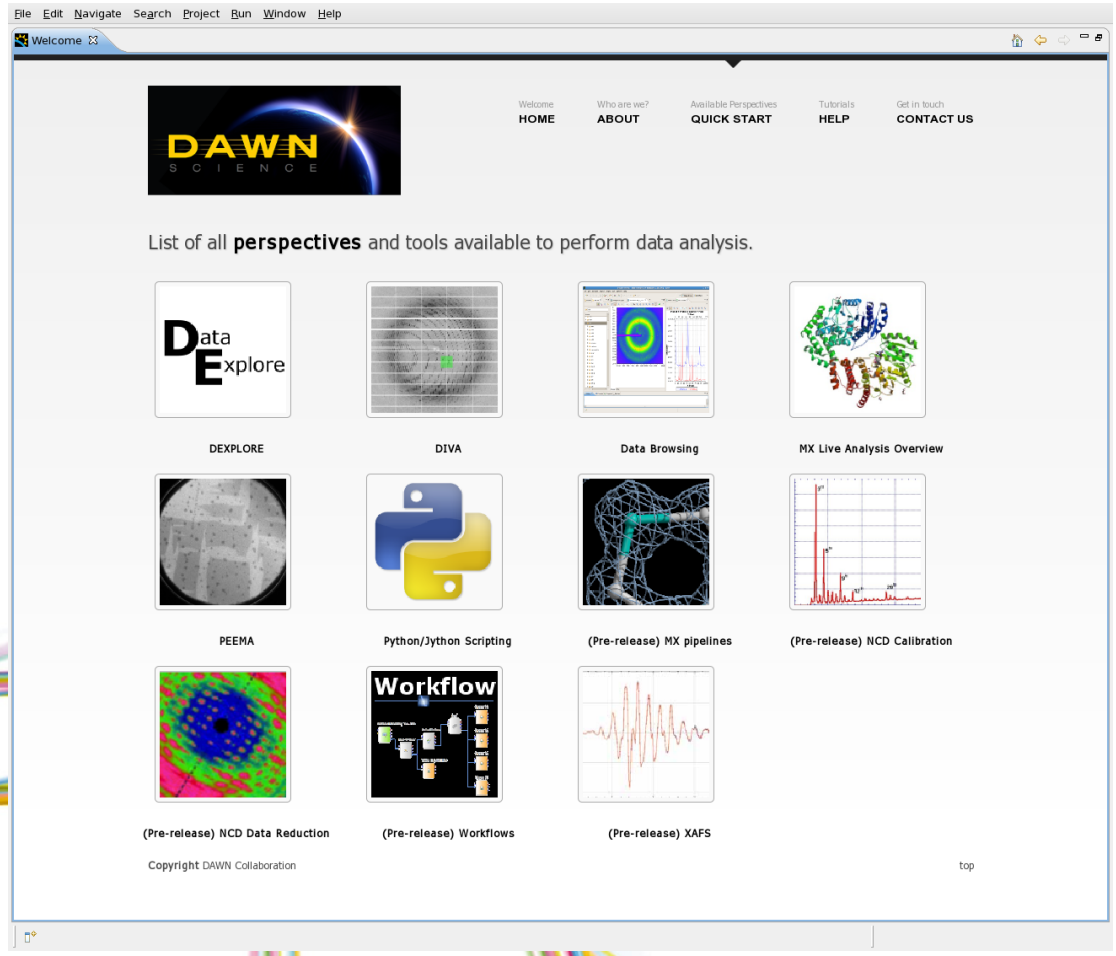
Small Angle X-ray Scattering data reduction using DAWN workbench

Irakli Sikharulidze, Tobias Richter, Peter Chang, Matthew Gerring, Bahá El Kassaby, Mark Basham, Marc Malfois, Nick Terrill and Alun Ashton

Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom

diamond

Data Analysis WorkBench (DAWN)



- DAWN workbench provides collection of tools for scientific data analysis.
- Software is implemented in Java using Eclipse RCP platform, allowing close integration with Generic Data Acquisition (GDA) framework.

diamond

Small Angle Scattering (SAXS) Data Reduction

Input data provided in NeXus files

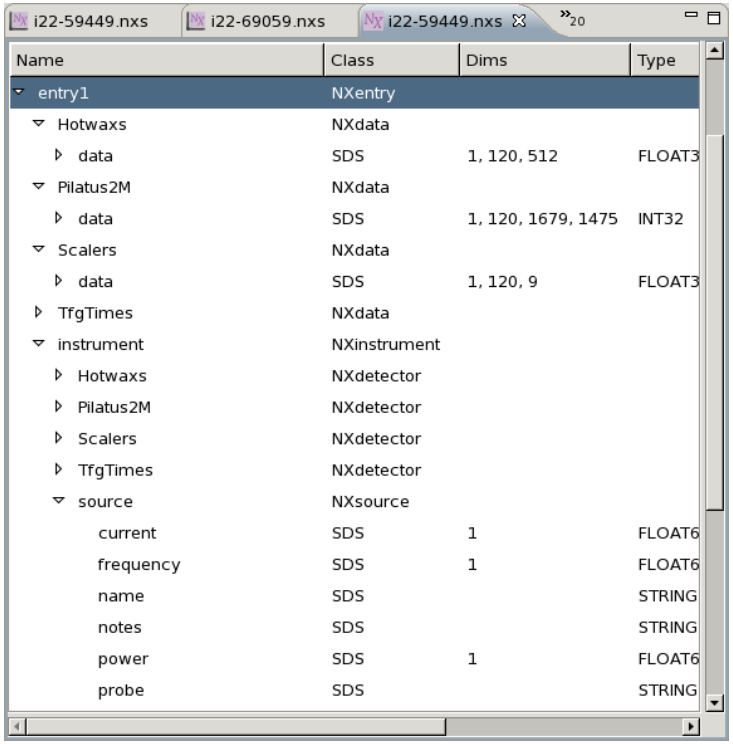
- Detector images (samples, buffers, calibrants)
- Beam monitoring data
- X-ray energy and detector pixel size

Processing requirements

- Calibrate detector in terms of scattering vector values
- Remove background and normalize to the same scale
- Ignore masked detector areas
- Calculate 1D profiles I(q)

SAXS Data Reduction Workflow

- Read detector information from input NeXus files
- Load calibrant image
- Select sector integration area
- Create detector mask
- Select peaks on integrated profile
- Specify x-ray energy
- Run calibration procedure
- Select data reduction stages
- Specify parameters for selected stages
- Select input data files and run data reduction



Name	Class	Dims	Type
entry1	NXentry		
Hotwaxs	NXdata		
data	SDS	1, 120, 512	FLOAT3
Pilatus2M	NXdata		
data	SDS	1, 120, 1679, 1475	INT32
Scalers	NXdata		
data	SDS	1, 120, 9	FLOAT3
TfgTimes	NXdata		
instrument	NXinstrument		
Hotwaxs	NXdetector		
Pilatus2M	NXdetector		
Scalers	NXdetector		
TfgTimes	NXdetector		
source	NXsource		
current	SDS	1	FLOAT6
frequency	SDS	1	FLOAT6
name	SDS		STRING
notes	SDS		STRING
power	SDS	1	FLOAT6
probe	SDS		STRING

diamond

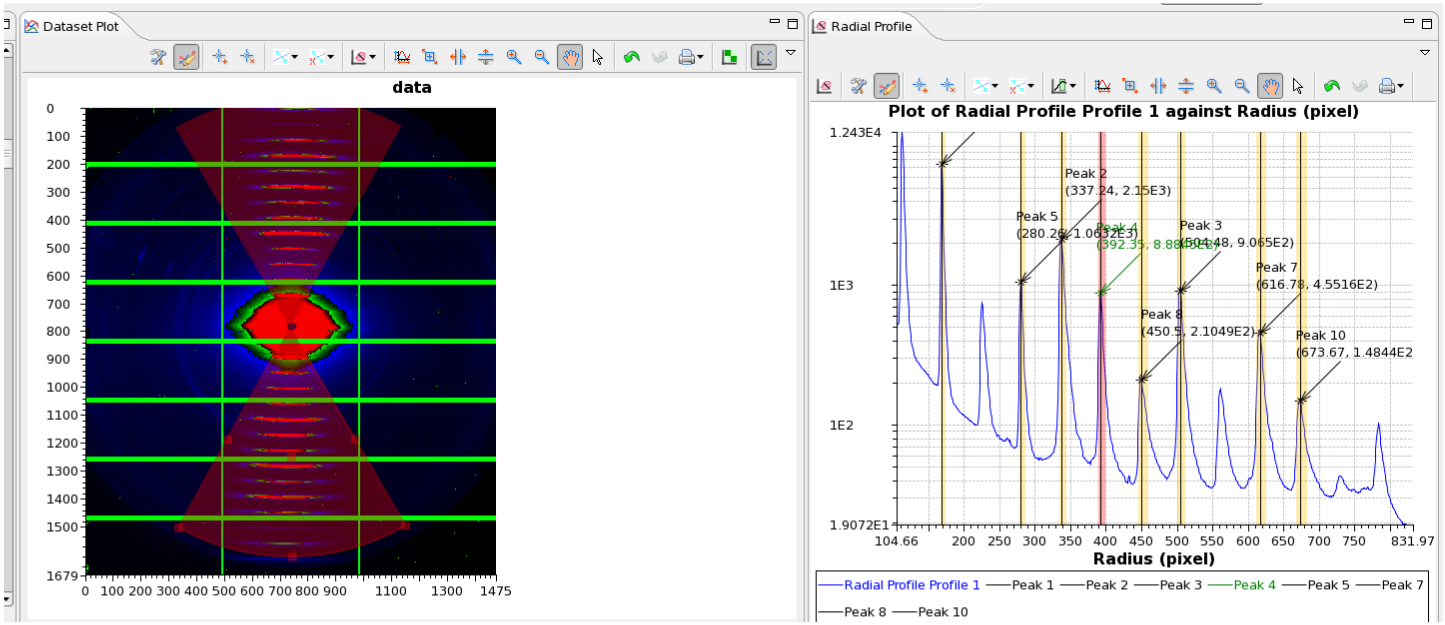
SAXS Detector Calibration

- In SAXS case we can approximate relation between scattering vector *q* and pixel position *x* with linear function.

$$q = \frac{4\pi \sin(\theta)}{\lambda} \approx \frac{2\pi}{\lambda D} x$$

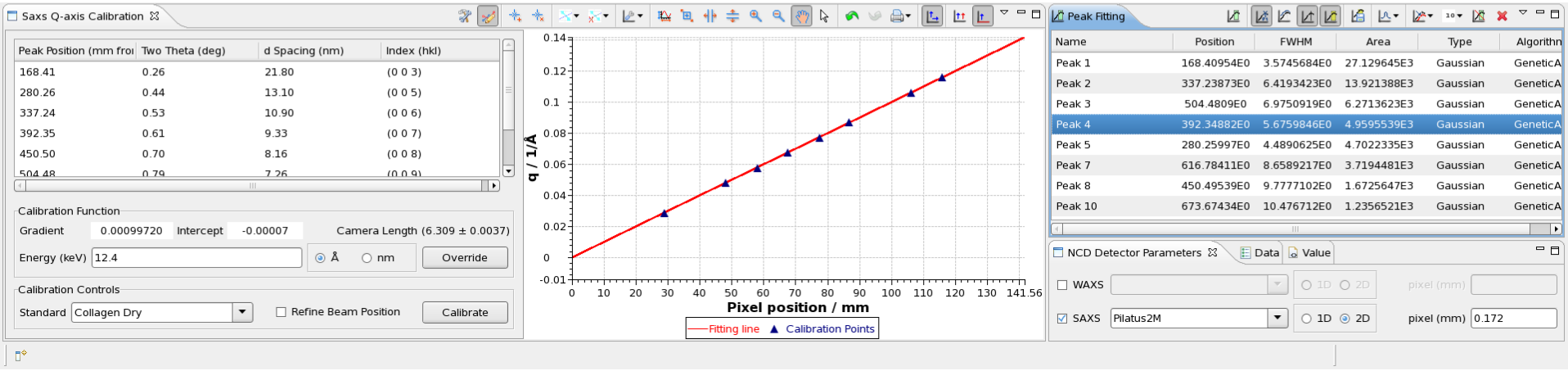
- Best linear fit $q = Ax + B$ is obtained by matching calibrant peaks with tabulated positions and adjusting beam center.

SAXS Detector Calibration



- Beam center position can be adjusted using ellipse fitting tool or symmetry related integrated sector profiles.
- Calibration data can be used for different sector sizes, but it needs to be updated if sector integration origin changes.

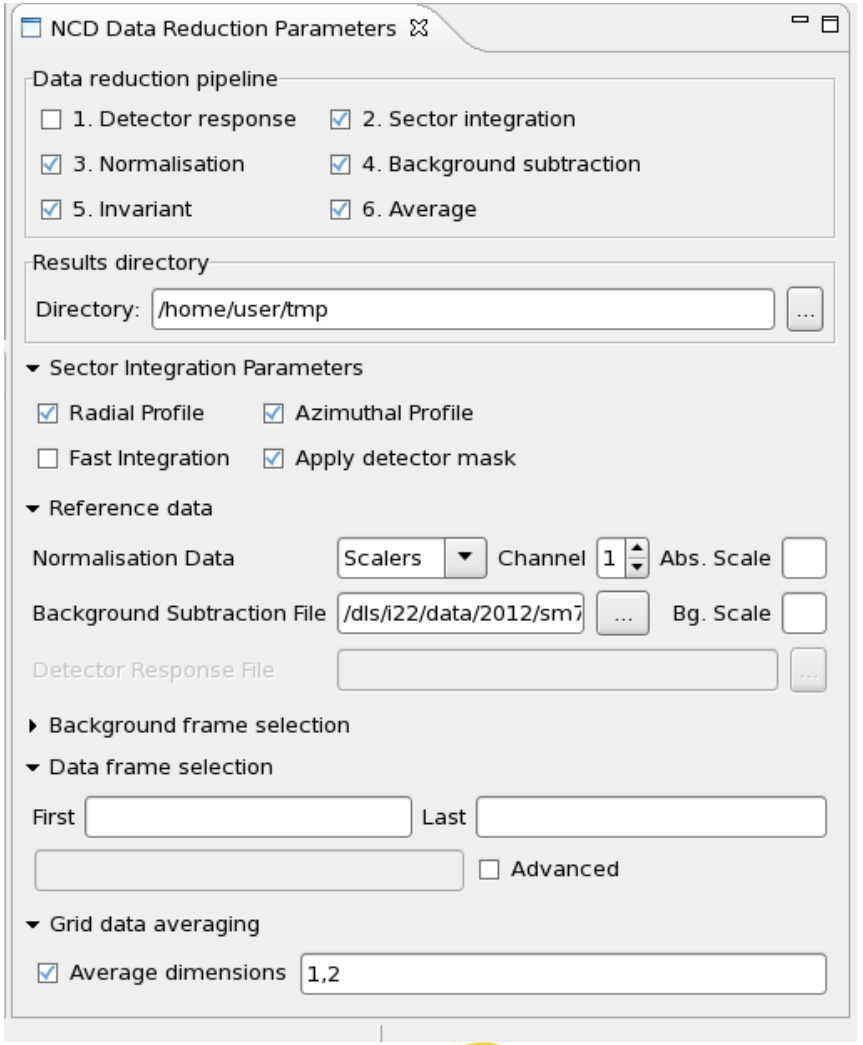
SAXS Detector Calibration



- Calibration procedure automatically indexes fitted peaks and estimates detector distance.
- Intercept value of linear fit function and detector distance estimate error provide measure for accuracy of calibration process.

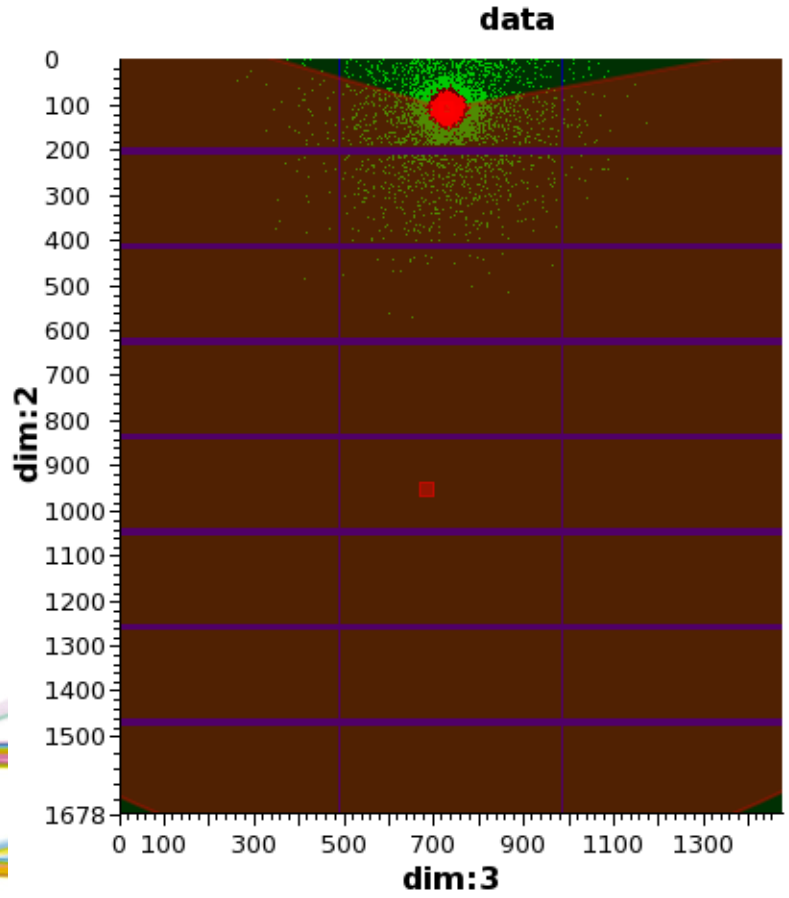
SAXS Data Reduction

- Experimental data files are processed in order
- Data from each file is split in chunks
- Chunks are run through the pipeline in parallel
- Results are written into the output NeXus file



diamond

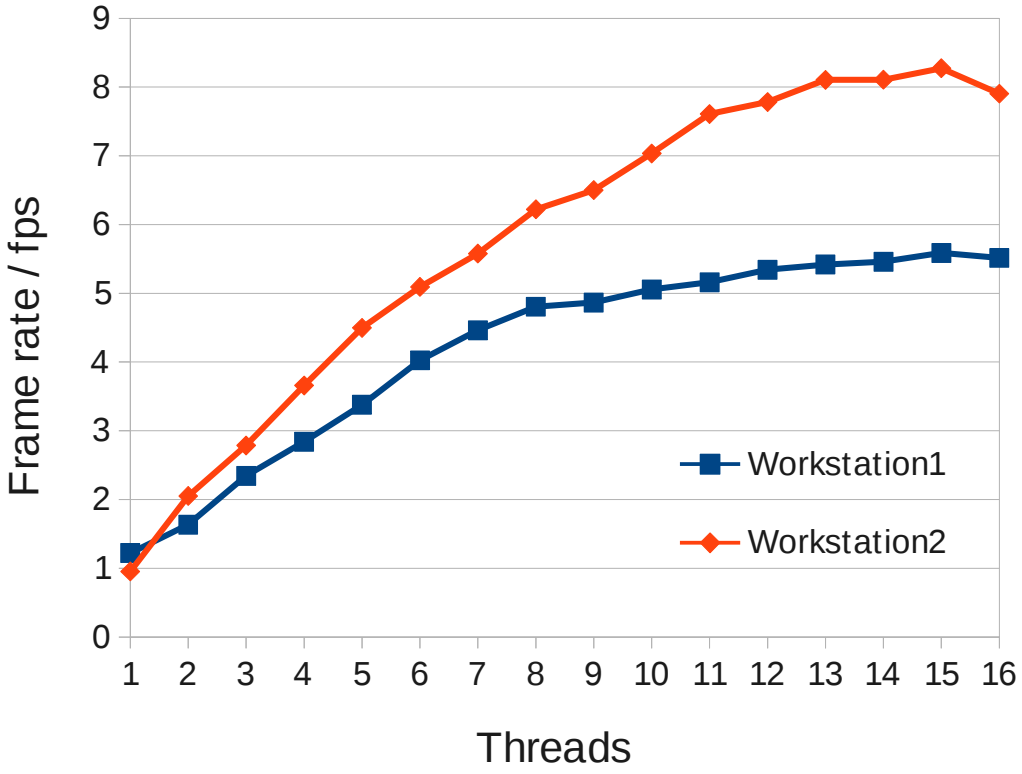
Sector Integration Profiling



- 120 Pilatus 2M frames 1679x1475 (1.11Gb)
- Sector radius 1696 px
- Sector angle 206.5°
- Single sector integration stage
- Interpolation algorithm
- No detector mask

diamond

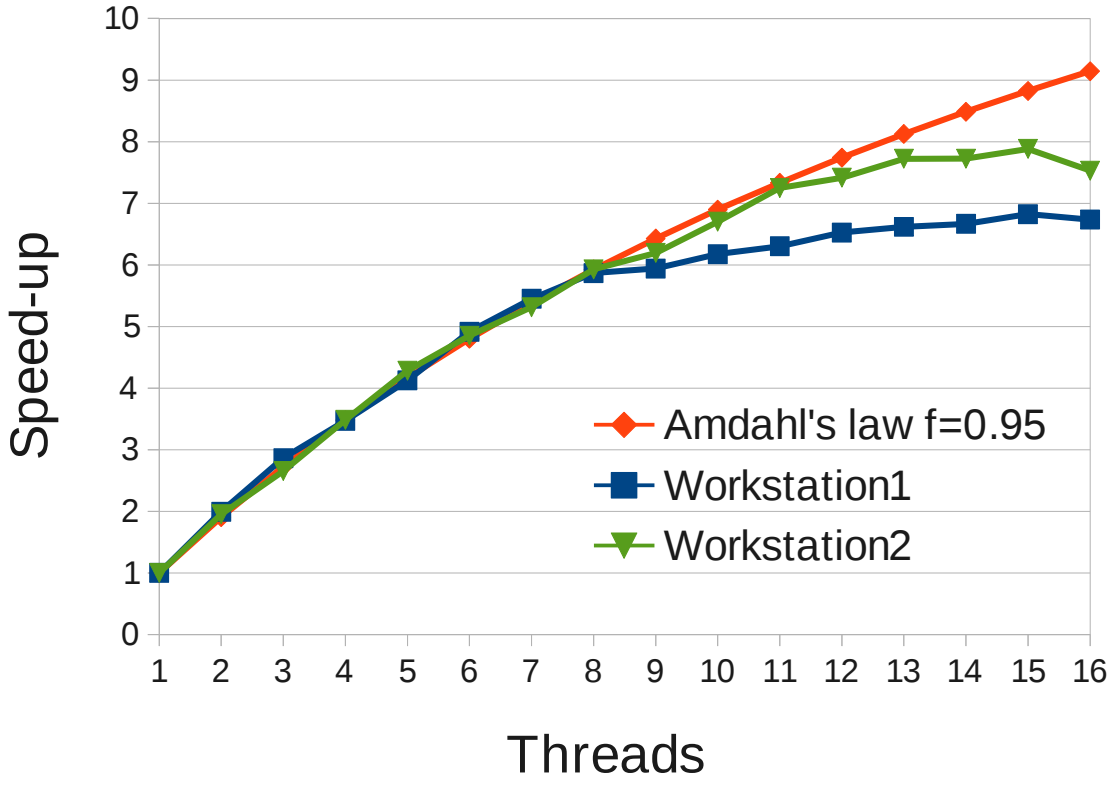
Sector Integration Profiling



- Workstation 1: 8x Intel Xeon L5520 @ 2.27GHz
  Workstation 2: 12x Intel Xeon X5660 @ 2.8GHz

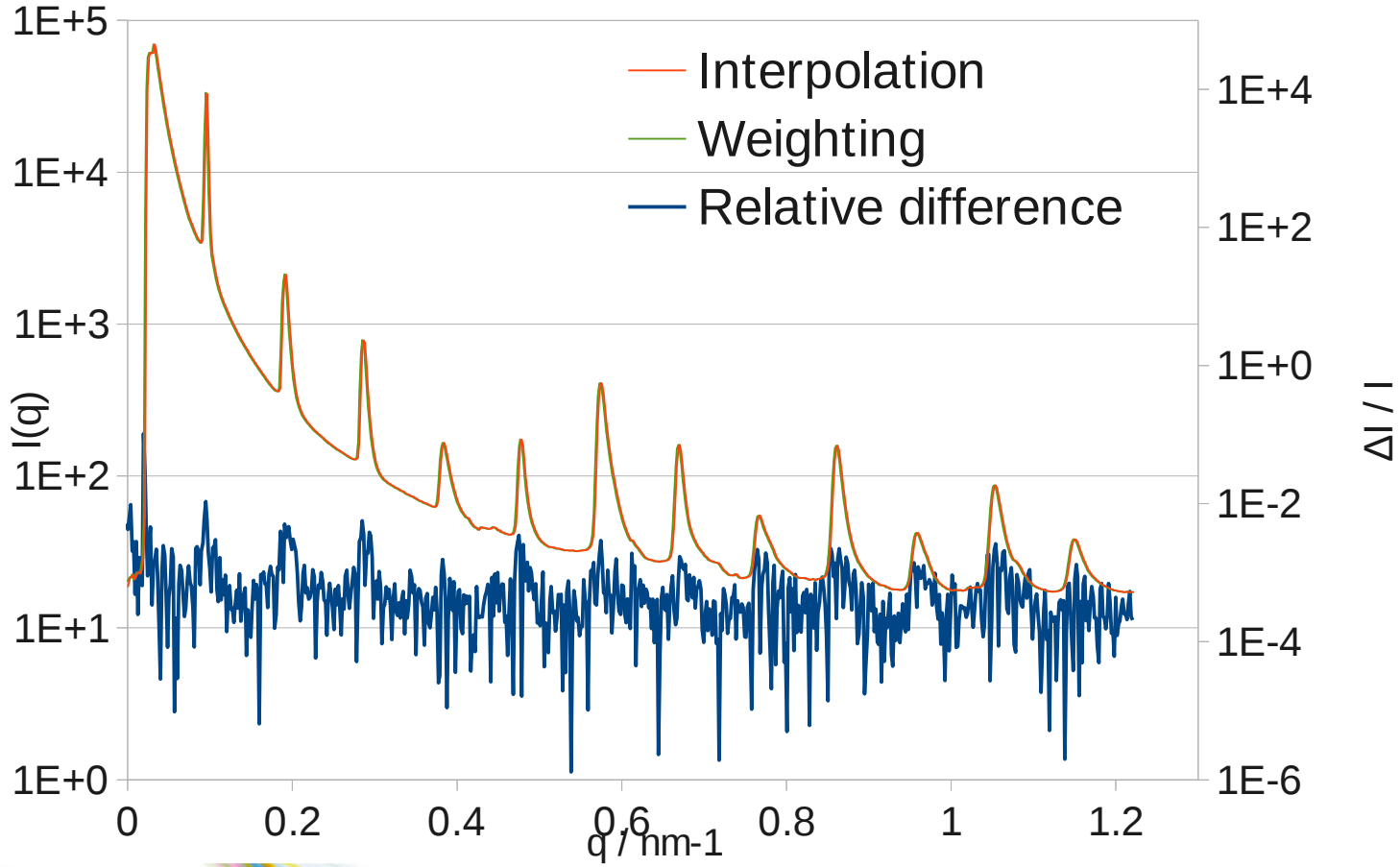
diamond

SAXS Data Reduction



- 20x theoretical speed-up limit

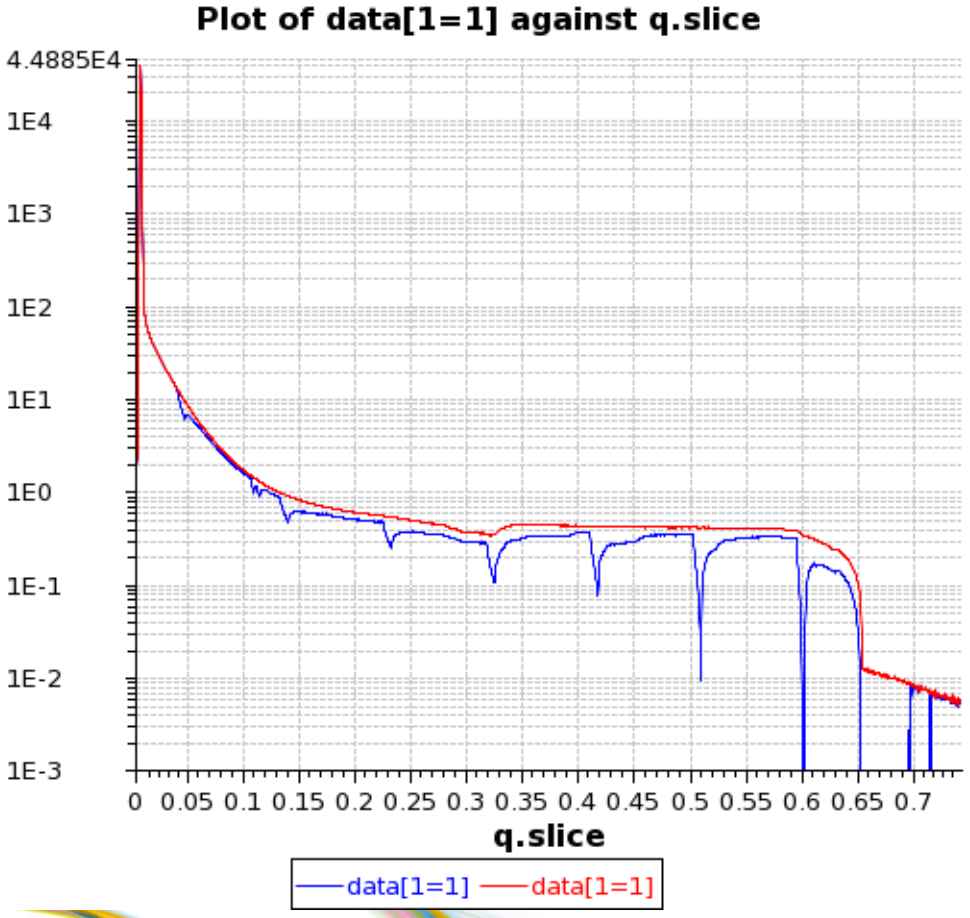
Sector Integration Algorithms

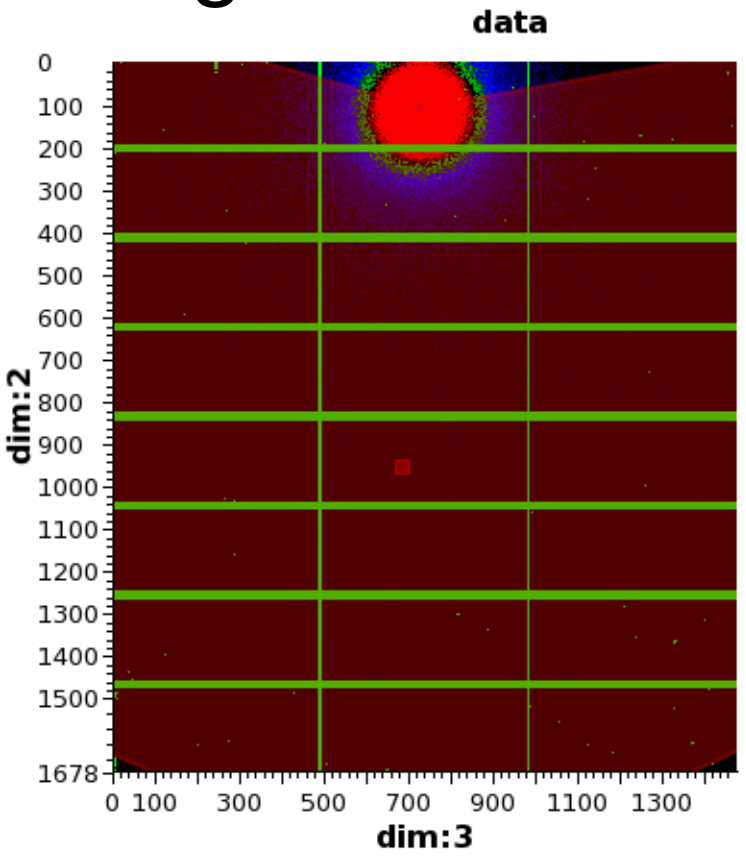


- Good agreement between two algorithms
- 2x speed gain in weighting algorithm

diamond

Detector Masking





- Data reduction performance (12x core workstation, ~8% masked area)
- 16.6s w/o mask, 19.8s with mask (Interpolation)
- 9.1s w/o mask, 10.8s with mask (Weighting)

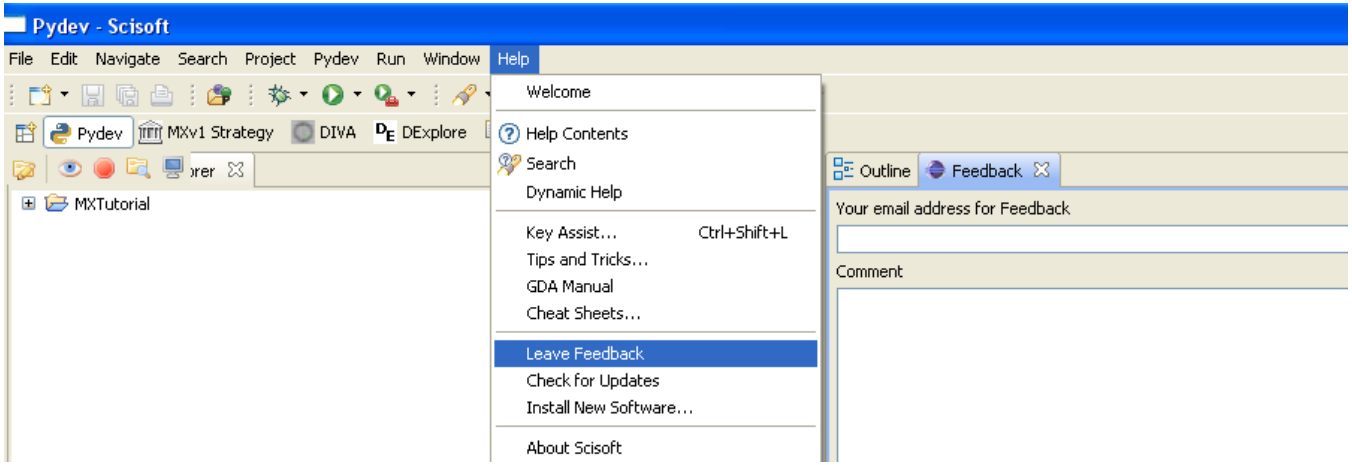
diamond

Future developments

- Improving GUI layout and usability
- Parallelization of basic dataset manipulation methods
- Cluster interface
- Integration with downstream processing software (e.g. EDNA ATSAS pipeline, Scatter, FISH...)

Feedback

- We welcome your input!



Calibration

Data reduction

DAWN collaboration http://www.dawnsci.org/

NeXus File Format http://nexusformat.org/

Diamond Scientific Software scientificsoftware@diamond.ac.uk

diamond