Issues For Other Software Developers

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Information highlighted

- F', f'' from the experiment
- Detector information (e.g. class, gain, pixel size……)
- Epoch of the measurement of this set (e.g. collected from THEN to THEN in seconds from 1970)
- beam current would be useful in the image CIF, or something like the ion chamber readout
- Entity which controlled the DC would be useful too.
- biological info like fluerescence scans or crystal content
- Cryo-Stream temperature for ADPs?

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Scope

…. issues that are interesting to those who write software that might follow data collection and reduction….

.... the essence of it is the data, not the format…

…. at the end of data reduction there should be an mmCIF with all useful meta data in addition to the "real" data of F's and sigmas…. during the experiment and in the use of "dna," [*or equivalent*] *we* will hold useful metadata within a database system…

… what data will you want, and in what form would you like to have them?

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Format?

- XML needs defining to be useful.
- mm/imgCIF is at least a recognised standard.
- You don't want EVERY file to carry all the info - ideally there would be a data base for each structure, but realistically, people like to keep some of the essential info on hand.

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issues that are interesting to those who write software that might follow data collection and reduction……

- Can we assume (correct) data collection starts at the bioinformatics stage and not at the collecting diffraction images stage?
- Can we assume that a persistent metadata catalogue will always be available, associated and 'with' the data?

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The last word.

- Anything as long as its correct.
- After much though and deliberation we have come to the conclusion that the most import thing that could be included would be the phases. They would make life a lot easier.

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1.75+ million man-hours	Electron Beam Energy	3 GeV
2,100 tons of steel	Circumference	561.6 m
35,000 m^3 of concrete	Diameter of outer wall	235 m
33,000 m^2 of roofing	Beam current	300 mA (500 mA)
	Emittance	2.7 nm rad
	Start March 2003: Users January 2007	

Phase I (2007)

- 3 MX (0.5 – 2.5 Å optimised for 0.98Å) with double crystal monochromator, Kirkpatrick Baez horizontal and vertical focusing mirrors; Focal spot size ~ 94 nm (h) x 17 nm (v) (FWHM); estimated flux at 12.6 keV 3.5 x 10^{12} ph/s; fully automated sample handler; cryo cooling; CCD detector.
- One station will have containment three facility for pathogenic samples

Phase II

- Microfocus beam line
- Fixed wavelength side station (0.96 Å) (MR & ligand binding studies)
- Long wavelength side station for Sulphur anomalous (1.5 – 2.5 Å)

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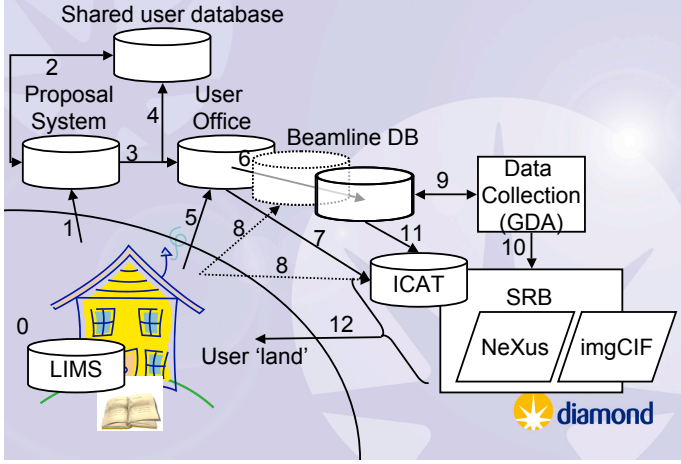
Data flow



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ImgCIF at Diamond

- CCD detectors that produce ImgCIF specified at time of tender.
- ADSC Q315.
- Chris Neilson and Harry Powell with help from others producing a working version.
- Diamond wanted images in an open standard
- Other than ImgCIF it is intended that NeXus will be the file format for all DLS beamlines.

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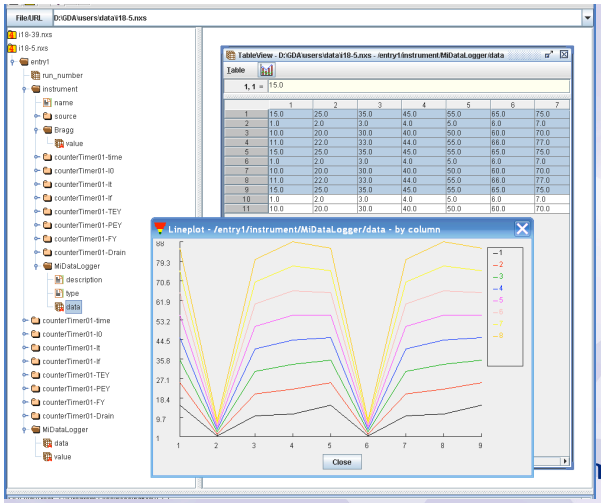

NeXus

- Based on a well established and supported format - HDF
- Allows storing of data, sample, environment, information together
- There is an experienced user community
- A common data format for synchrotron, neutron and meuon data (and from other sources)
- The format must worry about the implementation and support details

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diamond: www.diamond.ac.uk
DNA: www.dna.ac.uk
eHTPX: www.e-htpx.ac.uk
GDA: www.gda.ac.uk
ICAT: Information CATalogue
NeXus: www.nexus.anl.gov/index.html
SRB: Storage Resource Broker
www.sdsc.edu/srb/index.php/Main_Page

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Software for all DLS beamlines