POWDER DIFFRACTION REDUCTION

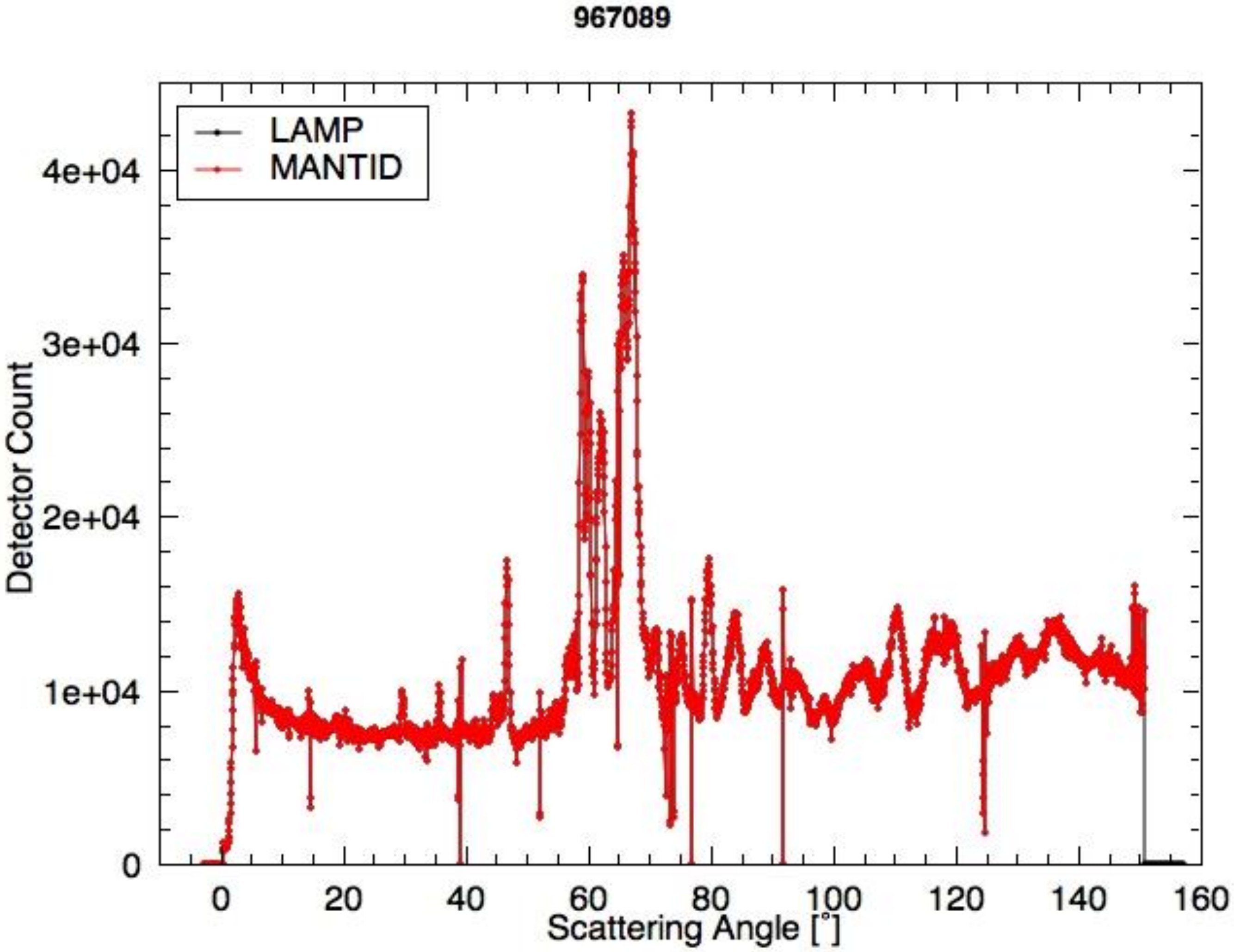
GAGIK, 22.09.2017, ILL

CURRENT STATUS

- ✓ Instrument geometry
- ✓ Loader validated
- ✓ Scanning detector loading
- ✓ Reduction algorithm
- ✓ Calibration algorithm
- ✓ Fullprof export

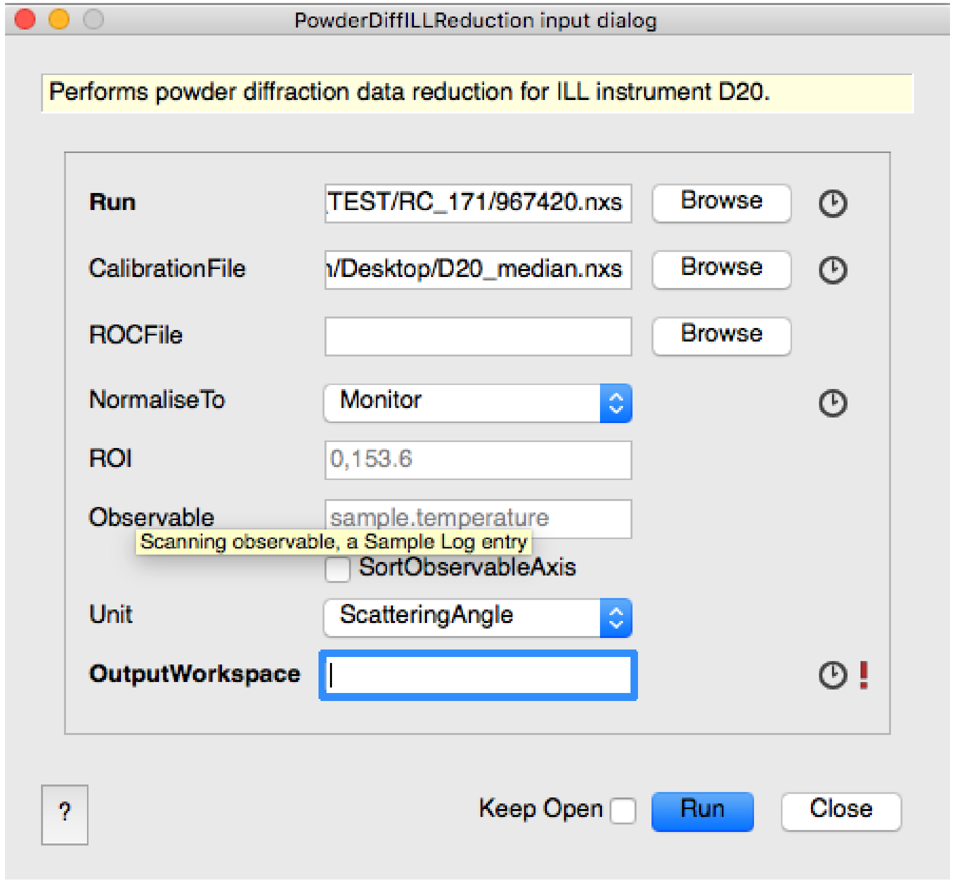
- □ Code cleanup and speedup
- □ Unit tests and documentation
- □ ROC correction
- □ GSAS export
- □ Omega scan
- □ D1B case

✓ LOADING VALIDATED



After final fix to the $2\theta_0$ rotation treatment and dead panels allocation (both on the right end), obtained a good match with LAMP in signed 2θ axis.

REDUCTION AND CALIBRATION ALGORITHMS

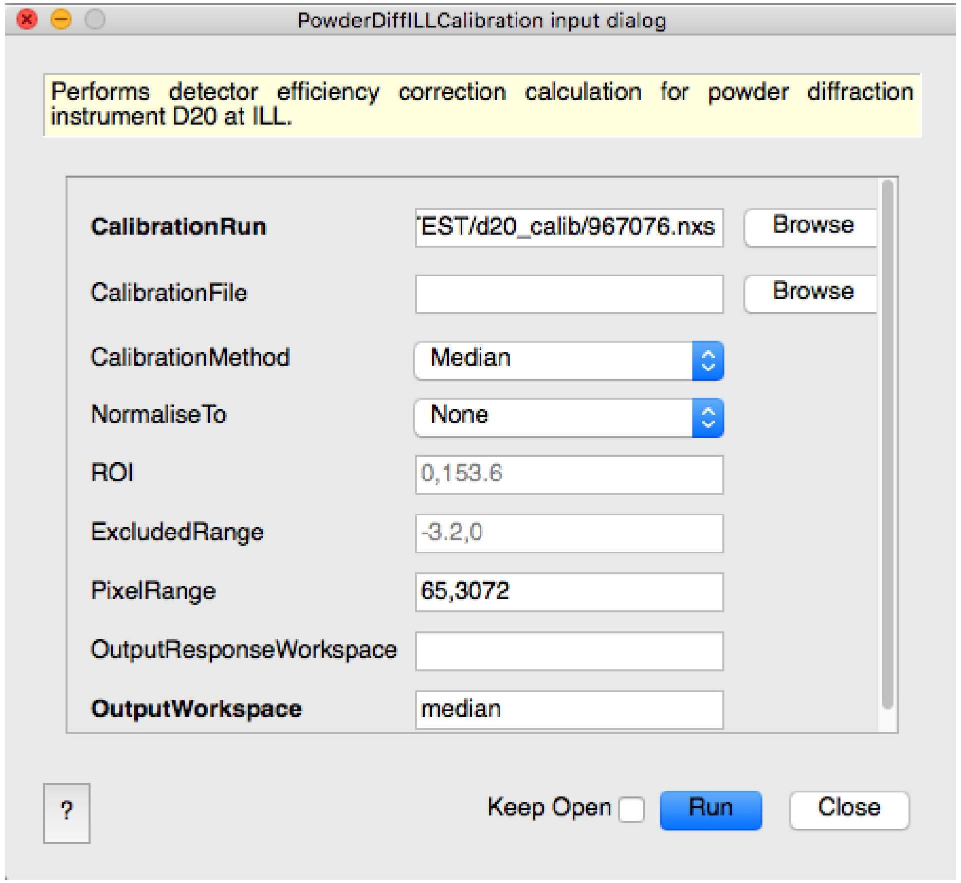


PowderDiffILLReduction input dialog

Performs powder diffraction data reduction for ILL instrument D20.

Run	TEST/RC_171/967420.nxs
CalibrationFile	\/Desktop/D20_median.nxs
ROCFile	
NormaliseTo	Monitor
ROI	0,153.6
Observable	sample.temperature
	□ SortObservableAxis
Unit	ScatteringAngle
OutputWorkspace	

Scanning observable, a Sample Log entry

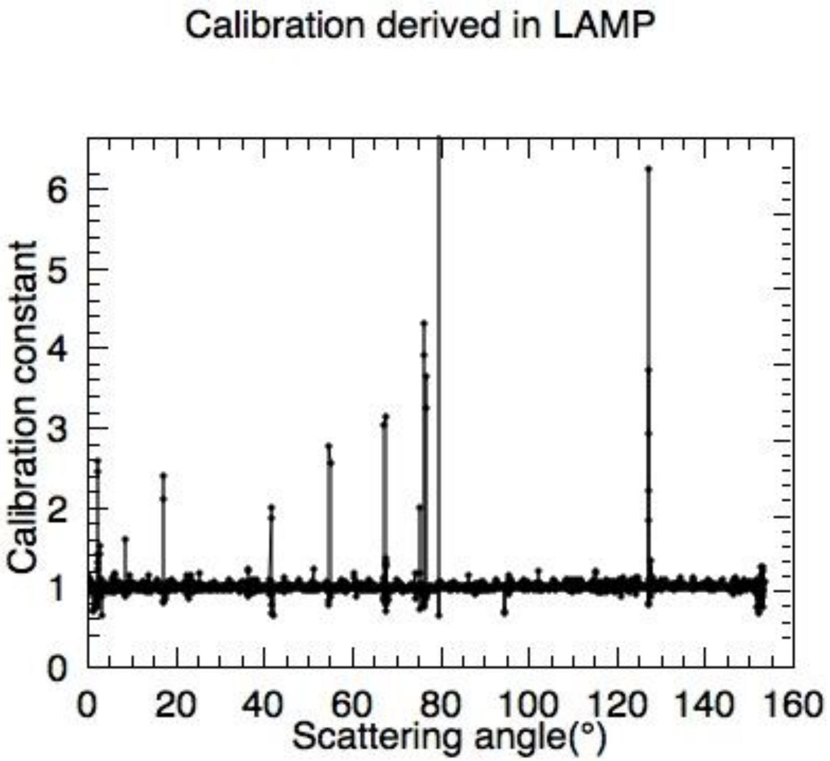


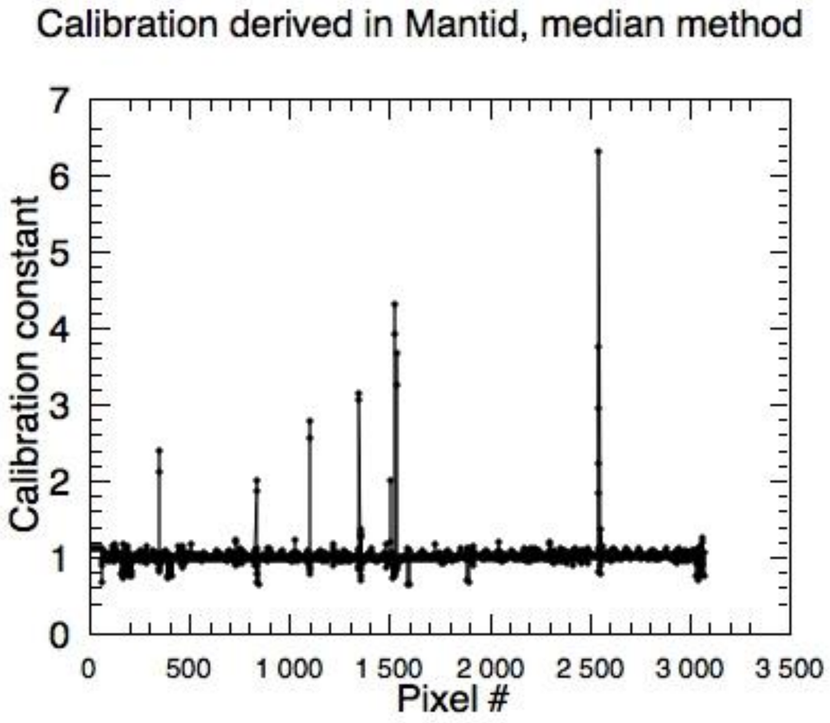
PowderDiffILLCalibration input dialog

Performs detector efficiency correction calculation for powder diffraction instrument D20 at ILL.

CalibrationRun	'EST/d20_calib/967076.nxs
CalibrationFile	
CalibrationMethod	Median
NormaliseTo	None
ROI	0,153.6
ExcludedRange	-3.2,0
PixelRange	65,3072
OutputResponseWorkspace	
OutputWorkspace	median

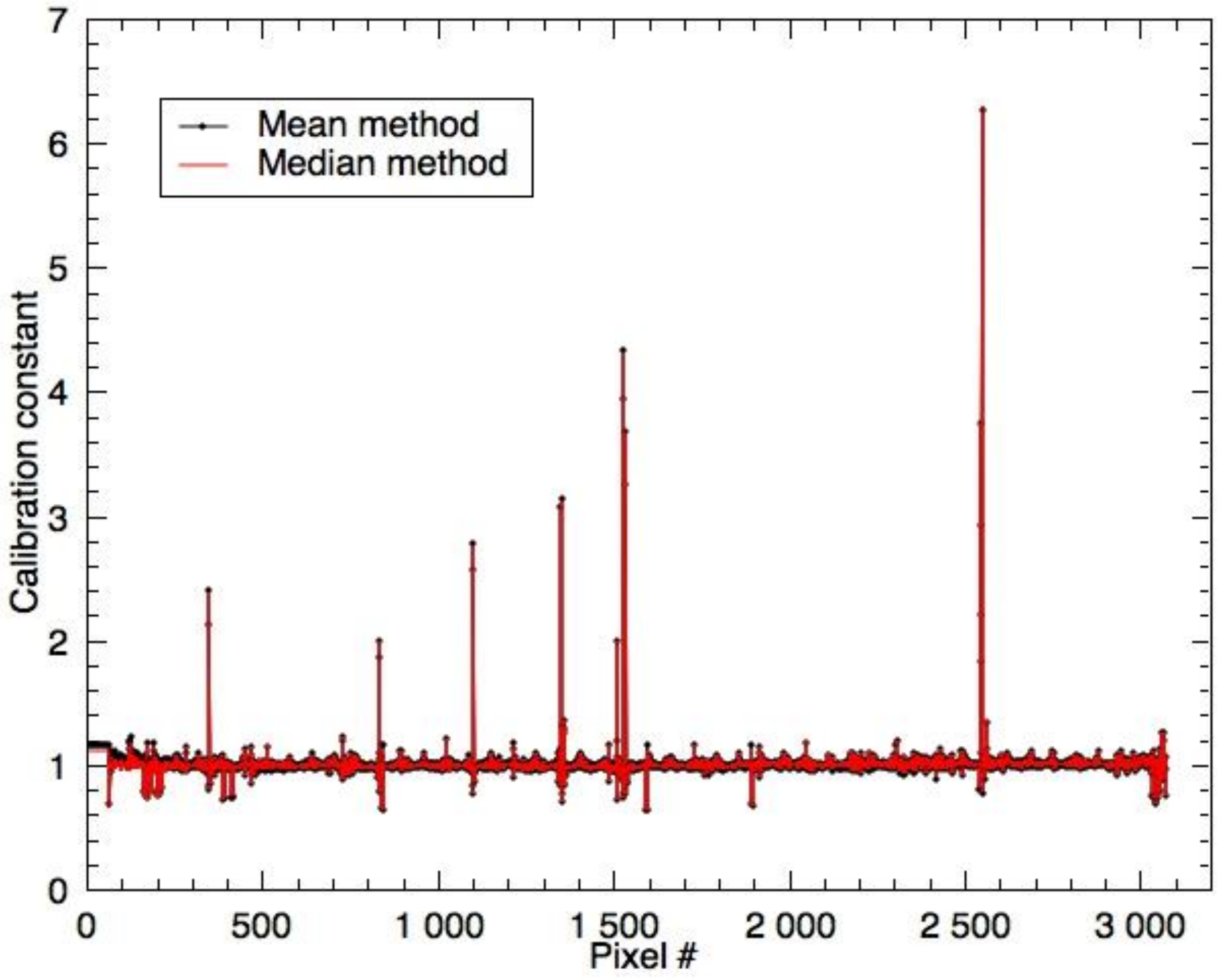
CALIBRATION CONSTANTS





- ✓ Similar results
- Note the different axes
- Note the different methods

CALIBRATION CONSTANTS

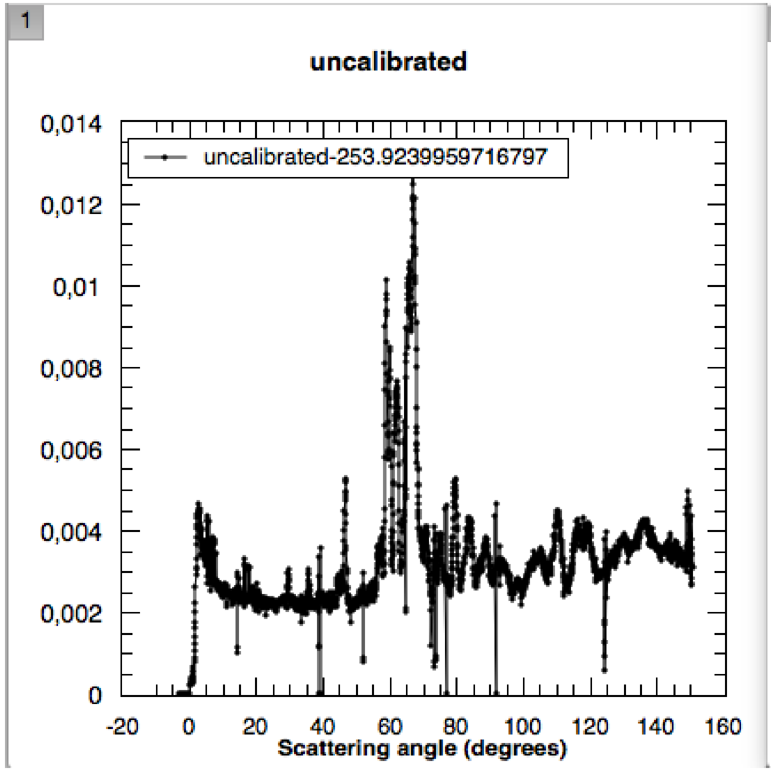


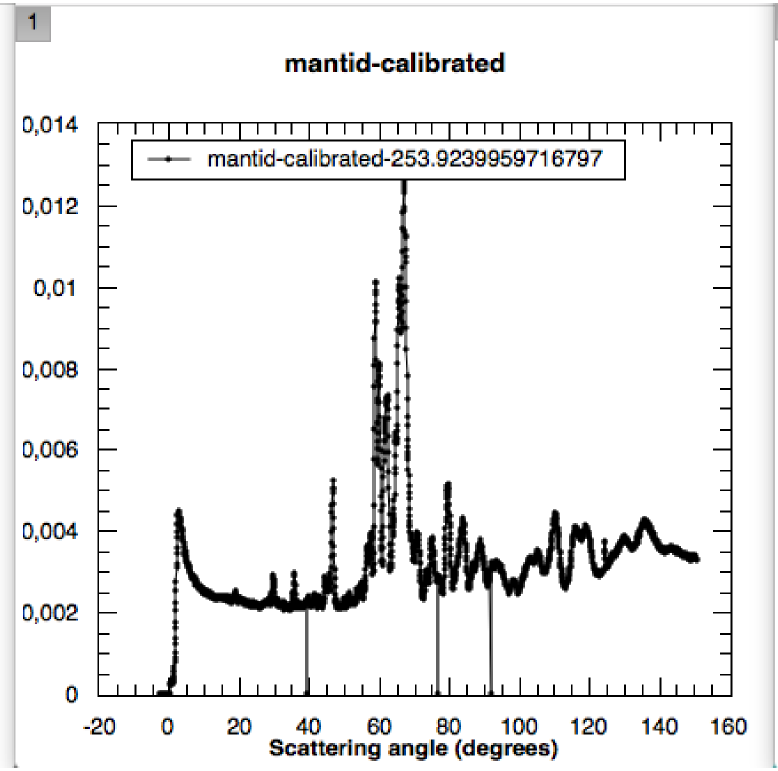
- ✓ Mean, median and max likely methods implemented
- ✓ Good (and similar) results
- ✓ Takes about 1m 30s for median and mean
- ❑ Maximum likelihood too slow (45m) in python
  - ❑ Investigate multiprocessing or C++?

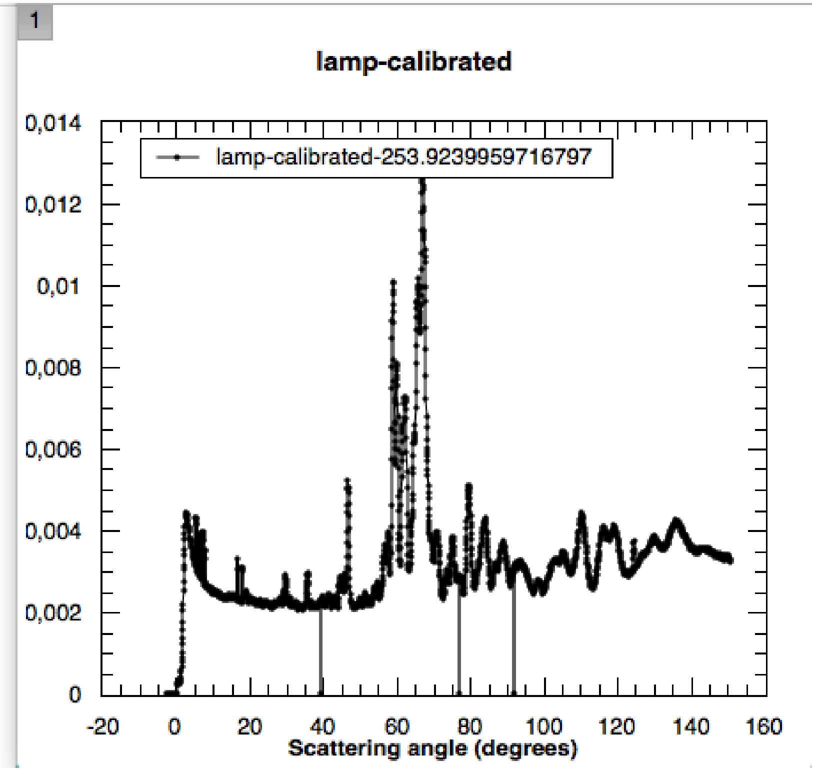
- ✓ Monitor normalisation
- ❑ Is time normalisation needed?
- ❑ What about ROI normalisation?
- ❑ Exclude dead pixels from final absolute scaling?

Currently no interpolation can be done
Assuming the scan step is integer multiple of the pixel size

CALIBRATED DATA COMPARISON

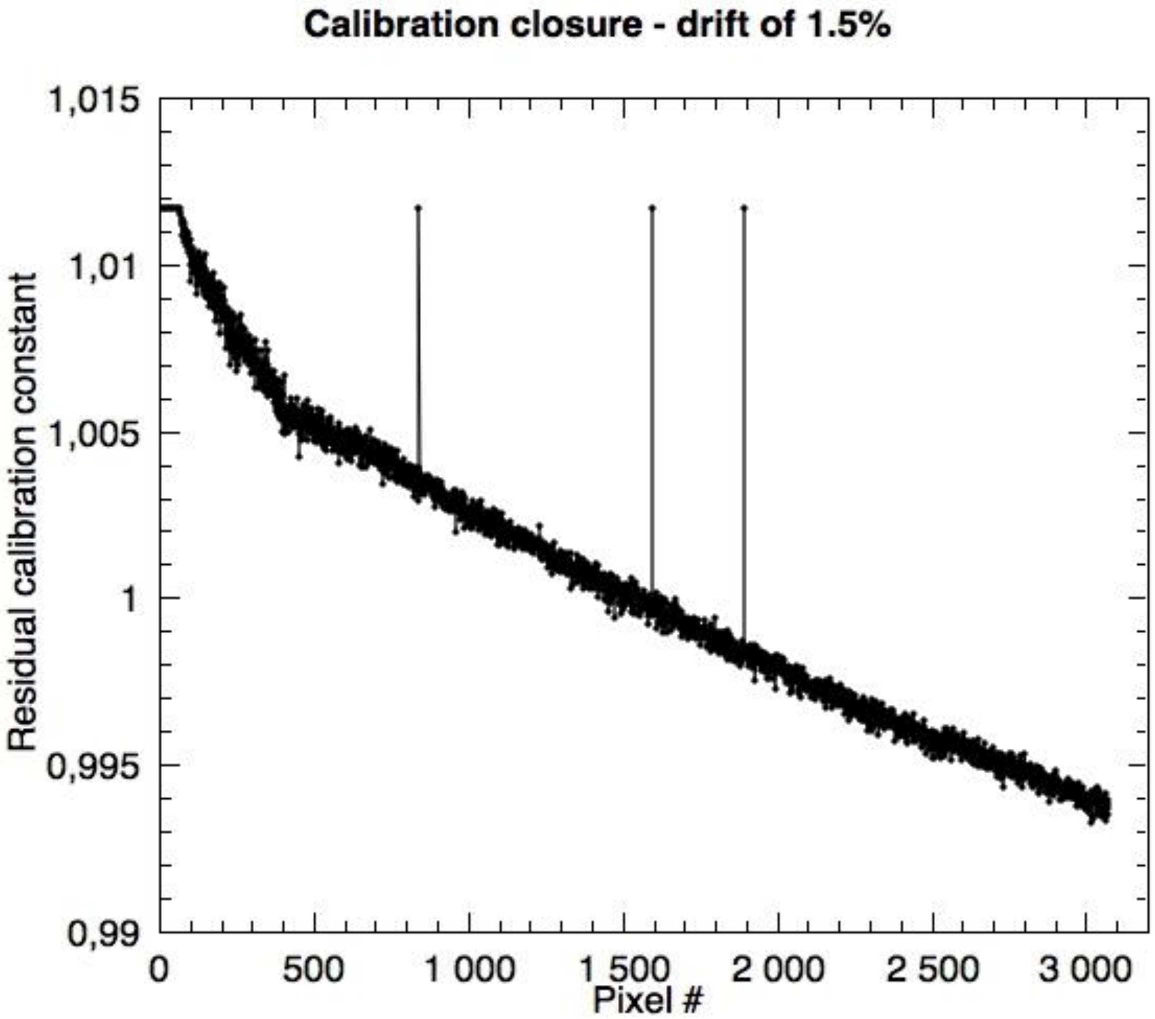

uncalibrated


mantid-calibrated

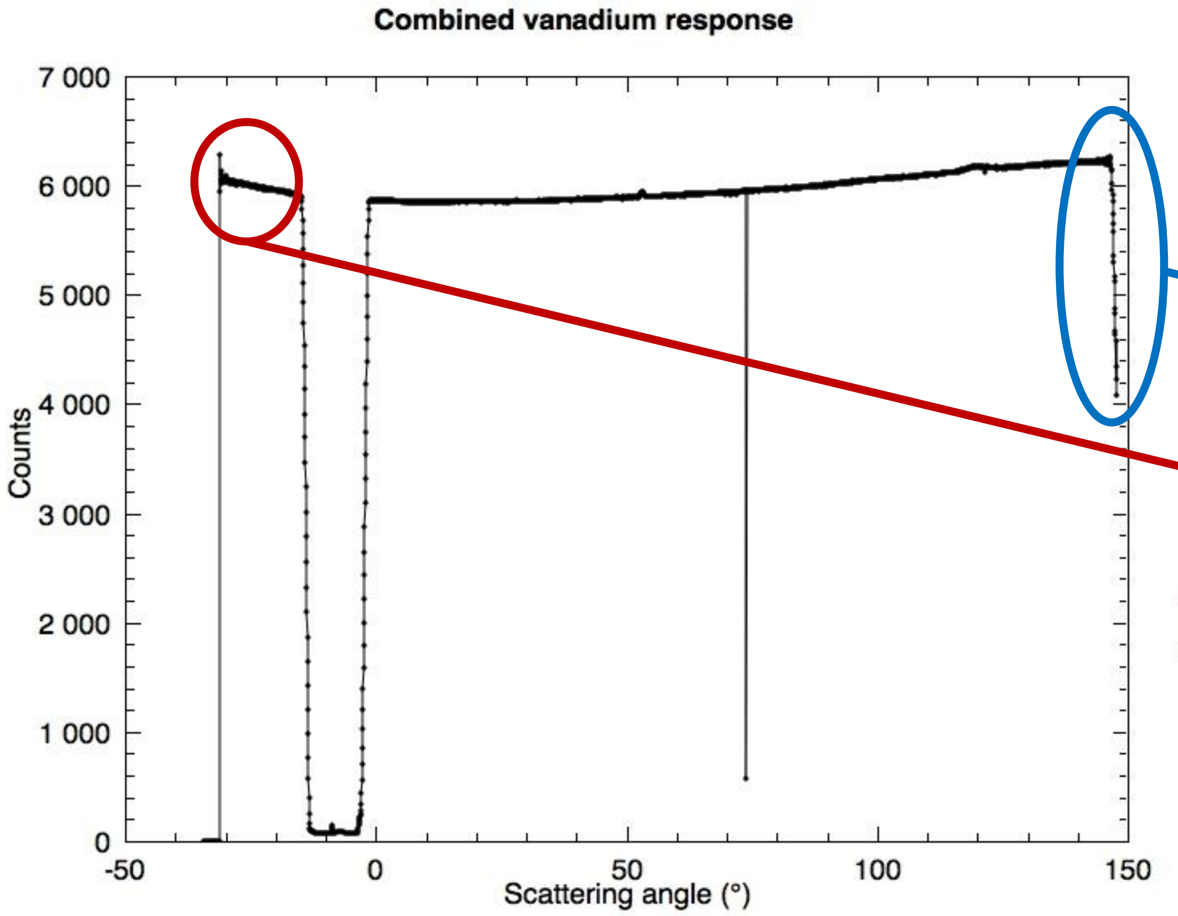

lamp-calibrated

✓ Calibration works

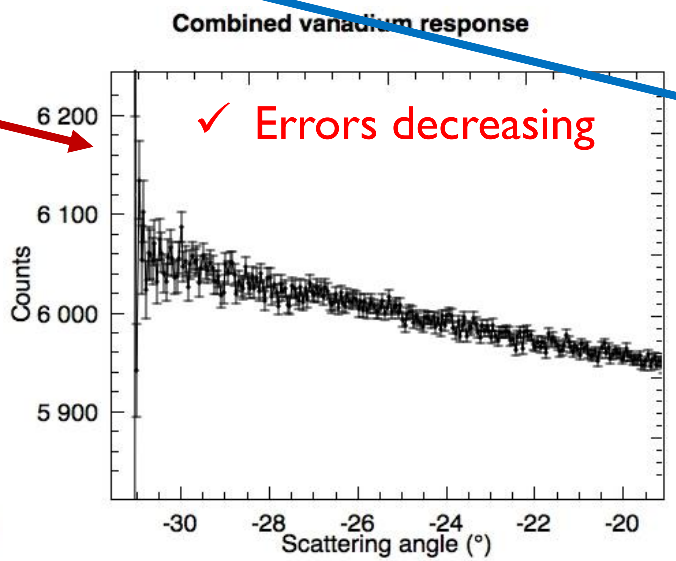
CALIBRATION CLOSURE - DRIFT



COMBINED RESPONSE FROM VANADIUM



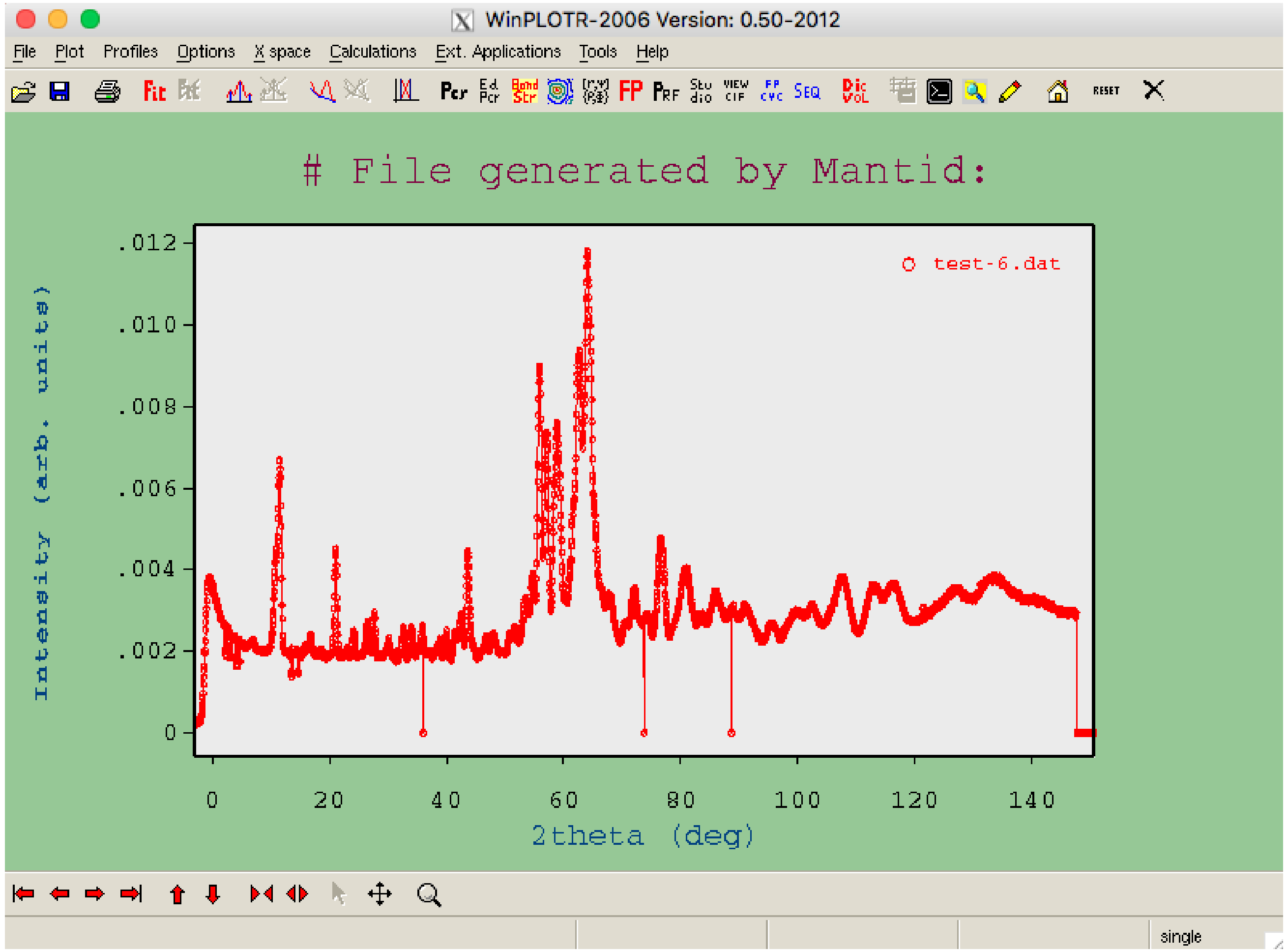
- Optional output of the calibration algorithm as a control plot
- Contains counts of all the pixels iteratively weighted-summed in the overlapping regions



✓ Errors decreasing

- Steep fall at the verge of the scan
- Present also in raw data
- Not an artifact from calibration procedure

FULLPROF EXPORT OPERATIONAL


WinPLOTR-2006 Version: 0.50-2012
File Plot Profiles Options X space Calculations Ext. Applications Tools Help
# File generated by Mantid:
.012
.010
.008
.006
.004
.002
0
Intensity (arb. units)
○ test-6.dat
0
20
40
60
80
100
120
140
2theta (deg)
single

- ✓ **SaveFocusedXYE** for FullProf format 10
- ❑ Need to add the temperature in the header of the file
- ❑ Need to crop out the dead pixels

TO DO

- ❑ Wrap up D20 calibration
- ❑ Build a package from the branch for testing
- ❑ Write unit tests, documentation, workflow diagrams, documentation tests and usage examples.
- ❑ Any other feature to include in the algorithms?
- ❑ GSAS export
  - ❑ Need to figure out how to load existing .gsa or .gda to GSAS II, then try to mimic the format
  - ❑ Research if the formats provided by SaveGSS existing in Mantid satisfy our case
  - ❑ Implement new format saving otherwise
- ❑ ROC Correction – **numors needed**
- ❑ Omega scan – **numors needed**
- ❑ D1B – **numors needed**