Powder Diffraction Reduction

Status Update

16.11.17, ILL

News since last meeting

- Large refactor of the calibration algorithm
  - Better organization of the code
  - Important speed-up (~1min max)
- Interpolation of overlapping 2theta angles
- ROI normalisation for calibration
- Fixed the exclusion regions for calibration

Open questions

Rebinning of the temperature axis

- Currently Rebin is used which is designed for histogram data
- It is not correct for non-equidistant points
- How exactly we want to group our points?
- New algorithm GroupPointData?

Picking up the scanning observable

- Currently this has to be typed by the user
- User should choose e.g. from [sample.temperature, Omega.Position]
- Can we define the most common parameters, and suggest a list?
- Can we make this fully automatic?

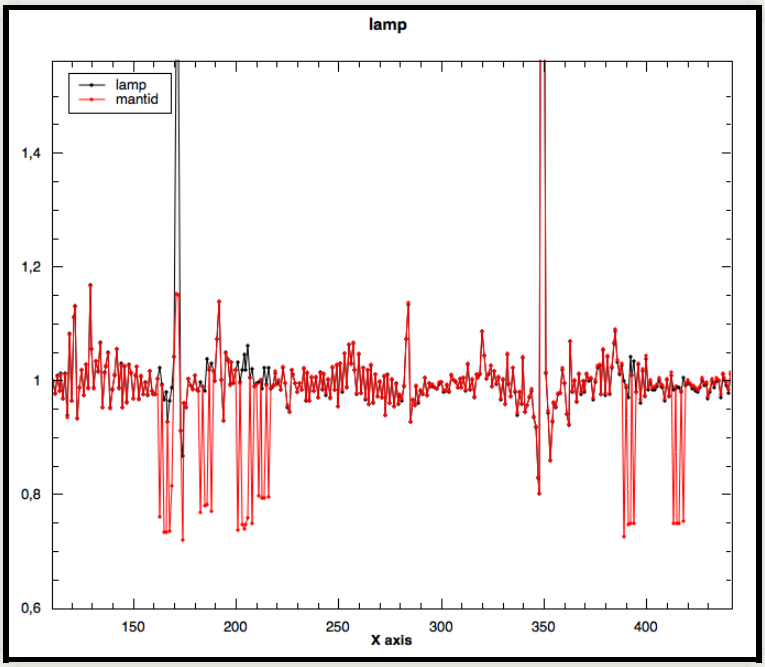
Detector scan data reduction

- Currently detector scan reduction logic is contained in the calibraiton algorithm
- Should we rename it to PowderDiffDetectorScan, with options [ProduceCalibration, Reduce]?
- And/or make 2 separate light-weight wrappers?

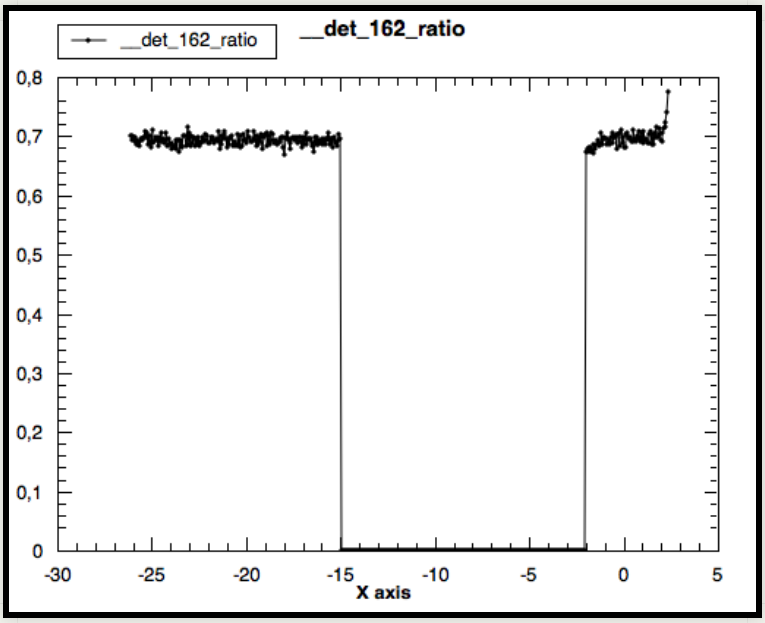
A side note about dead cell definition

- Few cells count 0, but not always
- A cell is treated as dead, if it counts zero in 80% or more cases

Investigated the difference in calibration constants for few cells

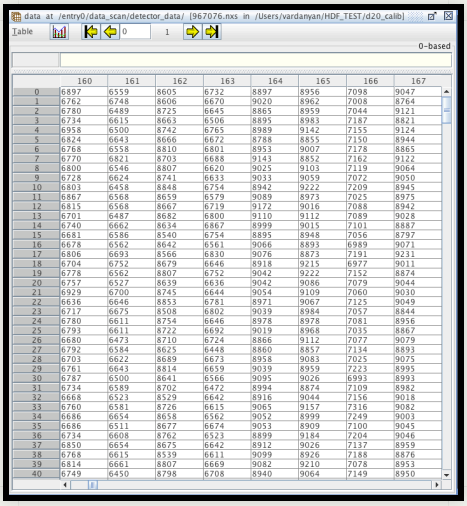


The ratio histogram for cell #162



Outside the beam-stop it is indeed about 0.7

It turned out that this comes from raw data.



	160	161	162	163	164	165	166	167
0	6897	6559	8605	6732	8897	8956	7098	9047
1	6762	6748	8606	6670	9020	8962	7008	8764
2	6780	6489	8725	6645	8865	8959	7044	9121
3	6734	6615	8663	6506	8895	8983	7187	8821
4	6958	6500	8742	6765	8989	9142	7155	9124
5	6824	6643	8666	6672	8788	8855	7150	8944
6	6768	6558	8810	6801	8953	9007	7178	8865
7	6770	6821	8703	6688	9143	8852	7162	9122
8	6800	6546	8807	6620	9025	9103	7119	9064
9	6728	6624	8741	6633	9033	9059	7072	9050
10	6803	6458	8848	6754	8942	9222	7209	8945
11	6867	6568	8659	6579	9089	8973	7025	8975
12	6815	6568	8667	6719	9172	9016	7088	8942
13	6701	6487	8682	6800	9110	9112	7089	9028
14	6740	6662	8634	6867	8999	9015	7101	8887
15	6681	6586	8540	6754	8895	8948	7056	8797
16	6678	6562	8642	6561	9066	8893	6989	9071
17	6806	6693	8566	6830	9076	8873	7191	9231
18	6704	6752	8679	6646	8918	9215	6977	9011
19	6778	6562	8807	6752	9042	9222	7152	8874
20	6757	6527	8639	6636	9042	9086	7079	9044
21	6929	6700	8745	6644	9054	9109	7060	9030
22	6636	6646	8853	6781	8971	9067	7125	9049
23	6717	6675	8508	6802	9039	8984	7057	8844
24	6780	6611	8754	6646	8978	8978	7081	8956
25	6793	6611	8722	6692	9019	8968	7035	8867
26	6680	6473	8710	6724	8866	9112	7077	9079
27	6792	6584	8625	6448	8860	8857	7134	8893
28	6703	6622	8689	6673	8958	9083	7025	9075
29	6761	6643	8814	6659	9039	8959	7223	8995
30	6787	6500	8641	6566	9095	9026	6993	8993
31	6734	6589	8702	6472	8994	8874	7109	8982
32	6668	6523	8529	6642	8916	9044	7156	9018
33	6760	6581	8726	6615	9065	9157	7316	9082
34	6686	6654	8658	6562	9052	8999	7249	9003
35	6686	6511	8677	6674	9053	8909	7100	9045
36	6734	6608	8762	6523	8899	9184	7204	9046
37	6850	6654	8675	6642	8912	9026	7137	8959
38	6768	6615	8539	6611	9099	8926	7188	8876
39	6814	6661	8807	6669	9082	9210	7078	8953
40	6749	6450	8798	6708	8940	9064	7149	8950

Some cells do count too much, and get a smaller calibration constant.

Status

- PR is open, ready for review
- New package is built
- Built on the server this time