Crystallography and Parallel Data Management

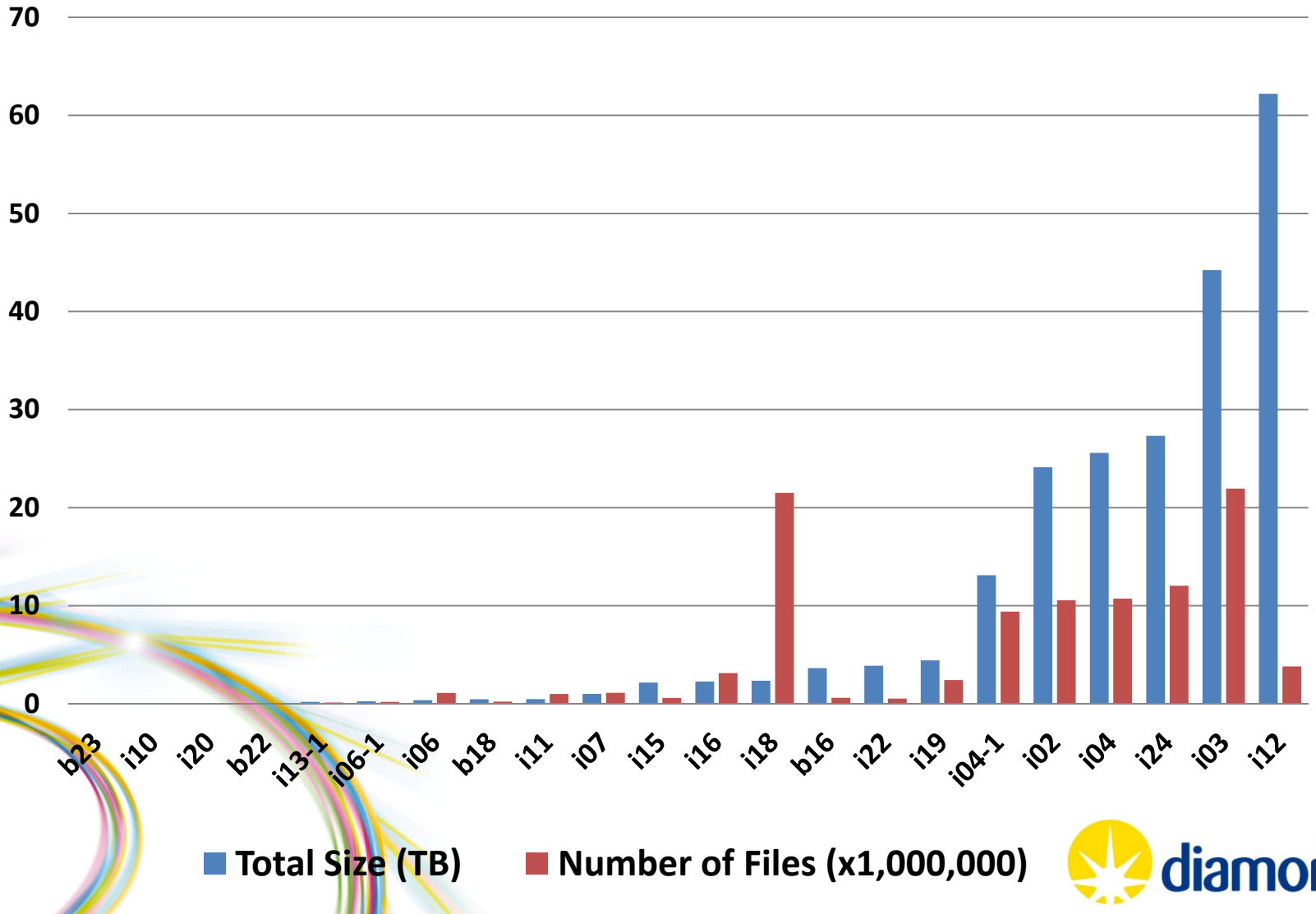
Alun Ashton

Scientific Software Team

Diamond.

With thanks to many groups and collaborators.

Total number of files and data volume per beamline



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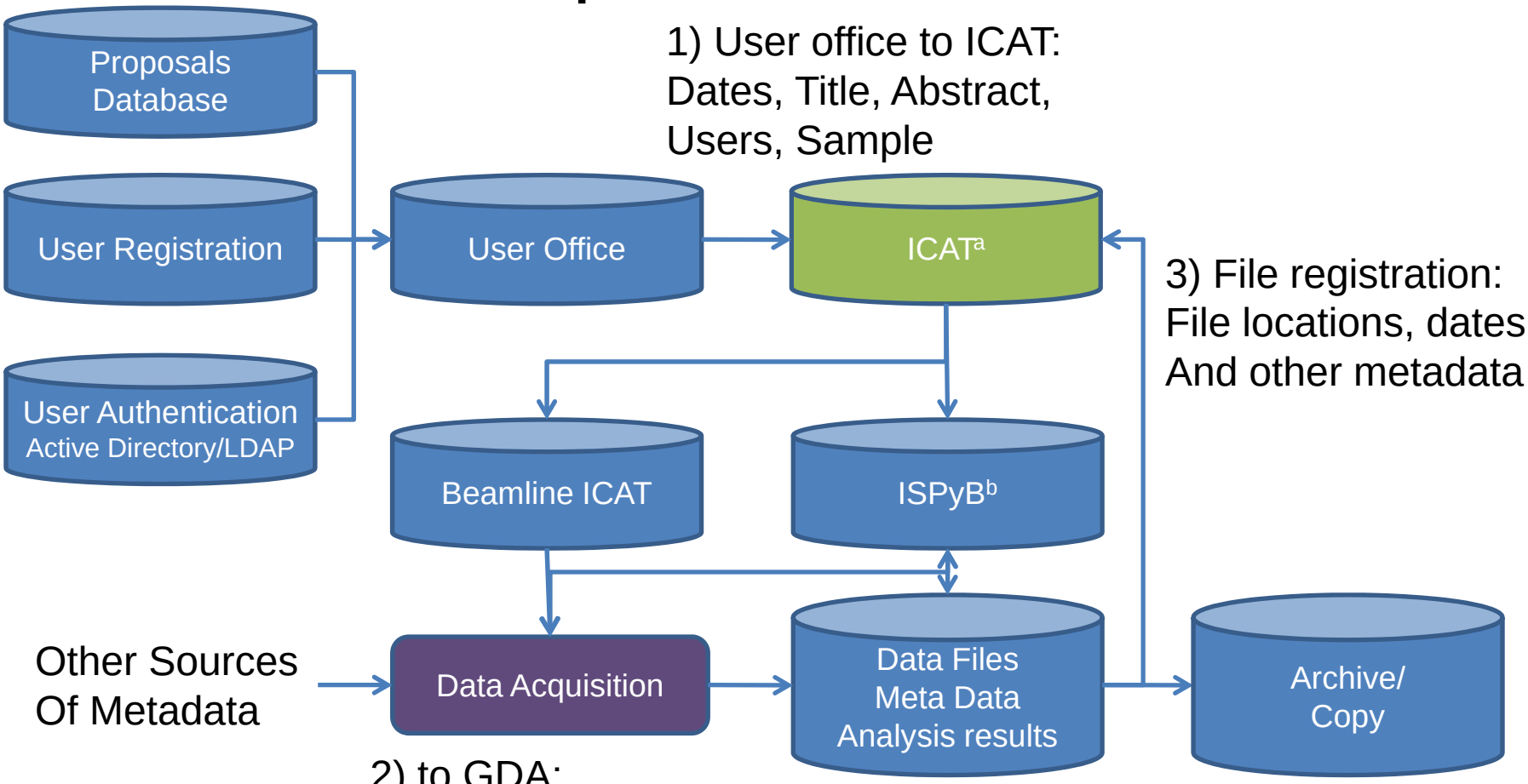
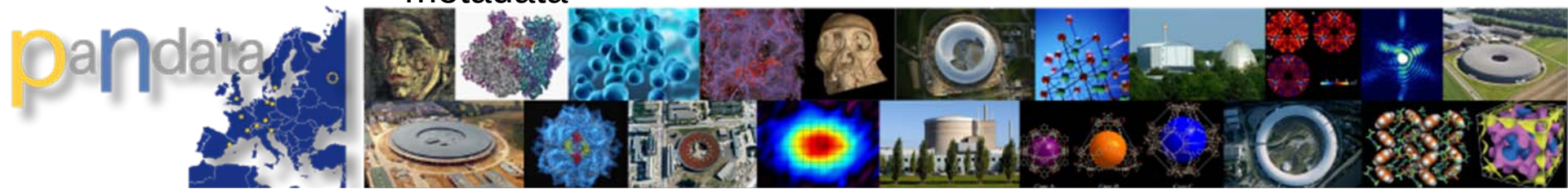
Metadata capture and data archive.

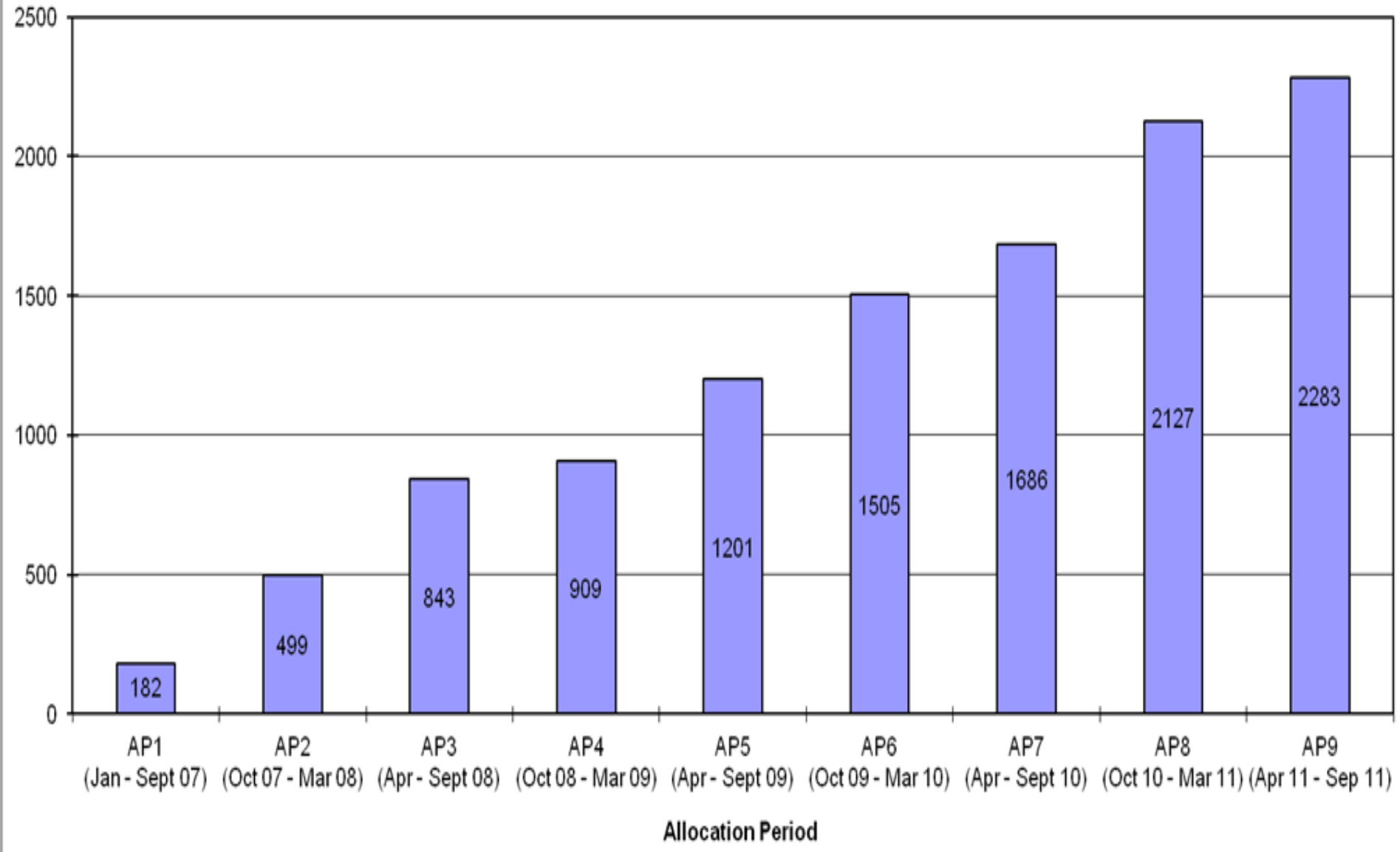




Data analysis and visualisation

IMMEDIATE (DURING EXPERIMENTS)	**SHORT TERM** (BEFORE THE USER GOES HOME)	**LONG TERM** (AT DLS/USER'S INSTITUTION)
"Real time" data processing, analysis and visualisation – to make experimental decisions Remote access/control	Data reduction and processing – Users go home with clean data free of instrument artefacts. Preliminary data analysis – helpful, but may require significant processing power and know-how	Detailed analysis – from data to information. Incorporating results from other techniques. Experiments: ➢Provide parameters for a model. ➢Test/verify a model or theory. ➢Show where a new theory or model is required.

Number of External Users on Experiments



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 SRSTLE='
',
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',
 &END
S1YCENTRE        Time     qbpm1
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-0.80950           0.20   0.24907
-0.70950           0.20   0.25041
-0.60950           0.20   0.25021
-0.50950           0.20   0.24987
-0.40900           0.20   0.25822
-0.31000           0.20   0.26743
0.090500           0.20   0.29894
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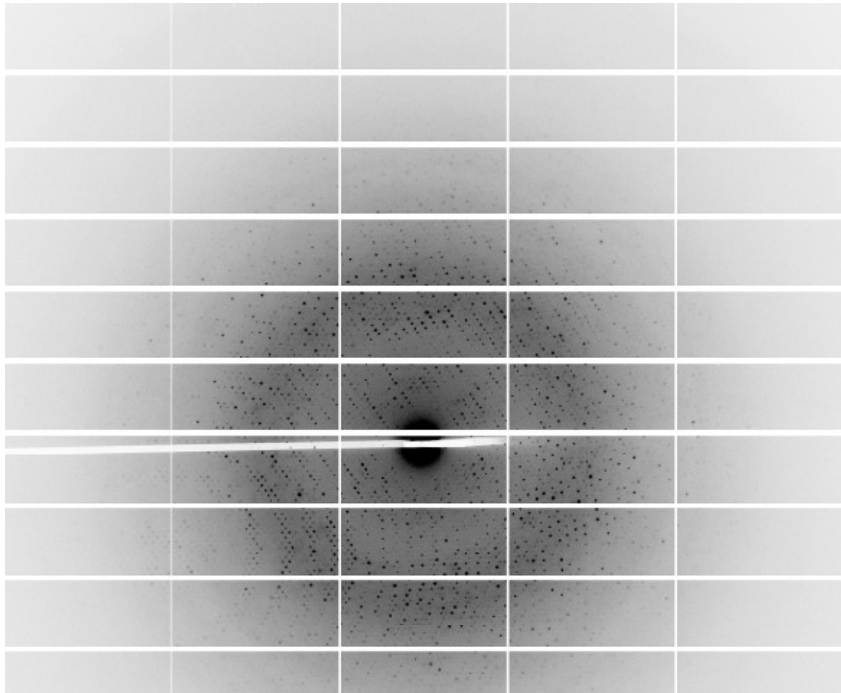
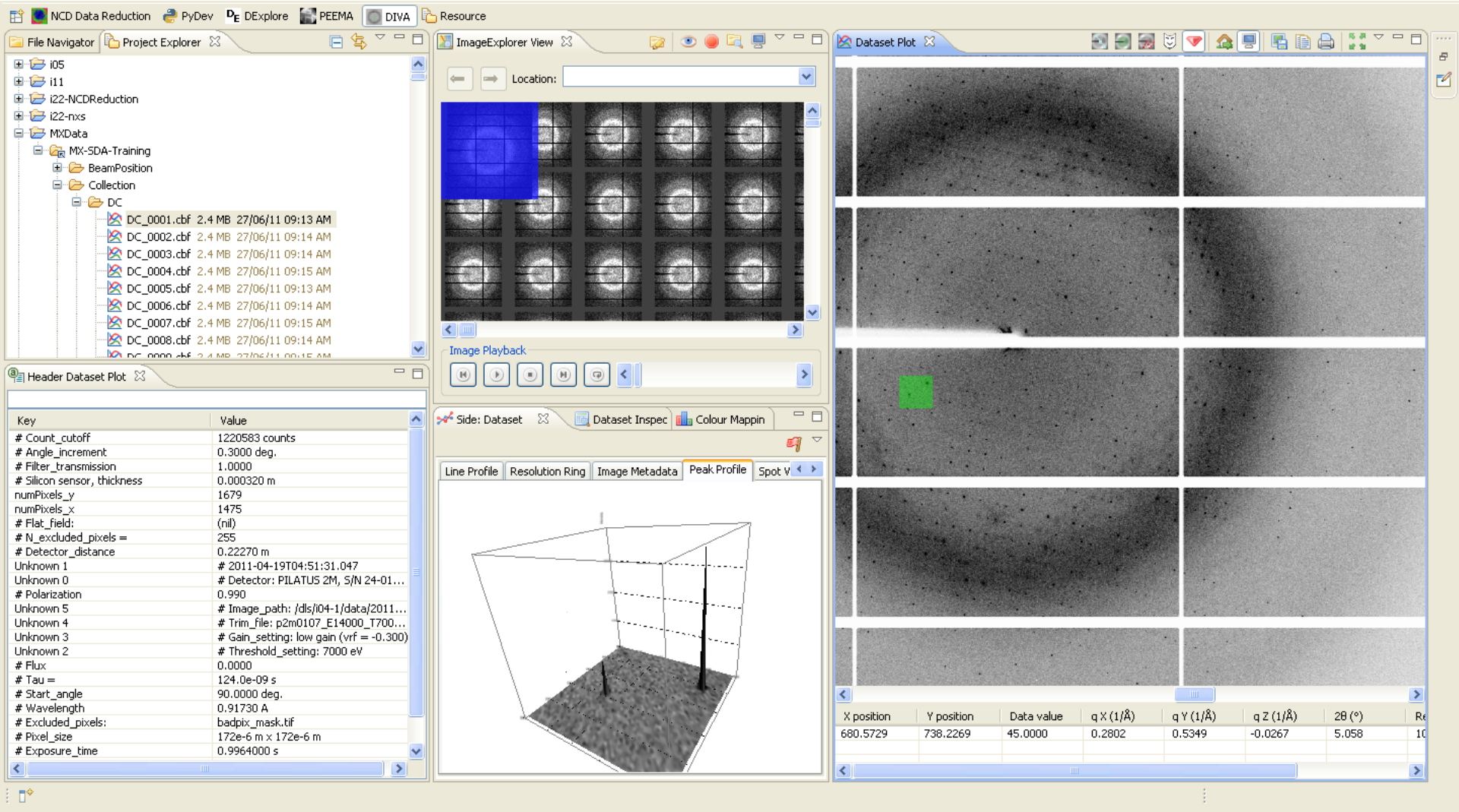
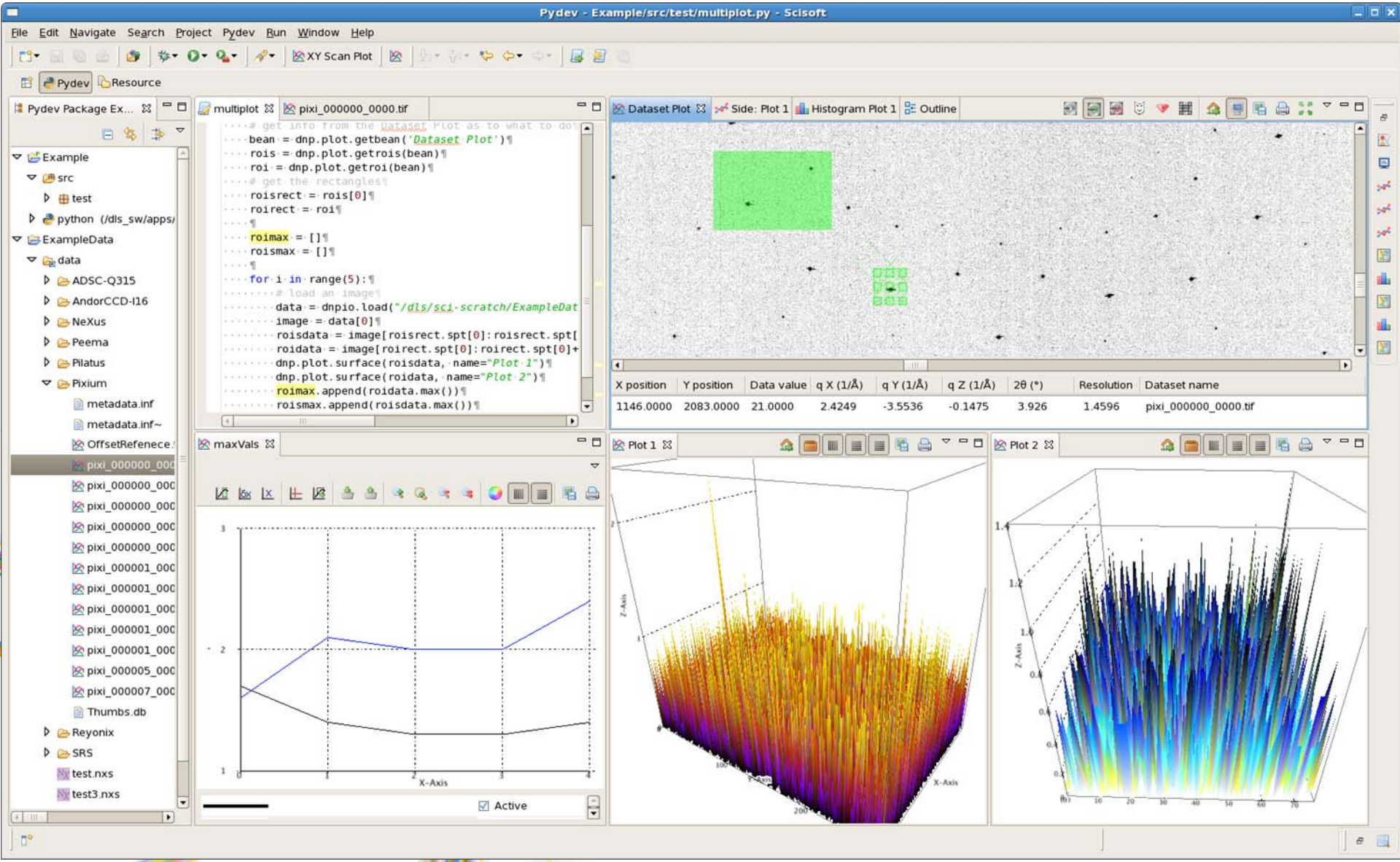


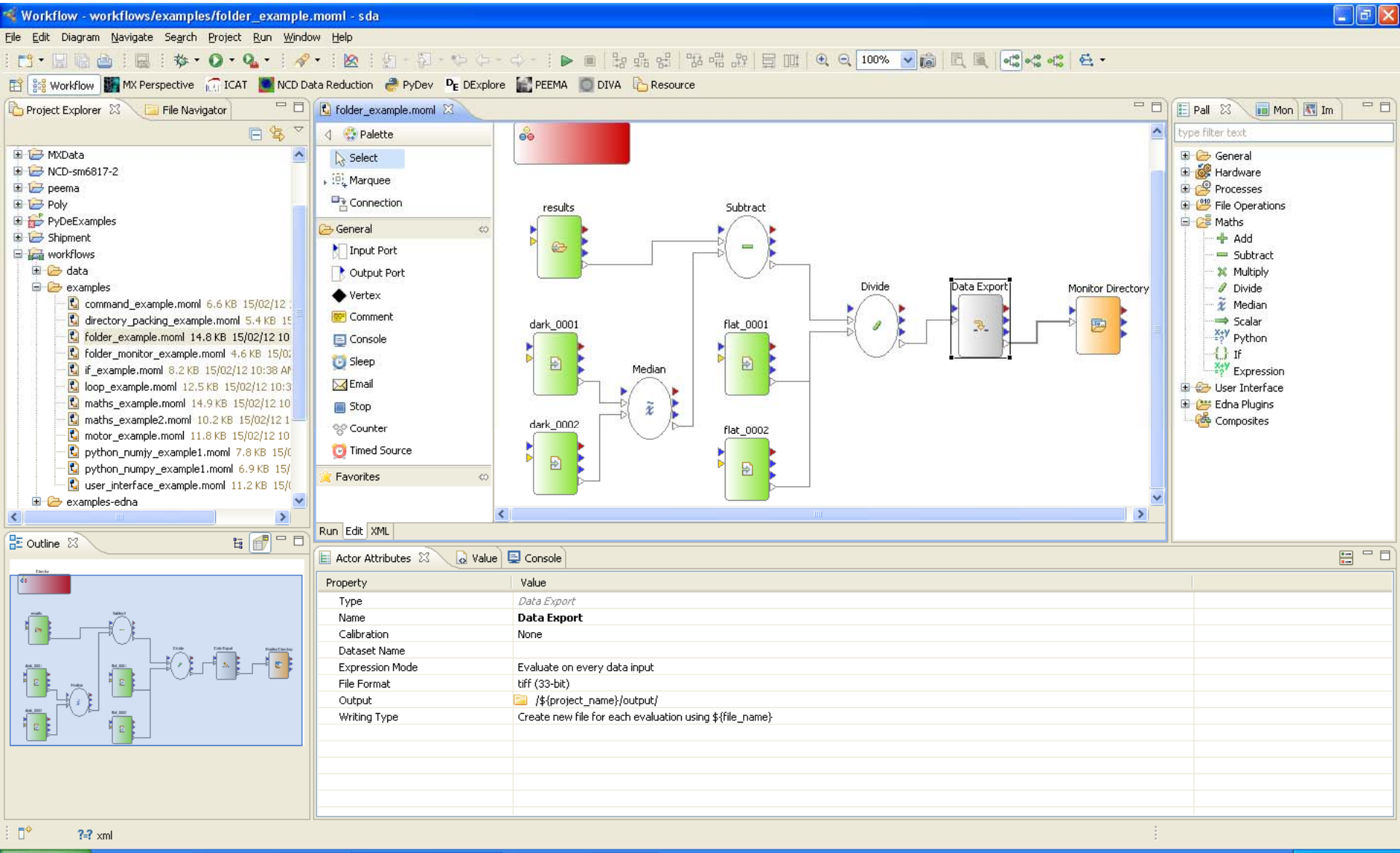
Analysis and visualisation tools



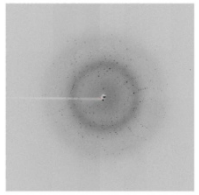
Analysis and visualisation tools

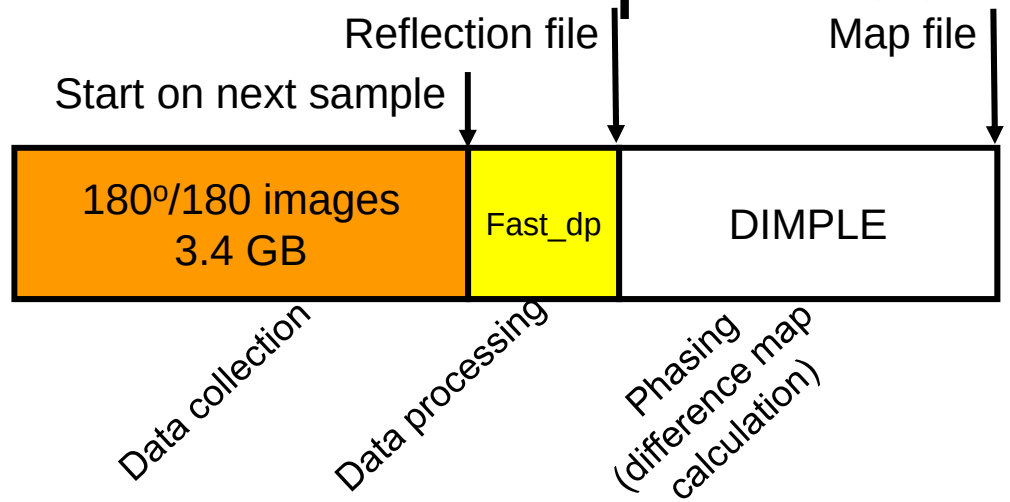


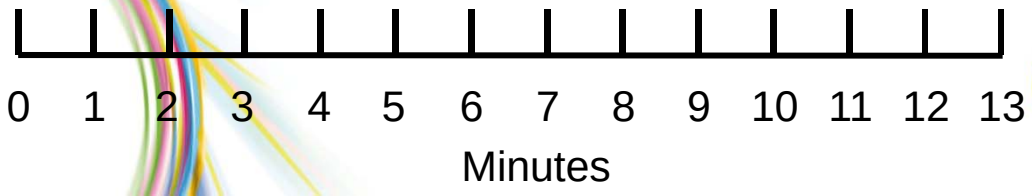
Analysis and visualisation tools



Automatic data processing







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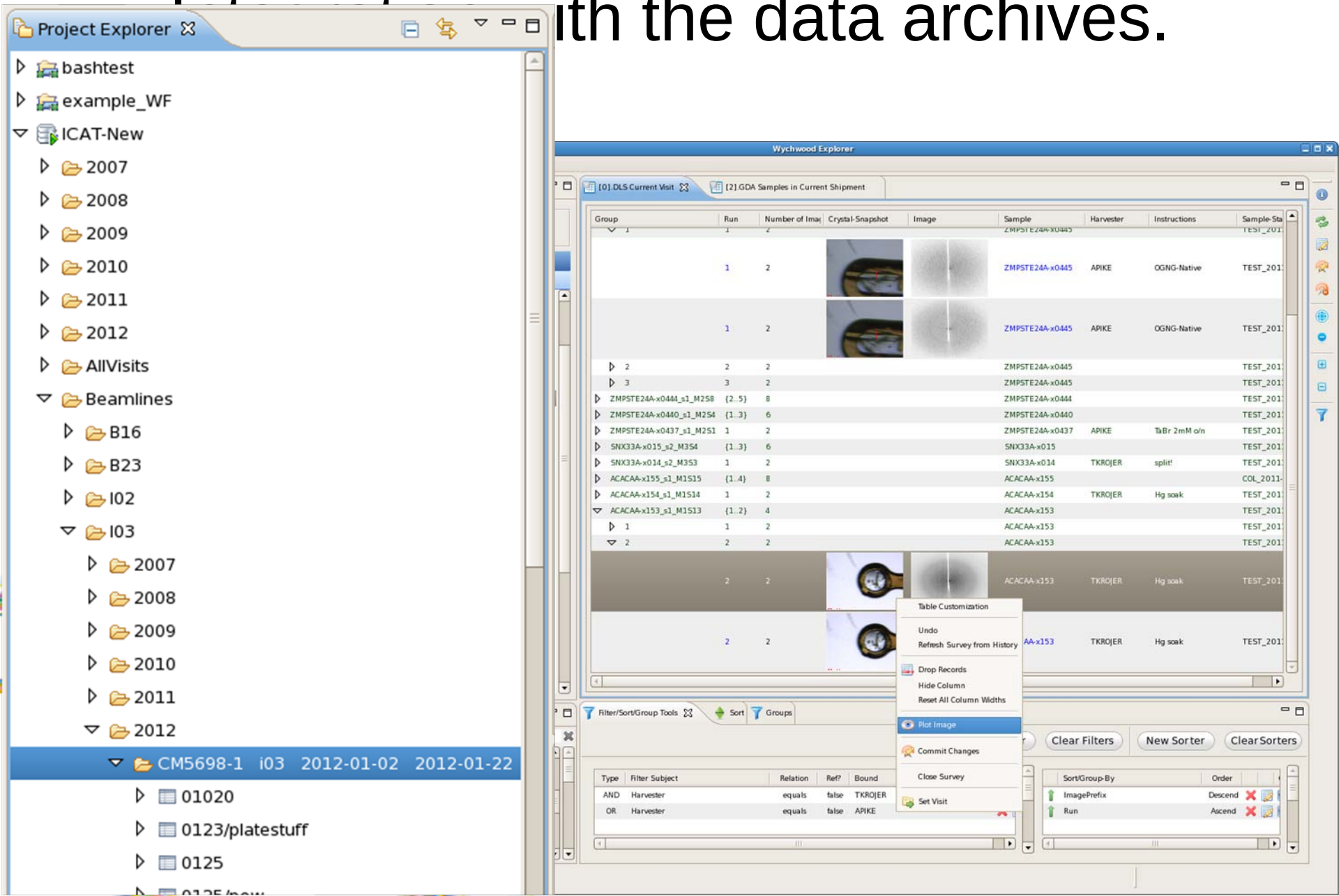
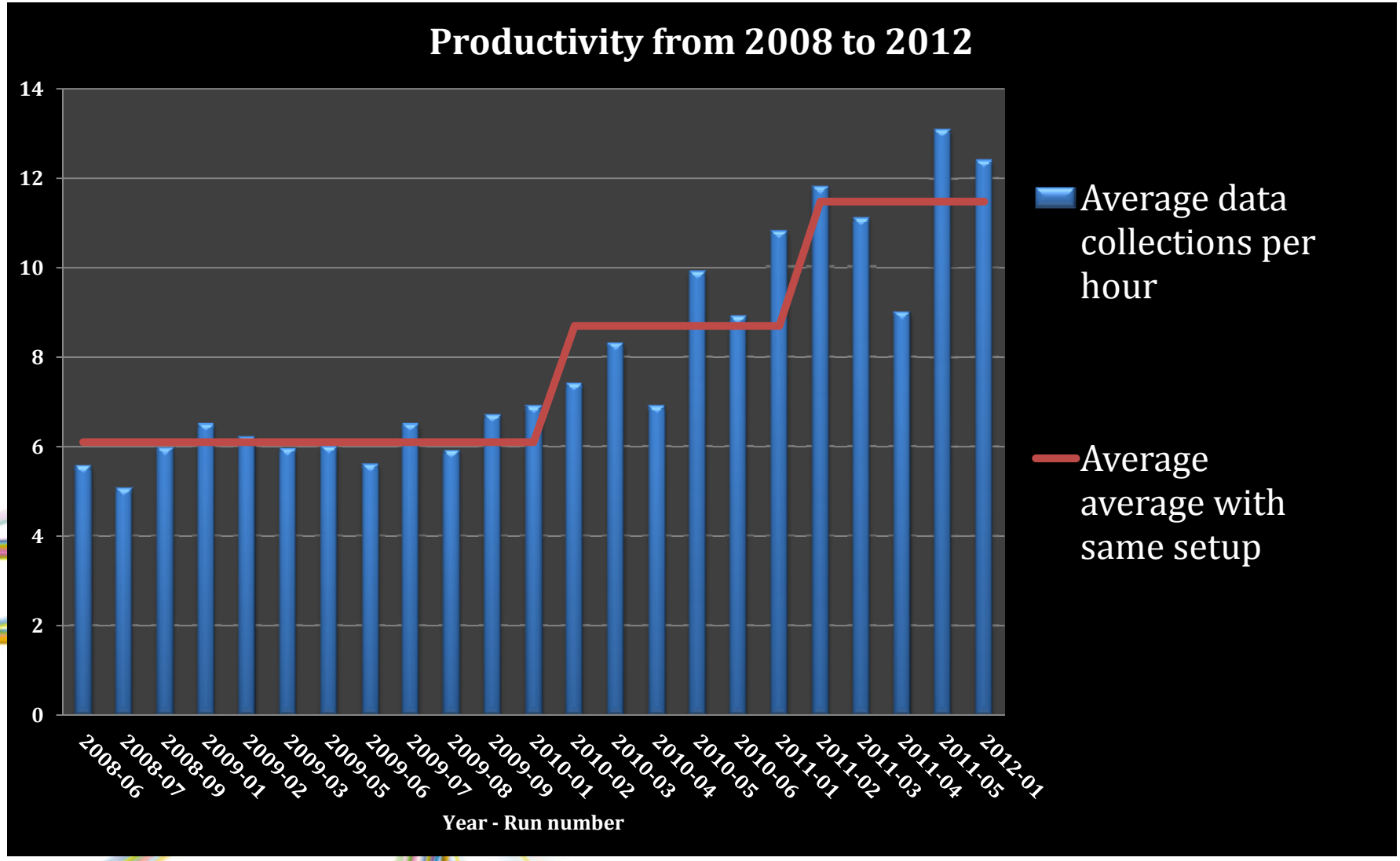
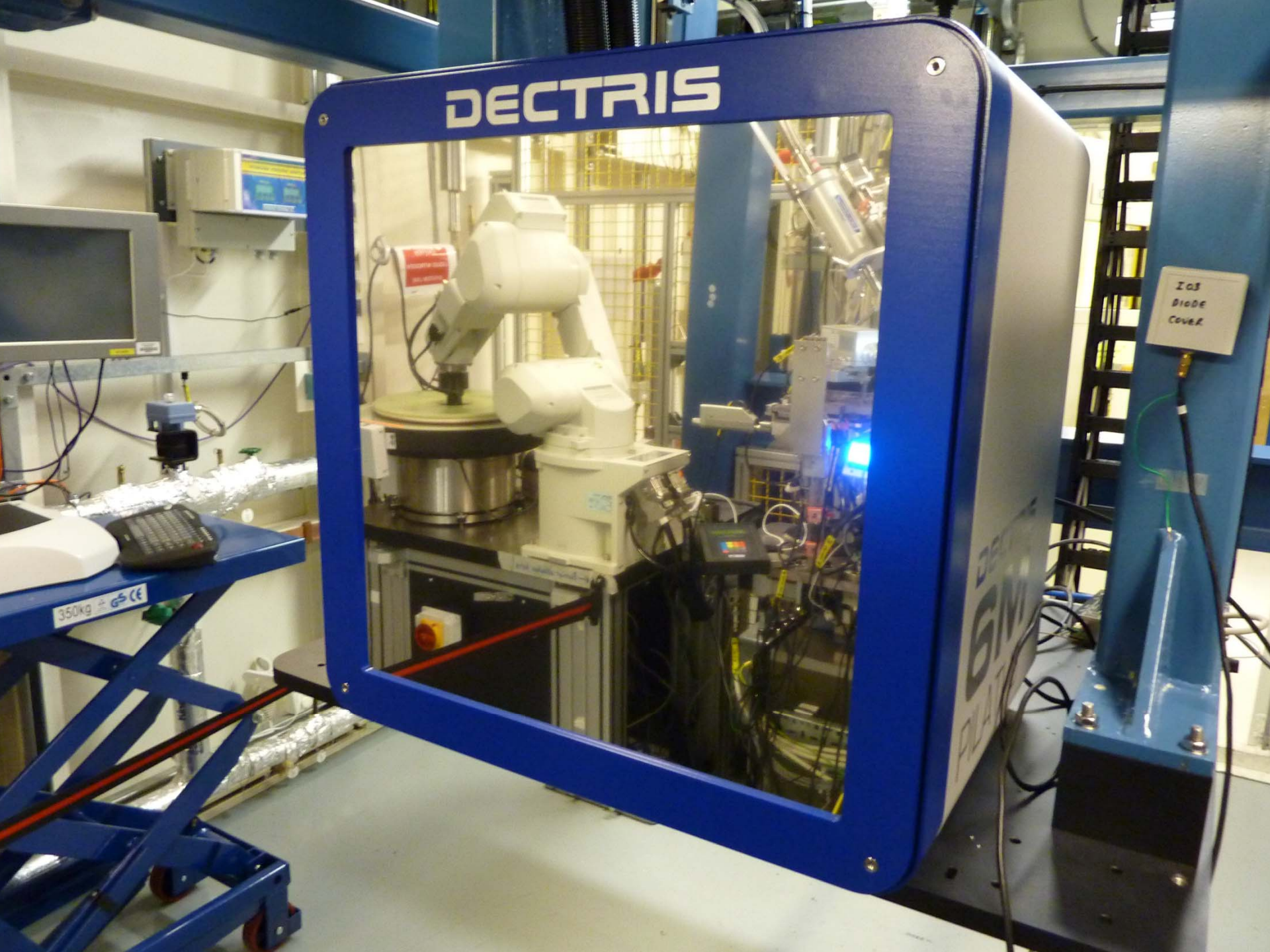
ith the data archives.

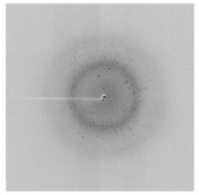


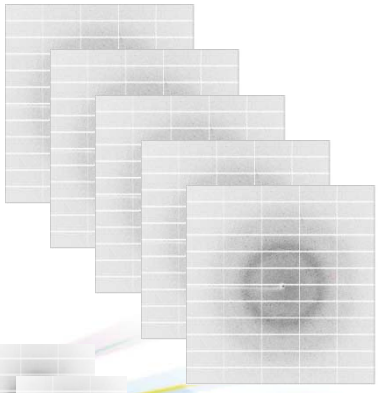
Increasing beamline ‘performance’




DECTRIS
350kg

Automatic data processing





Reflection file

Map file

Start on next sample

180º/180 images
3.4 GB

Fast_dp

DIMPLE

Data collection

Data processing

Phasing
(difference map
calculation)

180º
900 Images
5.6 GB

Fast_dp

DIMPLE

Data collection

Data processing

Phasing
(difference map
calculation)

180º
1800 Images
4.5 GB

Fast_dp

DIMPLE

0 1 2 3 4 5 6 7 8 9 10 11 12 13

Minutes

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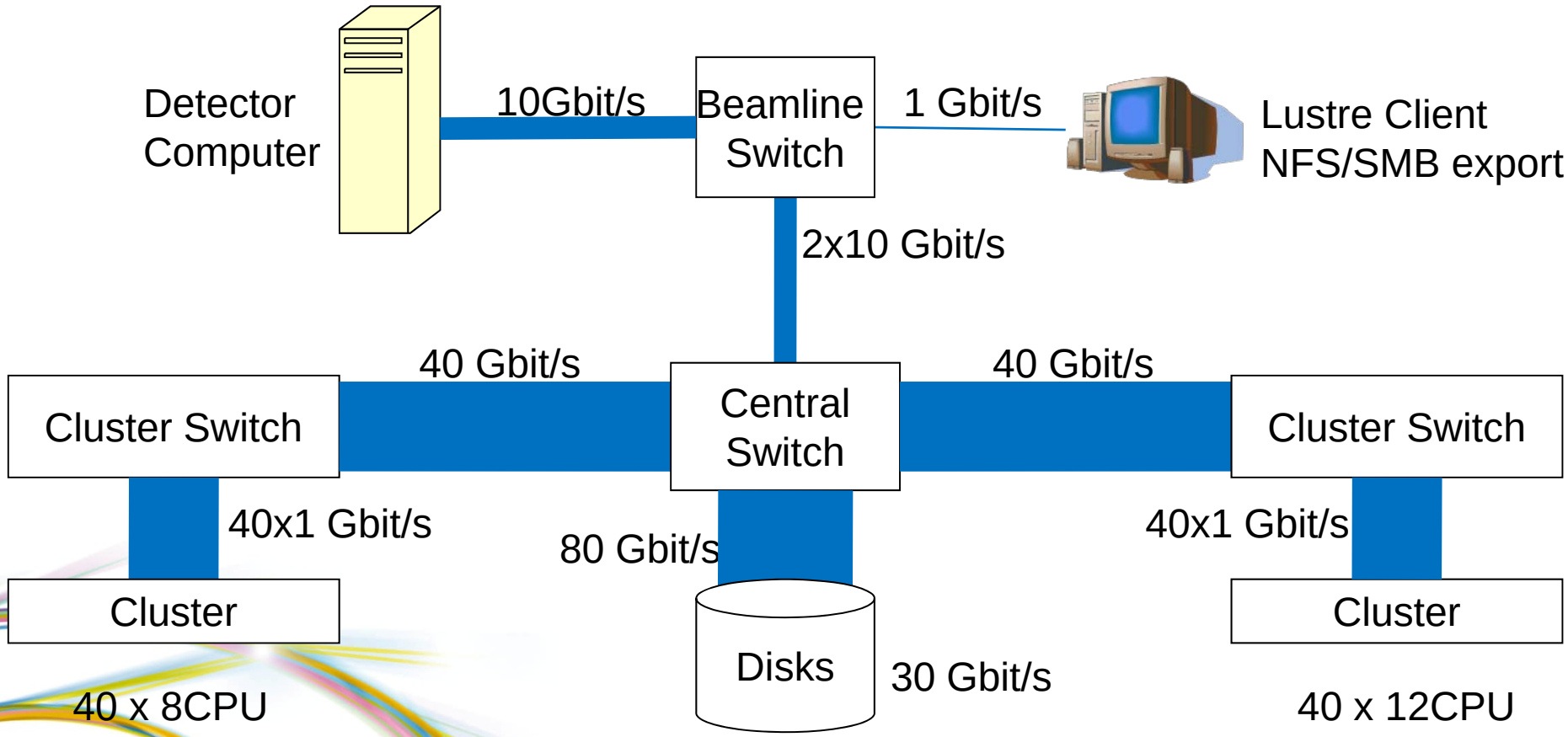
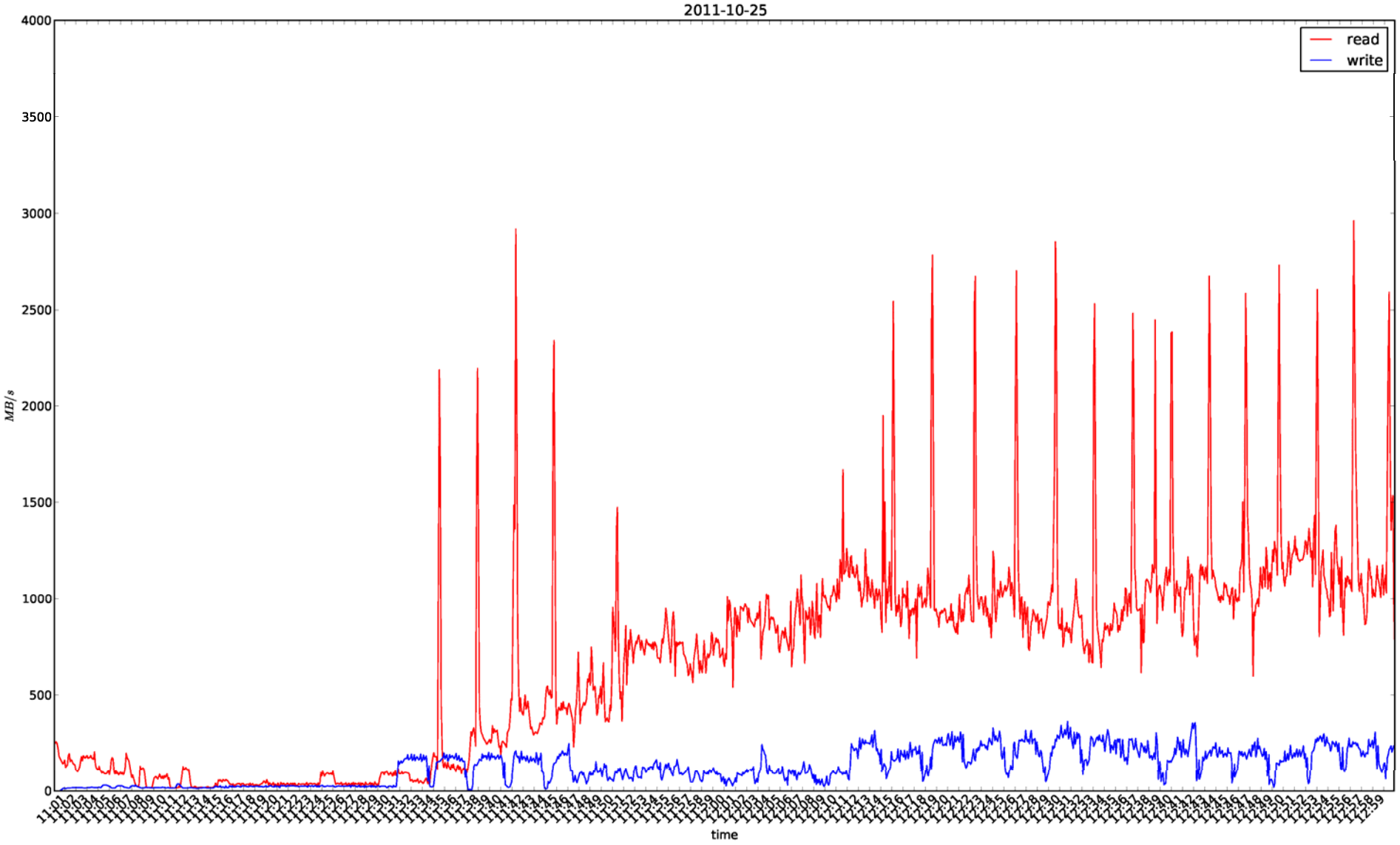
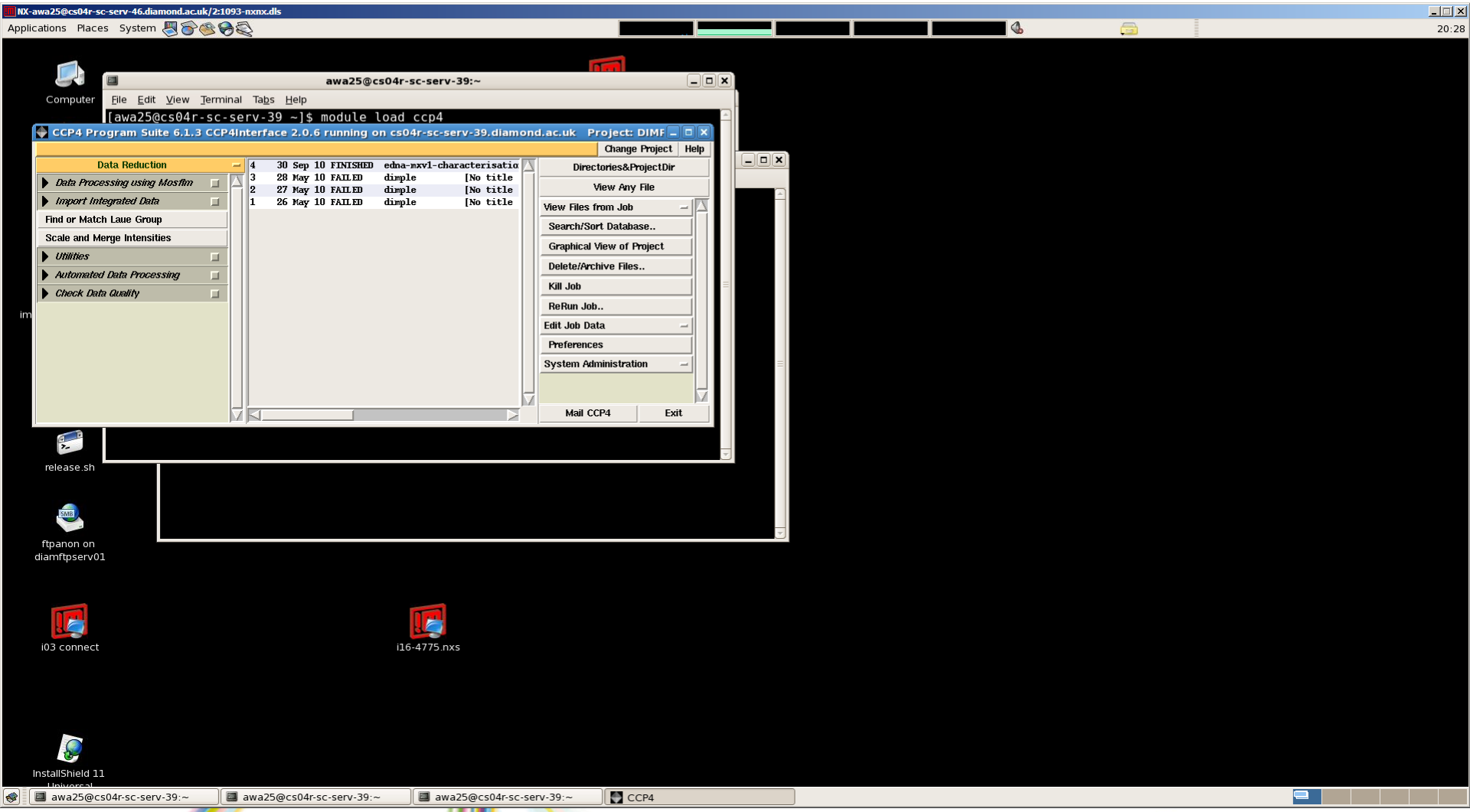
‘Local’ networking.



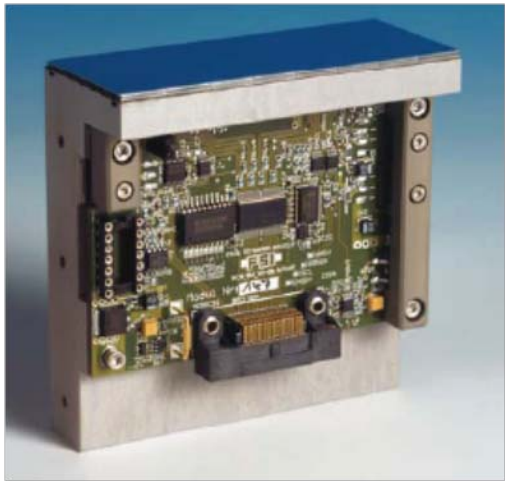
Data collection and processing data rates



A natural evolution…



Single module
8x2 chips
172 µm x 172 µm pixels



P6M
5x12 modules
~ 43x45 cm^2

- **Hybrid detector, 60 monolithic silicon sensors,**
- **Pixel size:** 172 um
- **No. of Pixels:** 2463 x 2527
- **Counter depth:** 20 bits
- **Frame rate:** 12 fps
- **Image size (Tif 32 bits):** ~23 MB
- **Compressed image:** ~ 6 MB
- **Data set:** ~ 1800 images
- **"Volume" of a data set:** 11 GB
- **P6M recently upgraded to 25 fps**
- **Future development P6M to 100 fps**

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Future scalability problems with crystallographic analysis

- Sheer number of files and data rates
  - Changing the file formats and structure, no longer perceived as a series of ‘films’
- Increased deployment of ‘longer’ running processing jobs
  - Use more disparate computing and exploit new hardware
- Continued use of legacy code
  - New initiatives to write code and new algorithms

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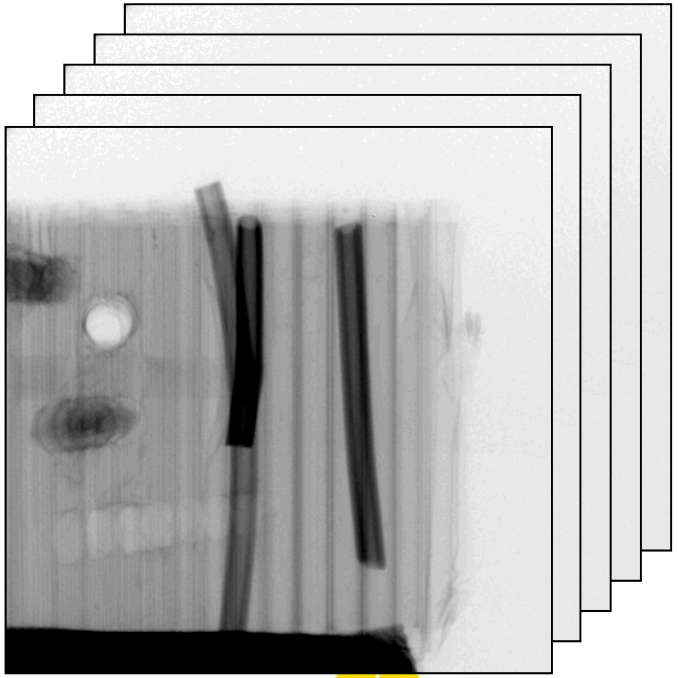
Tomography – Data Collection

- Data is collected straight to HDF5 3D data arrays

  - 4000x2600 pixel 16 bit greyscale image
  - Stored as an [4000,2600,6000] array
  - Totals around 120 GB of data
  - Collection Time can be as fast as 30 minutes.



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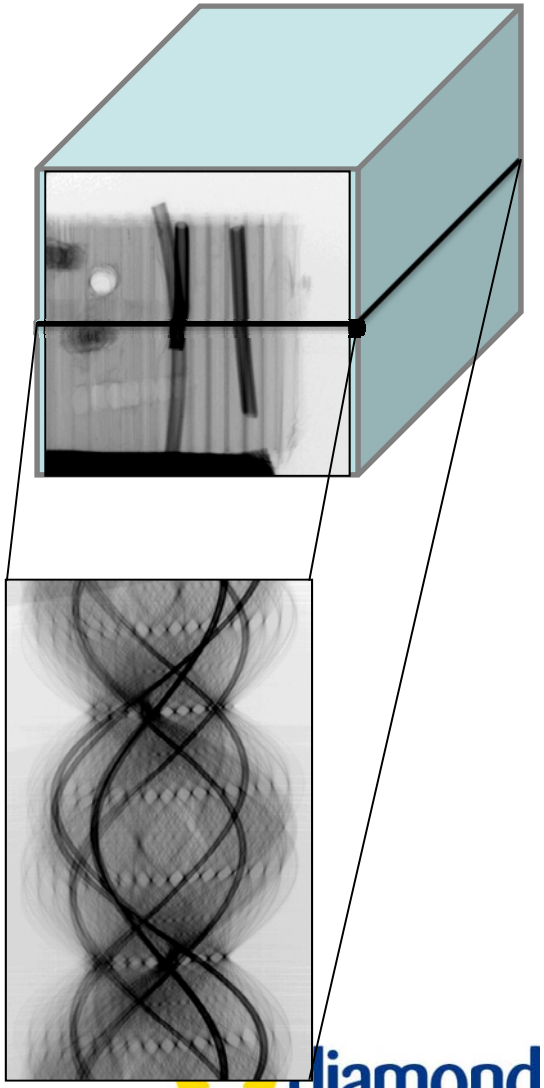
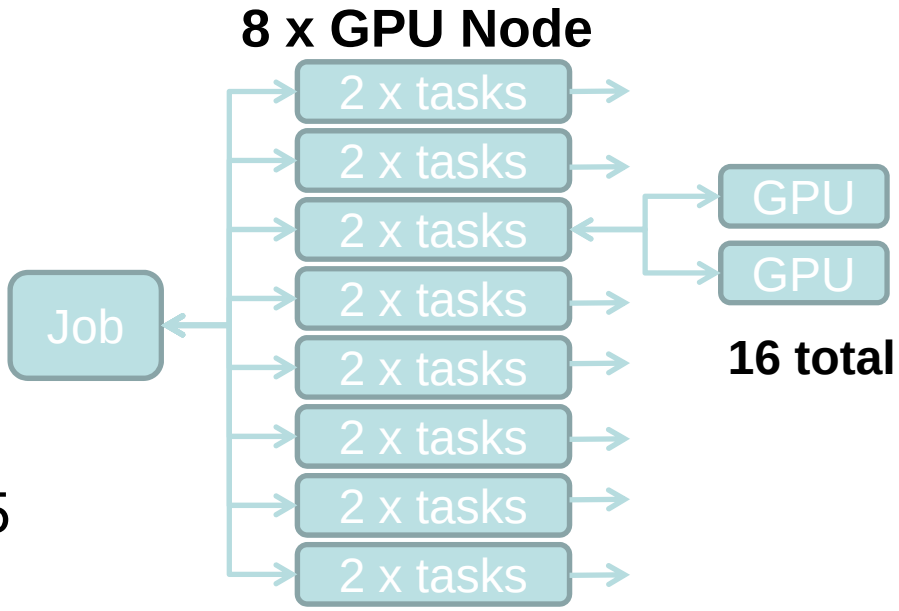
Tomography – Data Slicing

- The data is collected as [4000,2600,1] images
- The Camera software caches images though so that it can be written in [4000,16,8] chunks
- This is so that the data can be read out quickly as [4000,1,6000] sinograms, directly from the file.



Tomography – Data Extraction

- Data is read out as a stack of sinograms using parallel hdf5 across 8 dedicated GPU cluster nodes, running 2 tasks per machine.
- The bandwidth from the Lustre file system using parallel HDF5 is 25MB/s per Job, meaning a total parallel read speed of about 400MB/s
- We are hoping to push this closer to line speed (50MB/s) with further optimisations.



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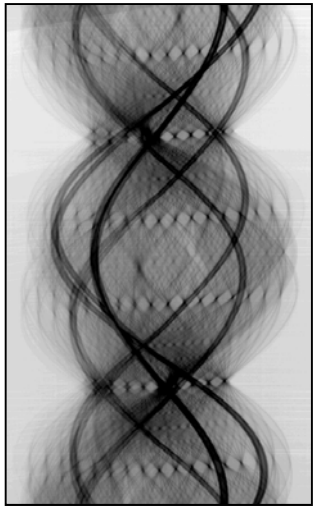
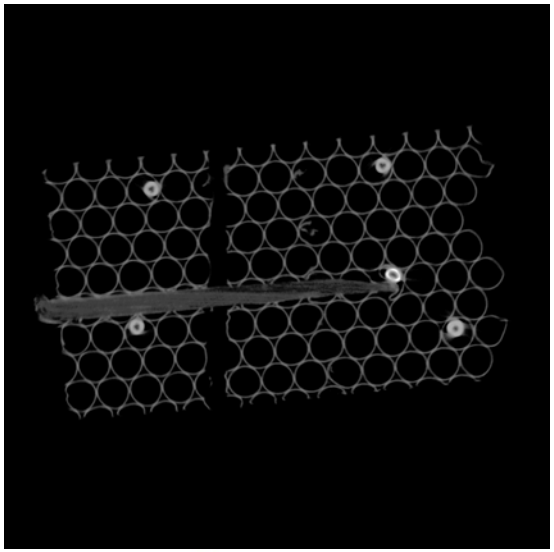
Tomography – Reconstruction

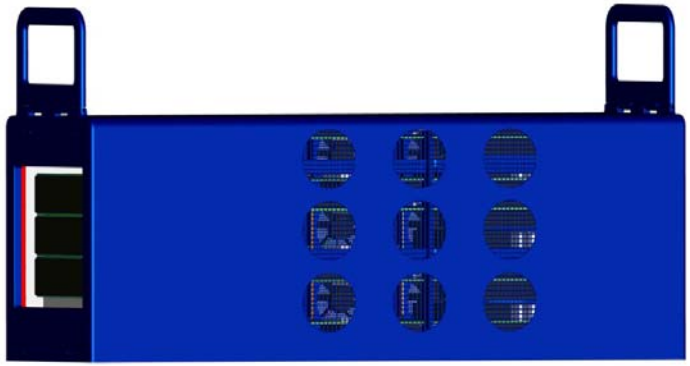


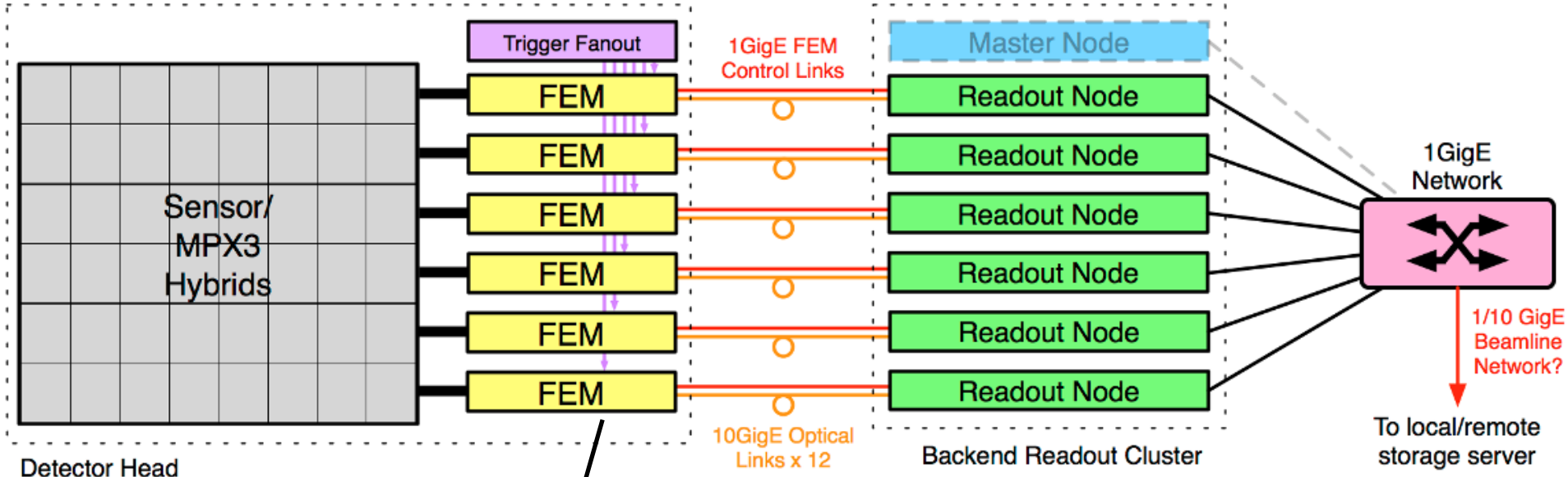
- Each of the 16 jobs then processes their set of sinograms using one of our GPUs
- Currently takes about 17 seconds per Sinogram, so this totals a reconstruction time of about 45 minutes
- We are currently looking to treble the number of GPU’s in this older cluster, and buy a new GPU Cluster to decrease times, and deal with more tomography beamlines coming on line.



EXCALIBUR

3 modules
3M pixels (11 x 10 cm)
8x2 MPX3/module
1 FPGA card / row of 8 MPX3s





Front-End Module (FEM) FPGA card

Readout backend: 6 Linux nodes

- Buffering, local storage & processing of image data
- Interface to EPICS for DAQ & control

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Conclusions.

Both during and after the ‘beamtime’:

- Data rates are increasing from larger or faster detectors.
- Data rates are increasing from beamline stability and performance.
- Data rates are increasing from ever growing automated processing, analysis, visualisation expectations.
- Structured hierarchical parallel well R/W file formats and structures can help to some extent with the data avalanche.
- Multiple data streams and keeping data in memory will help.
- Investment in new algorithms and exploitation of new hardware.