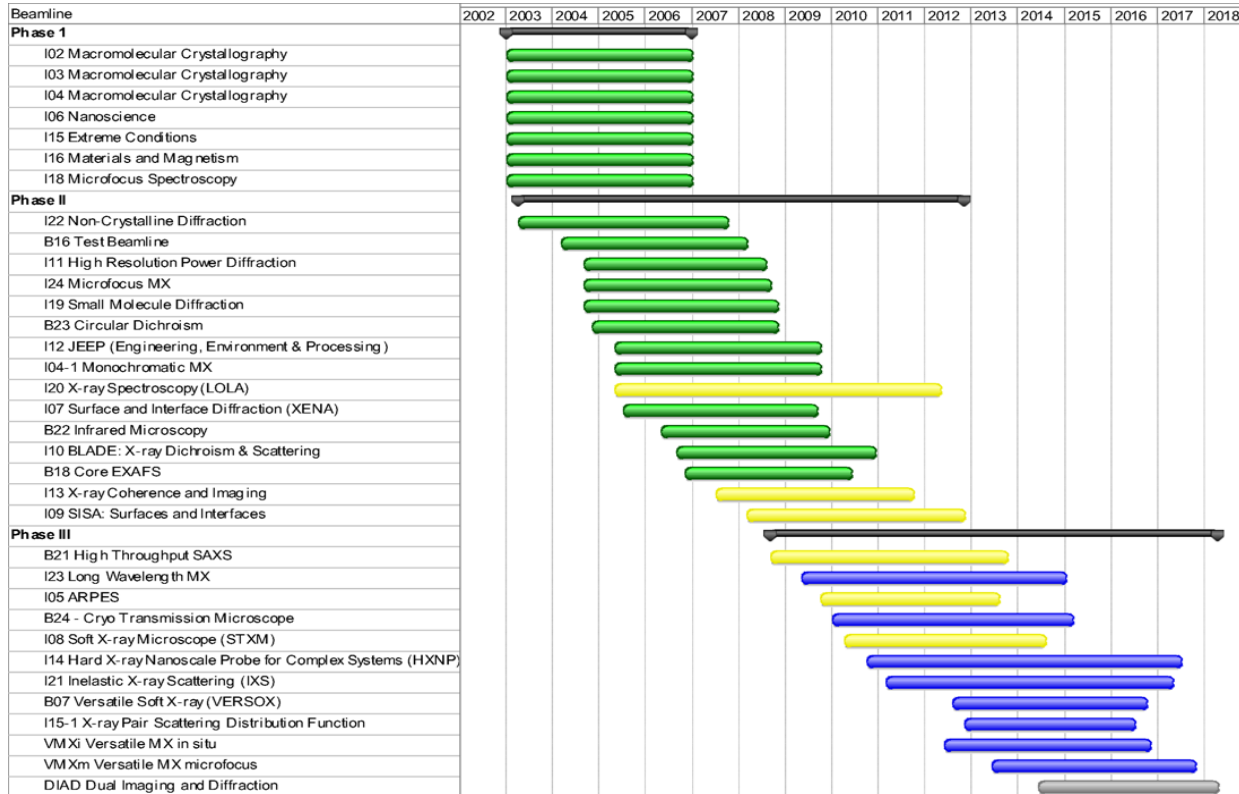# Mapping Developments at Diamond

Rob Walton

22nd October, ICALEPCS 2015, Melbourne

Scaling software at Diamond

| Beamline	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
Phase 1																	
I02 Macromolecular Crystallography																	
I03 Macromolecular Crystallography																	
I04 Macromolecular Crystallography																	
I06 Nanoscience																	
I15 Extreme Conditions																	
I16 Materials and Magnetism																	
I18 Microfocus Spectroscopy																	
Phase II																	
I22 Non-Crystalline Diffraction																	
B16 Test Beamline																	
I11 High Resolution Power Diffraction																	
I24 Microfocus MX																	
I19 Small Molecule Diffraction																	
B23 Circular Dichroism																	
I12 JEEP (Engineering, Environment & Processing)																	
I04-1 Monochromatic MX																	
I20 X-ray Spectroscopy (LOLA)																	
I07 Surface and Interface Diffraction (XENA)																	
B22 Infrared Microscopy																	
I10 BLADE: X-ray Dichroism & Scattering																	
B18 Core EXAFS																	
I13 X-ray Coherence and Imaging																	
I09 SISA: Surfaces and Interfaces																	
Phase III																	
B21 High Throughput SAXS																	
I23 Long Wavelength MX																	
I05 ARPES																	
B24 - Cryo Transmission Microscope																	
I08 Soft X-ray Microscope (STXM)																	
I14 Hard X-ray Nanoscale Probe for Complex Systems (HXNP)																	
I21 Inelastic X-ray Scattering (IXS)																	
B07 Versatile Soft X-ray (VERSOX)																	
I15-1 X-ray Pair Scattering Distribution Function																	
VMXi Versatile MX in situ																	
VMXm Versatile MX microfocus																	
DIAD Dual Imaging and Diffraction																	

- 31 beamlines
- 43+ end stations
- Ever higher demands of software
- Focused on scaling
  - Deploy
  - Automation
  - **Mapping**

Mapping

- Many beamlines perform mapping experiments
- Move sample under focused x-rays
- Continuous or trajectory motion (a.k.a. fly scan)
- Interactions include e.g.:
  - **Fluorescence (XRF)**
  - Absorption
  - Scattering
  - Diffraction
  - **Electron emission (ARPES)**
- Process
  - Reduce data to create a map (image)
- Visualization
  - Show map of reduced data
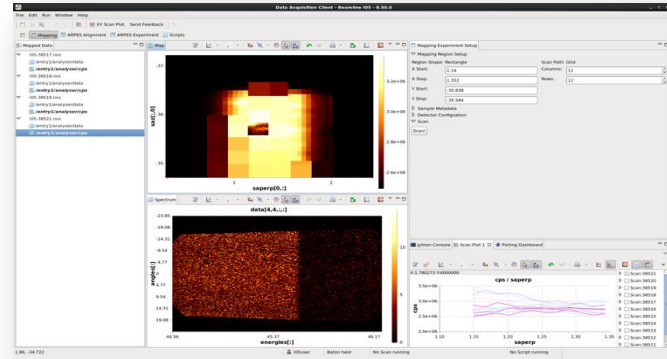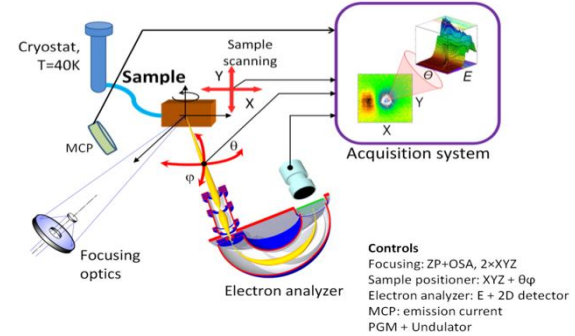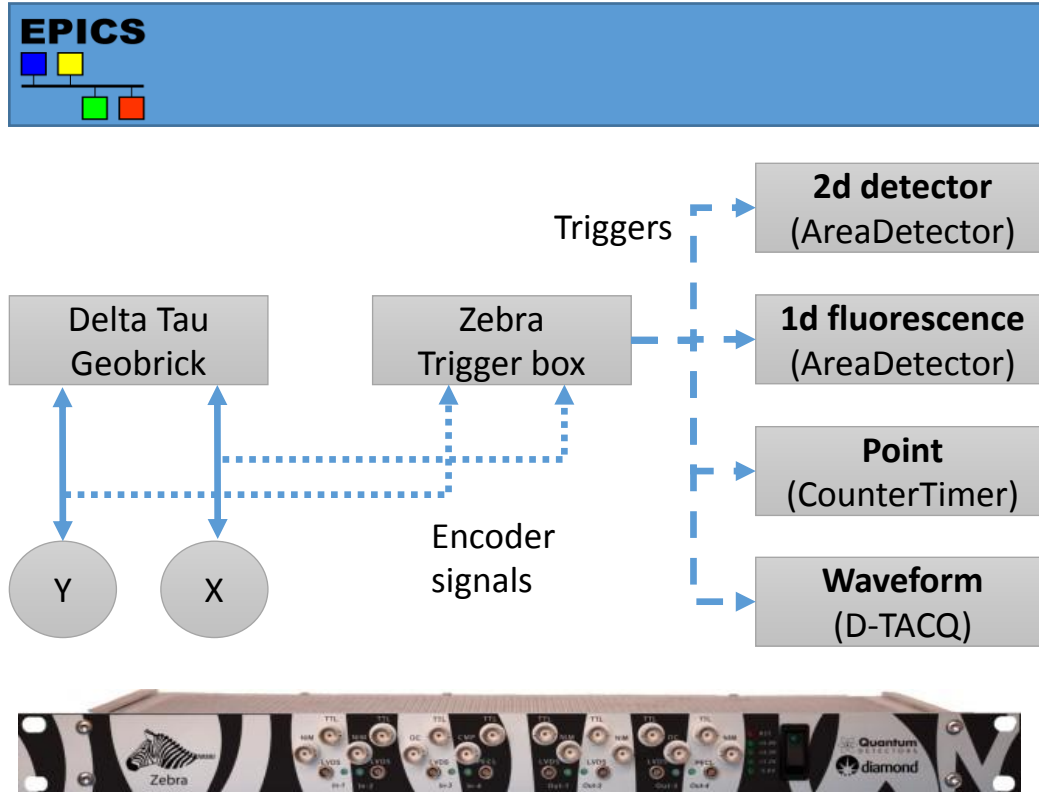 - Click to see raw or detailed data

Fluorescence

Nano-ARPES

www.aps.anl.gov
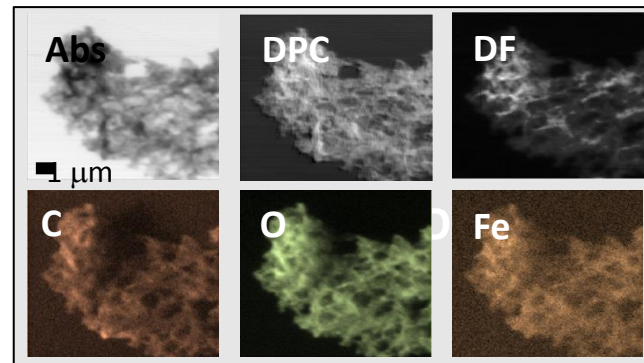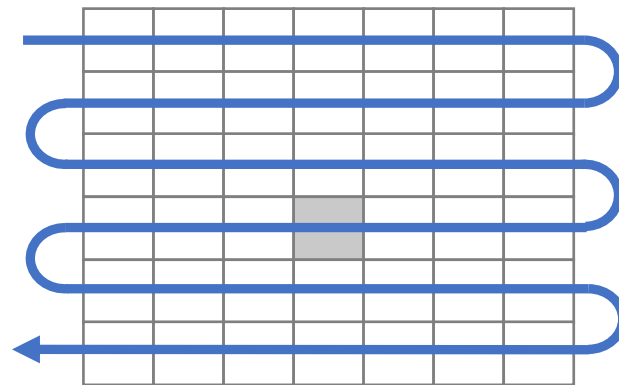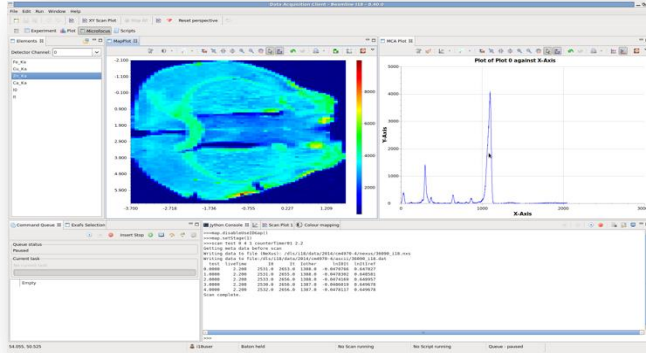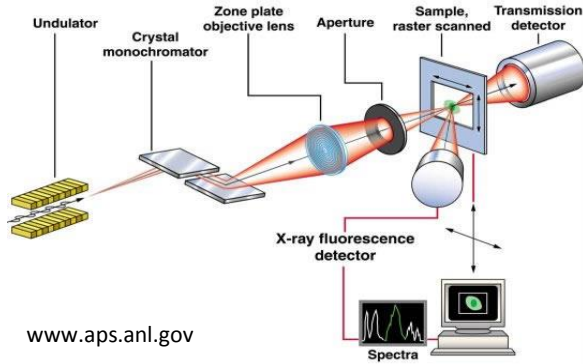
Map of zinc content, detail is spectrum

Map of measure of electron momenta, detail is energy v's angle

Hardware

Diamond's "Mapping project"

- Create generic solutions
- Target beamlines
  - 5 diverse to start
  - More to follow MX (7), Other (5+)
- Scope:
  - User work flow
  - Streamlined data flow
  - Generic continuous scanning framework
  - Standardise processing and visualisation
  - Reusable GUI components
- Cuts across many systems and groups

		XRF	XAS	Diffraction	ARPES	SAXS
I05-1	Nano-ARPES				■	
I08	Scanning x-ray microscopy	■	■	■		
I13	X-Ray Imaging &Coherence			■		
I14	Hard X-ray nanoprobe	■	■	■		■
I18	Microfocus Spectroscopy	■	■	■		

Initial target beamlines

User work flow

- Interactively explore surface
    - Take visual image
    - Perform scan, selecting
        - Detectors
        - Parameters
        - Region, line or point
    - Process to create map or other data
    - Add to history
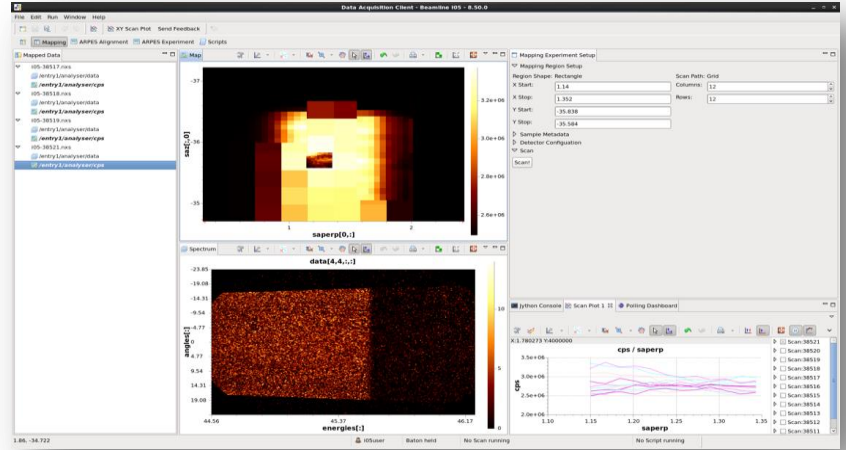
(Prototype RCP interface)
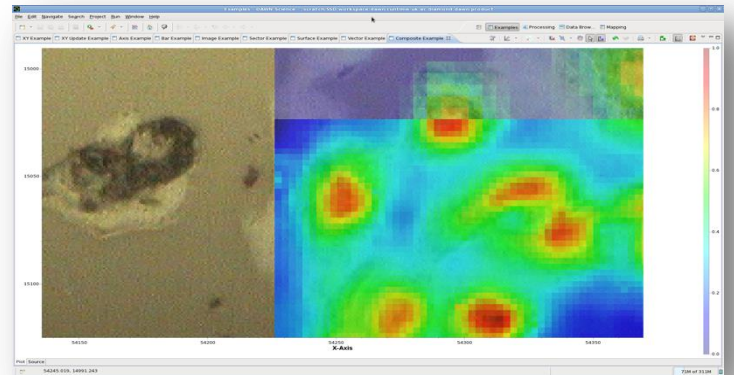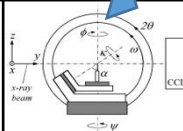
Streamlined data flow

- Committed to NeXus
  - Multidimensional
  - Multimodal (multiple techniques)
  - Geometry
  - Metadata (e.g. sample environment)
  - = Great for pipelined analysis (descriptive)
- Backed by HDF5
  - Combatable with centralized file storage
    - (small files load Lustre & GPFS metadata server)
  - Detectors write data
- But cannot be read as written
  - **HDF SWMR to the rescue**
    - **S**ingle **W**rite **M**ultiple **R**ead
    - HDF5 1.10 Spring 2016 (beta available)

Components

Access to all data live

- SWMR
  - Single path for data
- Same processing used live and after a collection
  - DAWN analysis pipeline
    - Calibrated powder diffraction
    - ARPES analysis
    - Tomography reconstruction
  … with access to cluster
- Same visualisation used live and after a collection
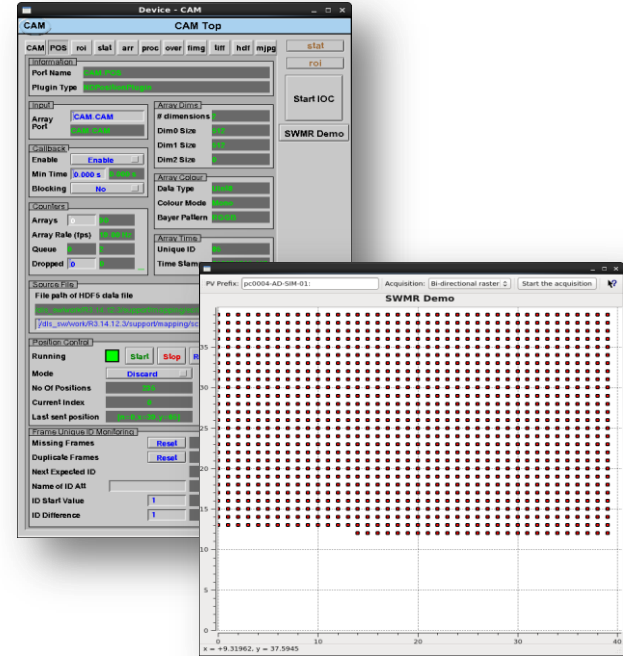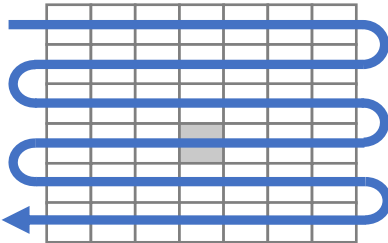 - DAWN (dawnsci.org)

DAWN Analysis Pipeline
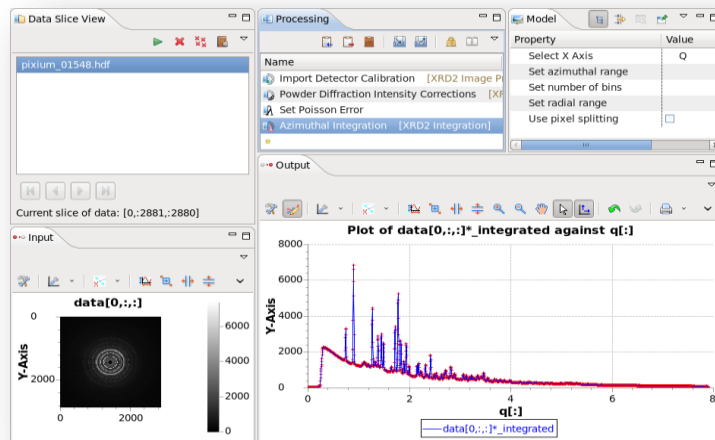
DAWN Hyperspectral viewer
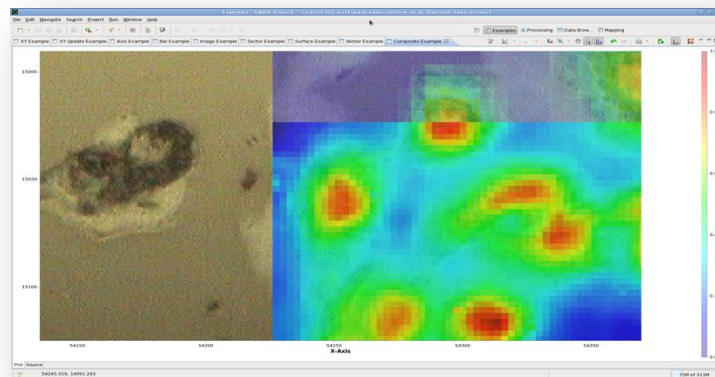
AreaDetector & Zebra SWMR enhancements

- HDF writing upgraded:
  - write HDF SWMR
  - write multidimensional data
  - Fill dataset in arbitrary order matching beam's path across surface
- E.g. Bi-directional raster scan
  - 2d (scan) + 2d (detector) = 4d
  - Snake path

Epics AreaDetector writing bi-directional data during a raster scan using new plugin accessed by HDF plugins

New Malcolm EPICS service

- API for a generic continuous scanning framework
- Malcolm in the middle between acquisition server and EPICS
- Configure-Run state machine
  - config(), run(), pause(), abort(), reset()
- Nestable
- Currently:
  - Python server with JSON over websocket or zeroMQ
  - Java declarative OSGI service
  - Prototyping nano-ARPES stage and electron analyser
- Future:
  - pvData over pvAccess
  - C++ port for AreaDetector
  - More scans types
 - More detector combinations
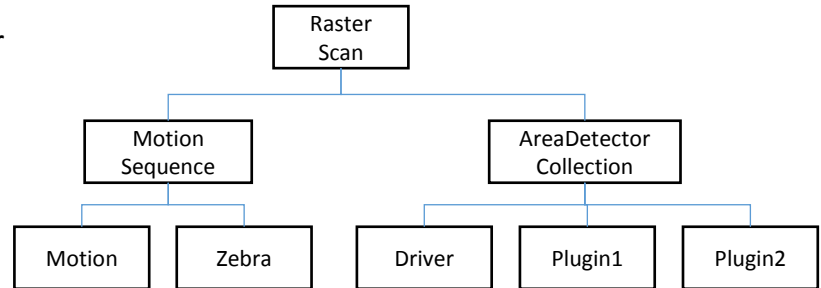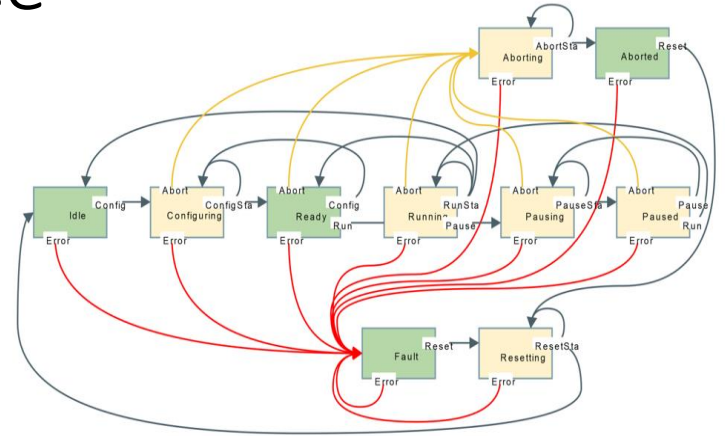
User interface views

- Eclipse RCP
- Eclipse IDatasets
  - From NeXus file
  - From Remote Dataset service
- Light to maintain
  - Auto generated parameter editors
  - Compose for different beamlines
  - Future: Adapt to server?
- Build views into
  - GDA client
  - DAWN
  - Anything RCP
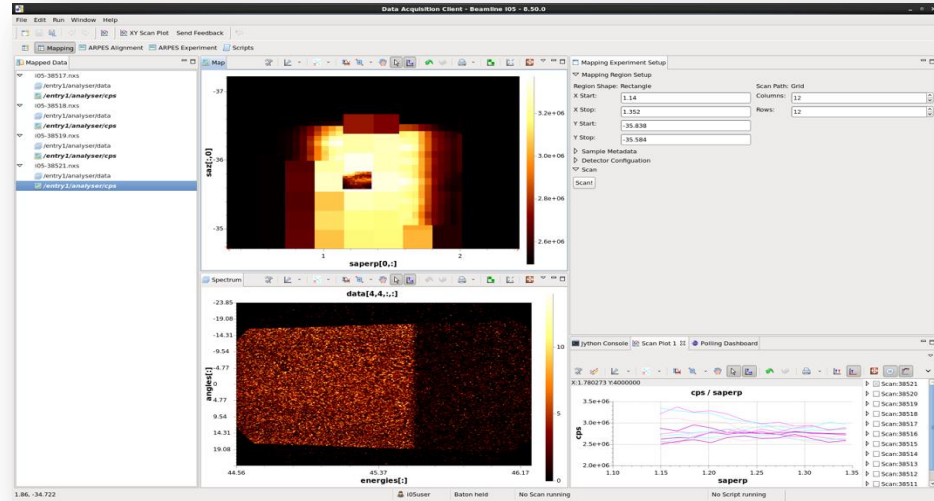
Acquisition server

- Acquisition Server contains:
  - NeXus Writer service
  - Malcolm OSGI service
  - Remote Dataset service for client
- JMS Broker (Active MQ)
  - Server to DAWN Pipeline analysis
  - Server to client
- Build acquisition server into
  - GDA server (splitting up)
  - Decoupled OSGI declarative services
    - Anything Java
    - Anything RCP (OSGI)
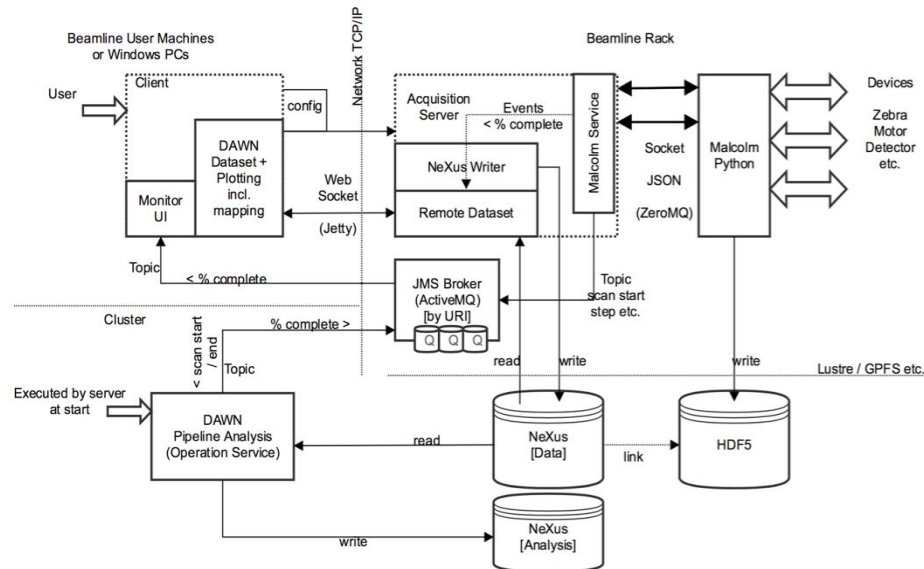
Status

- 6-8 months into project
- Tested on one beamline
- Deploying next Spring and Summer to 3 more
- 2 years to 'complete'

Conclusion

- Focused on 5 beamlines with more to follow
- We like NeXus HDF5 and with SWMR we looking forward to seeing out data like the good old days!
- Malcolm providing a promising API for continuous scanning
- Breaking down GDA software
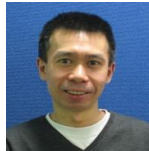- Line scans are just 1 x N mapping scans

Acknowledgements

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