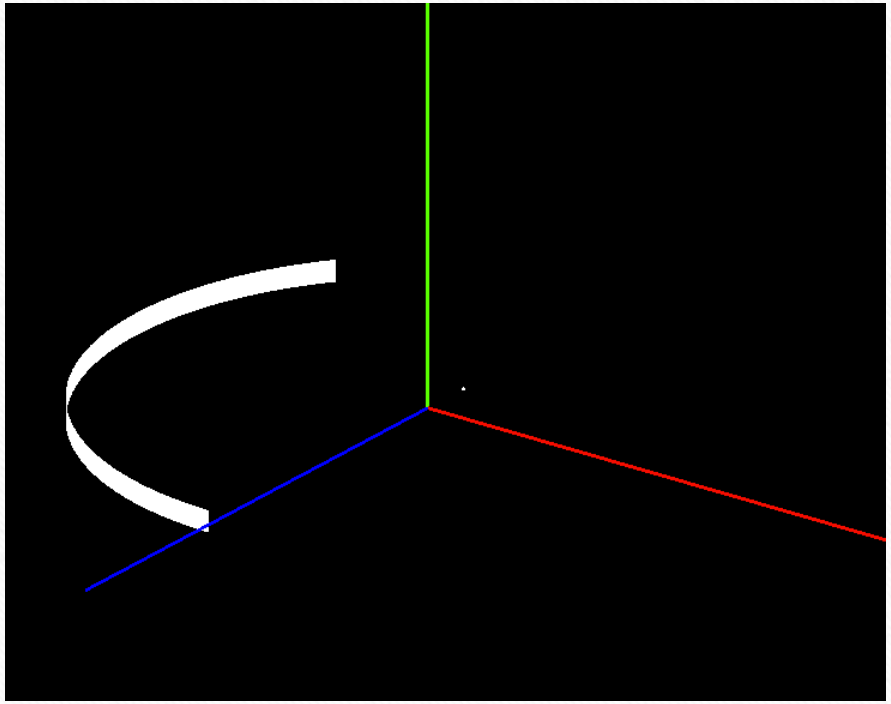
- Definition existed already
- **Monitor is missing**
- 128 evenly spaced tubes
- $5° < 2\theta < 165°$



D1B

- L2 = 1.5m
- 1280 cuboid cells with height of 0.1m
- Width is such, that each cell covers ~0.1^0 in 2θ
- Each cell is facing the sample
- $0.8^0 < 2\theta < 128.8^0$

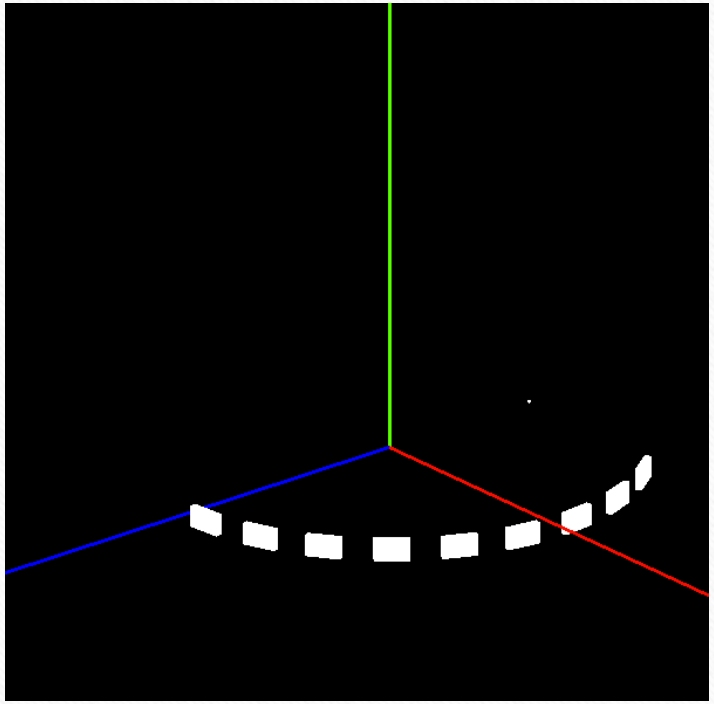
L1 = ?
Monitor = ?



D4

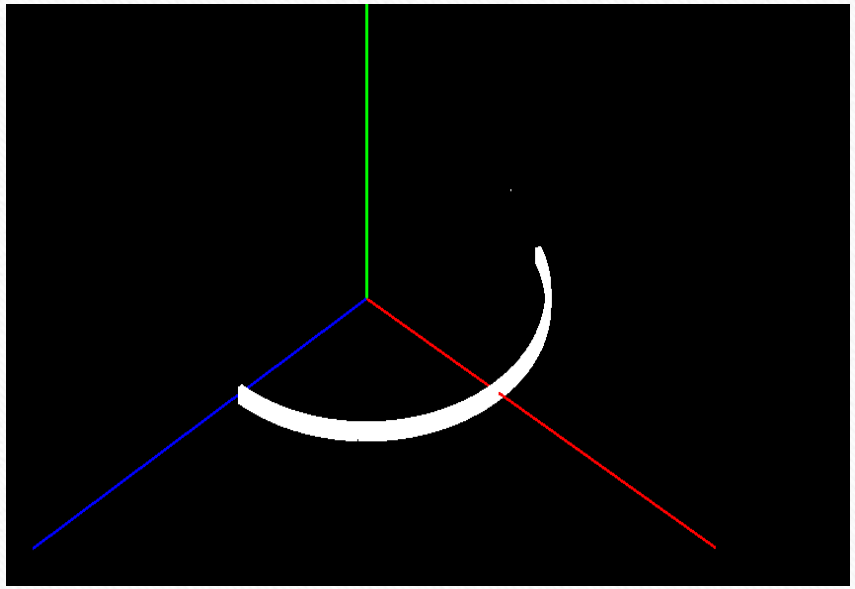
- L2 = 1.146m m
- 9 flat panels in polygonal arrangement, facing the sample
- Each panel covers 8^0, gap between two panels is 7^0
- Each panel has 64 evenly spaced cuboid cells, ~0.125^0 each
- $1.5^0 < 2\theta$

L1 = ?
Monitor = ?



D20

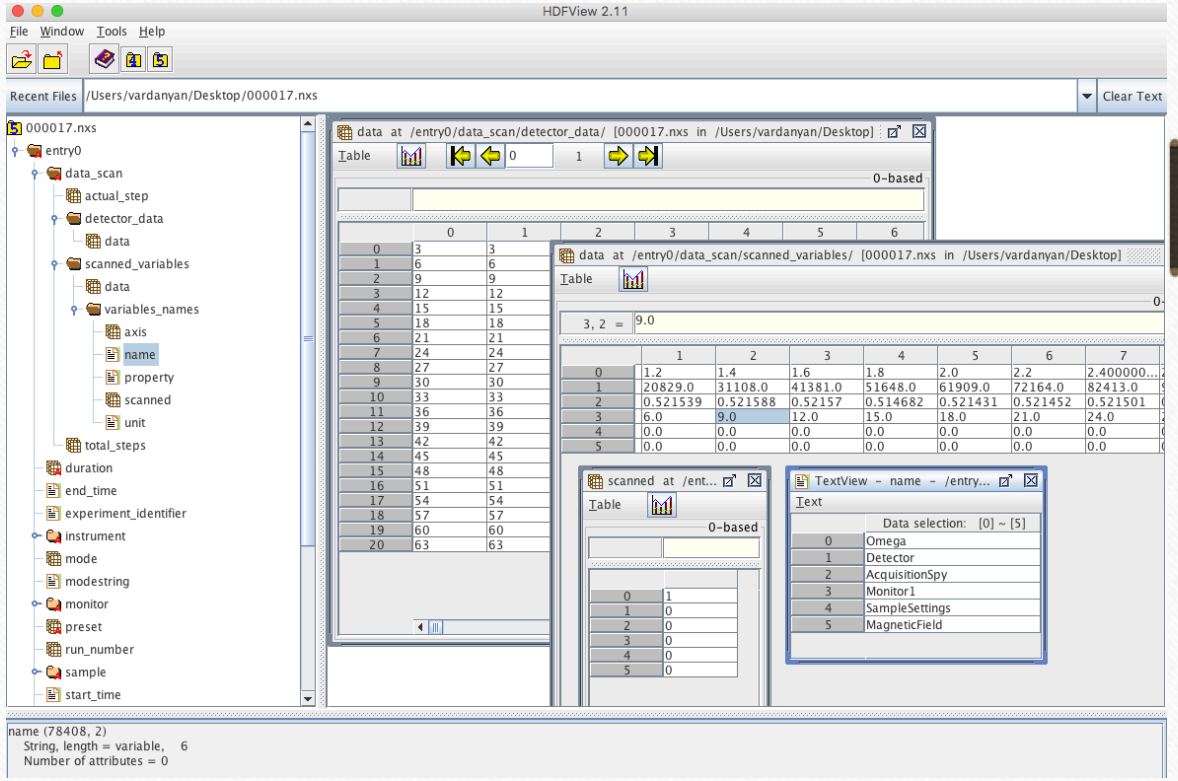
- L2 = 1.471m
- 48 flat panels in polygonal arrangement
- Panels facing the sample
- Each panel has 32 cuboid cells of width 0.002568m
- Each cell covers ~0.1^0
- $0 < 2\theta < 153.6$
- L1 = 3.2m
- Monitor = 2m



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)