Background

- Much existing data acquisition (e.g. PXGEN) old and developed independently, difficult to develop.
- SR Colleges and Synchrotron Radiation computing group (SRCG) formed.
- Greater collaboration between data acquisition developers in different scientific areas.
- Data acquisition hardware changing with increasing variety on different stations.
- Have to continue to maintain and develop existing software whilst incrementally developing better solution.

SRCG Objectives

- Increased cross college collaboration.
- New software to be developed through the use of more shared code, a common framework and standards.
- Easier to develop solutions and cope with changes, plug and play construction.
- Scripting language to facilitate easy configuration of experiments, based on Python.
- Distributed solution to cope with multiple hosts where required.
- Deployable to DIAMOND.

PX Objectives

- Replacement for PXGEN offering greater functionality.
- Uniform interface across stations, detectors, cameras etc.
- Simple GUIs that make set up and data collection easy.
- Automation wherever possible.
- Link data acquisition and processing.
- Flexibility to cope with future changes.
- Remote monitoring and control.

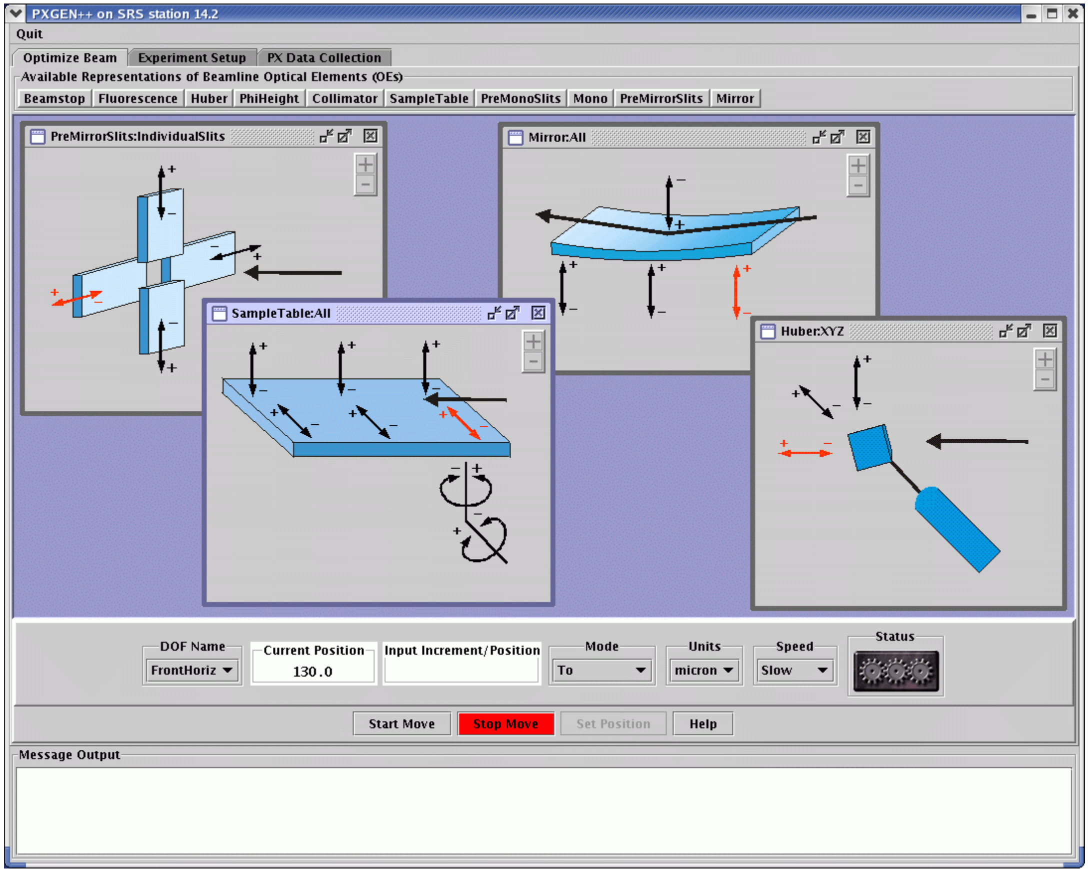
GDA – Generic Data Acquisition

- Object-oriented “plug and play” toolkit - easier to maintain and create configurable software systems.
- Common and technique specific classes part of the same overall package, GDA.
- Core object oriented development, Java, flexible and transportable.
- Objects to represent real beam line hardware e.g. detectors, cameras, sample changers, tables, mirrors etc.
- Use interfaces to give plug and play.
- Configuration of objects via XML files or database.
- Underlying levels can be in any language, interfaced by GDA classes.
- Use scripting for flexible control.
- Provide common ‘look and feel’.
- Allow a variety of network protocols to enable distribution (e.g. CORBA, sockets, SOAP).

PXGEN++ so far

- GUI has tabbed ‘look and feel’.
- Uses common GDA elements e.g. beam optimisation, XAFS.
- PX specific classes built as part of, and utilising other components from GDA. Likely to be refactored to be partly or wholly general.
- Basic functions for experiment set up and single wavelength data collection developed.
- Use of Rigaku sample changer included.
  - Standard Rigaku loop centring.
- Image display started but presently done via adxv.

Align beamline



DOF Name: FrontHoriz

Current Position: 130.0

Input Increment/Position:

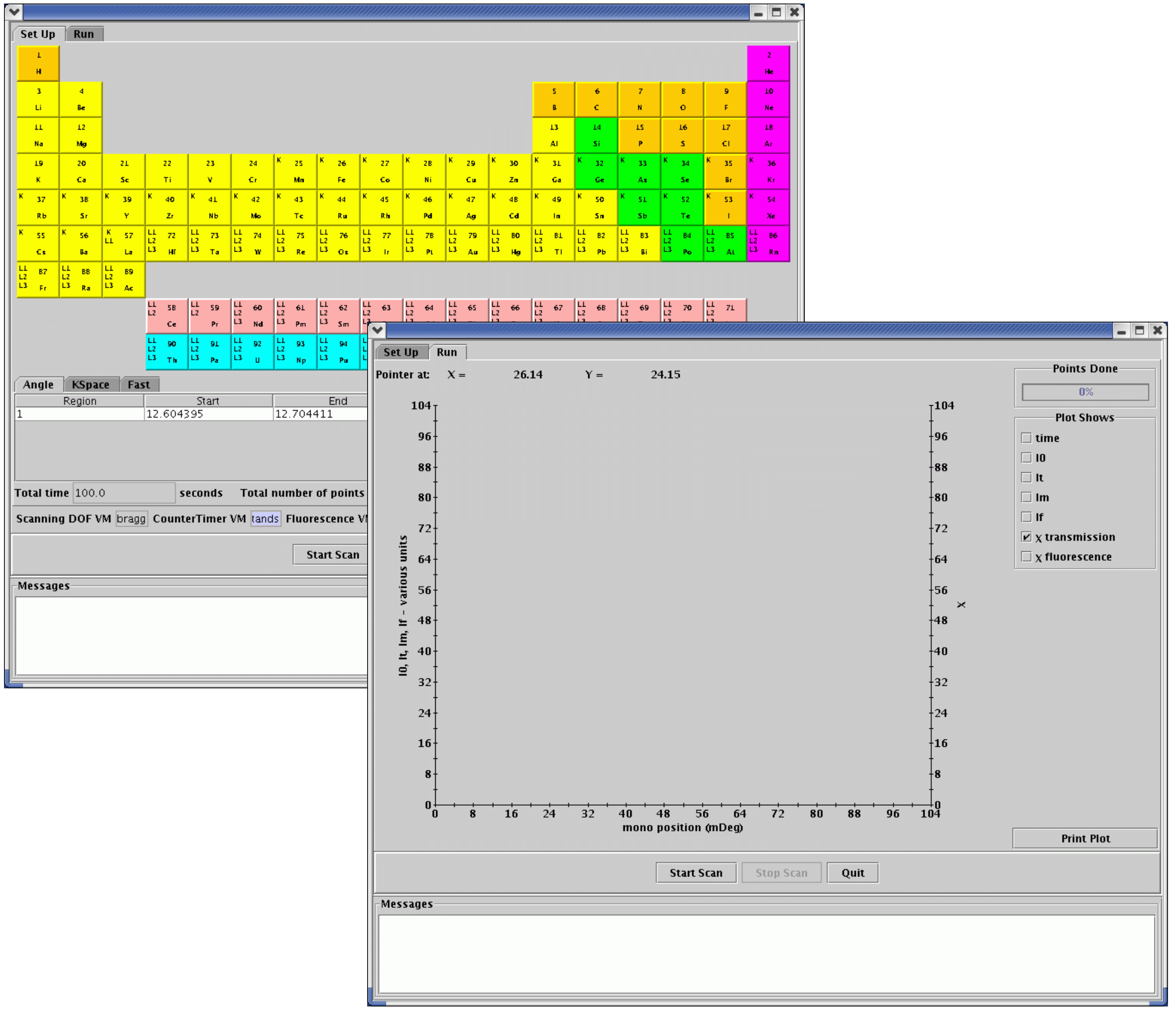
Mode: To

Units: micron

Speed: Slow

- Manually align beamline for data collection.
- OEMove provides a standard tool to allow the control and set up of Optical Elements.
- Easily configurable for different stations.
- All OEs implement a standard interface.
- Configuration loaded at runtime.
- One tool meets needs of many projects.
- GDA standard.

Xafs



Region	Start	End
1	12.604395	12.704411

Total time 100.0 seconds Total number of points

Scanning DOF VM bragg CounterTimer VM tands Fluorescence V

Pointer at: X = 26.14 Y = 24.15

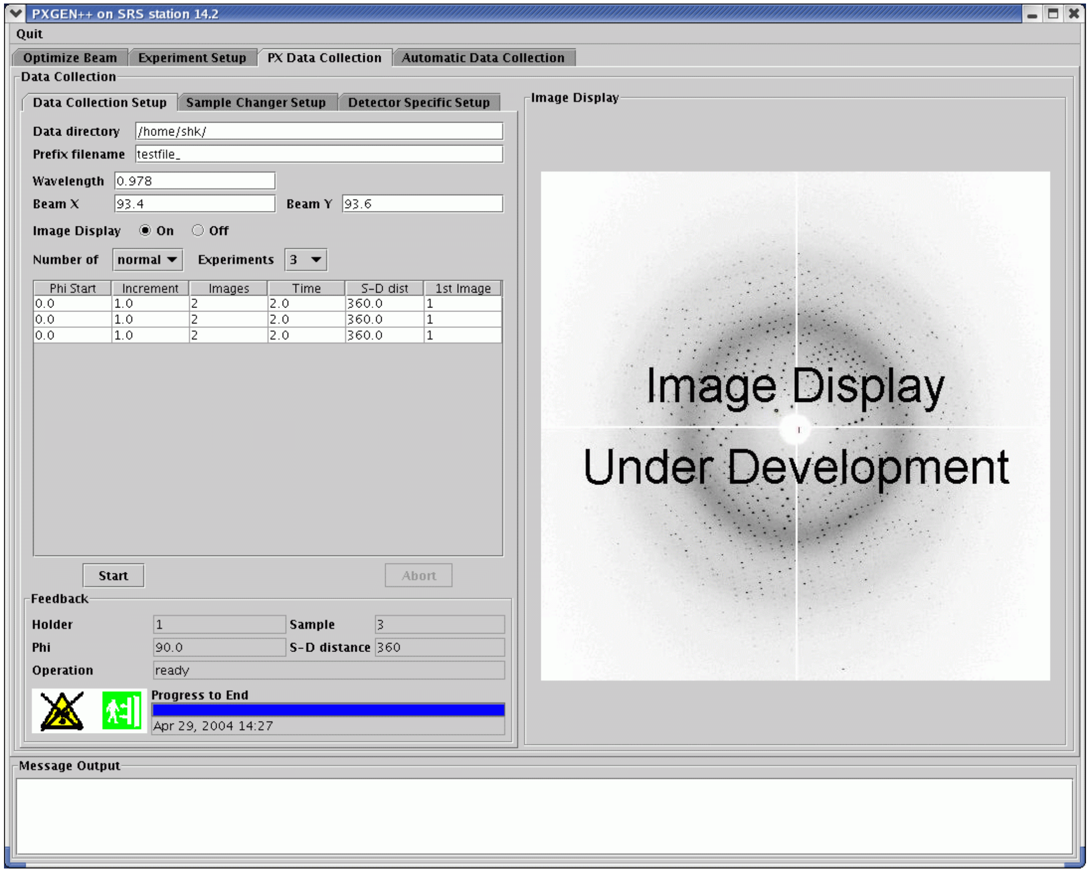
Points Done 0%

Plot Shows

☐ time
☐ I0
☐ It
☐ Im
☐ If
☑ χ transmission
☐ χ fluorescence

- Standard absorption edge scan interface and control.
- Will support multiple modes, Angle, KSpace and Fast.
- GUI completely detached from control.
- Scans done via scripting language.
- GDA standard.

Data collection



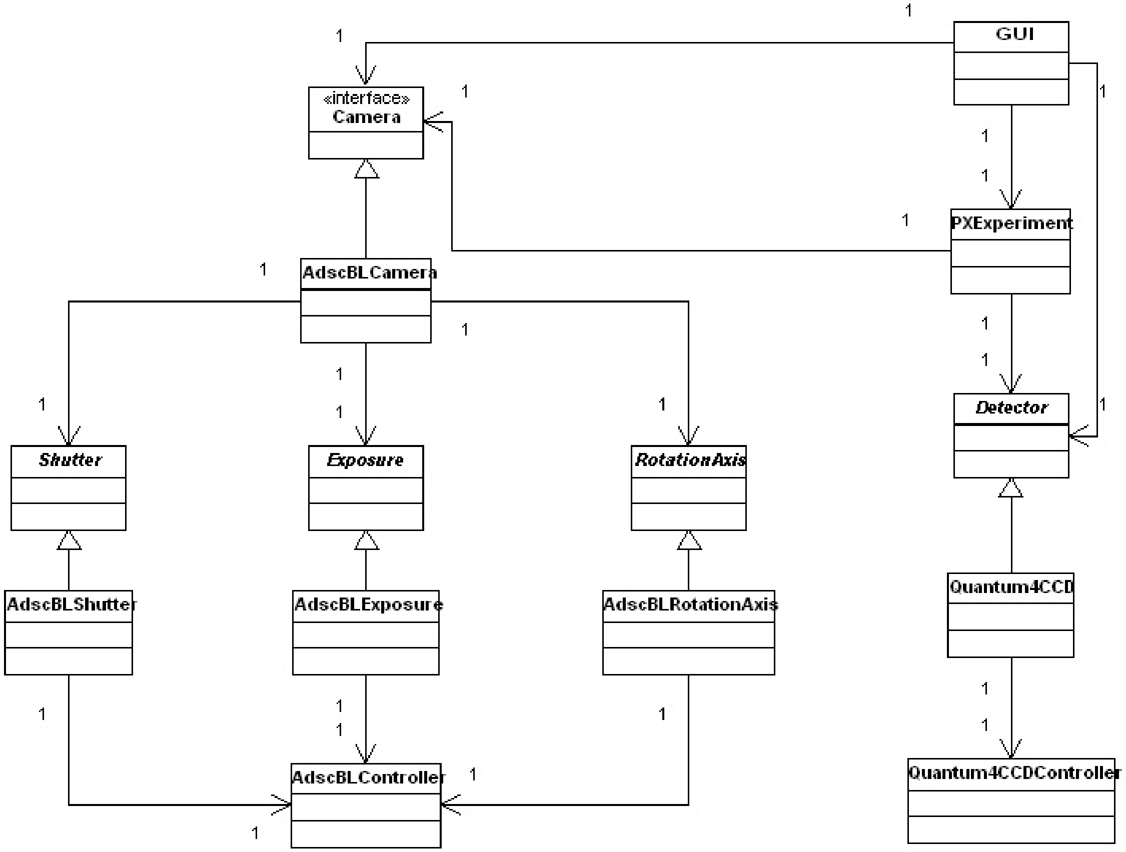
Data directory /home/shk/
Prefix filename testfile_
Wavelength 0.978
Beam X 93.4
Beam Y 93.6
Image Display ● On ○ Off
Number of normal
Experiments 3

Phi Start	Increment	Images	Time	S-D dist	1st Image
0.0	1.0	2	2.0	360.0	1
0.0	1.0	2	2.0	360.0	1
0.0	1.0	2	2.0	360.0	1

Holder 1
Sample 3
Phi 90.0
S-D distance 360
Operation ready
Apr 29, 2004 14:27

- Standard data collection software on 9.6 and 14.2.
- Same GUI independent of detector in use.
- Can use Q4, MAR180 & MAR345 detectors.
- Can use standard adsc control daemons or MAR control software.
- Rigaku sample changer included.
- PX specific.

PX Data Collection



Scripting

- GDA using Jython for ease of access to Java objects.
- JClam scripts on top of Jython. Easier general purpose scanning and backward compatibility.
  - pos LeftSlit 2.0 RightSlit 2.0
  - scan Slit 1 1 5 qcr 1
- More natural language? Jython add on.
  - open shutter
  - move detector to 200 mm
  - collect dataset

PXGEN++ future development

Ever increasing list of “general” requirements

- Scripting for PX data collection control.
- Integration of XAFS for monochromator calibration.
- MAD data collection protocol(s).
- XAFS for MAD wavelength selection.
- Manual crystal alignment.
- Other detectors e.g. MAR CCDs.
- Other sample changers e.g. MAR DTB.
- General scanning interface.
- Development of diffraction image display.
- Camera image (crystal) display.

PXGEN++ Automation

- Beam Alignment
    - Collimator to beam, Slits, Mirror/Monochromator focussing.
- Sample rather than loop alignment.
- Crystal screening (DNA - collaboration).
- Analysis of data integration (DNA - collaboration).
- Automatic logging of data collection from DNA/PXGEN++ (PXWEB/database server– collaboration).
- BIOXHIT post – Automation of Protein Crystallography beamlines (beamline alignment, sample handling etc).