(Automatic) MX Beamlines at the ESRF

Gordon Leonard ESRF MX Group 31/10/2007







Acknowledgements



ESRF

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ESRF MX Beamline characteristics

Beamline	ID14-1	ID14-2	ID14-3	ID14-4	ID23-1	ID23-2	ID29
E (keV)	13.270	13.294		9.6-14.5	6-20	14.2	6-20
λ (Å)	0.934	0.933		0.9-1.3	0.62- 2.07	0.873	0.62- 2.07
Beamsize* (µm)	20-200	20-200	XS	20-200	60	7 x 5	60
Detector	ADSC Q210	ADSC Q4r	SA	ADSC Q315r	ADSC Q315r	Mar 225	ADSC Q315r
Max ^m Resolution (Å)	1.0	1.0		0.9	0.6	0.9	0.6
Flux (phot/s)	5.8×10 ¹⁰	1.3×10 ¹¹		1.8×10 ¹²	1.5×10 ¹²	4.0×10 ¹¹	1.0×10 ¹³

MX Experiments at the ESRF

Experiment duration typically 3 shifts (24 hrs), 6 shifts at weekends.

Over 600 user experiments per year :
 ~ 45% of all ESRF exp'tal sessions.

Over 2000 user visits per year :
 ~ 40% of all ESRF user visits.

- Rapid turnover of experiments.
- Simplification/automation/consistency of equipment.

 <u>Above figures for academic users only -</u> <u>MX BLs also host a flourishing industrial</u> <u>activity.</u>





A common BL control GUI (mxCuBE)

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The typical MX 'experiment' can be automated



monitoring

Automating X-ray beam provision and maintaining & monitoring beam integrity on the MX Beam-lines



Automating Alignment of Optics Hutch Elements [ID23-1, ID29]



Automating X-ray beam provision

e.g. Primary Slits :

- Initialisation using limit switches
- Series of scans allow proper centering around white beam





Analogous protocols for secondary slits, monochromator, mirror. Soon to be combined into 'one button' procedure and 'rolled out' to all MX BLs

Automatic Calibration of Monochromator

Initialisation using absolute encoder. Calibration using Pt foil (transmission @ at L_{III} edge)



Validation procedure (if desired) using scans of Fe K, Cu K, Pt $L_{\rm III}$, Pt $L_{\rm II}$, Zr K and Mo K absorption edges.

Aligning the Mirror

Mirror Alignment :

- Utilisation of encoders
- Prealignement of the mirror
 - In height
 - In horizontal translation



• Automatic optimisation of bender, tilt, yaw on-going

Automation in the experimental hutch



Slits: alignment in same way as PS etc..



YAG screen: allows automatic alignment of X-ray beam to goniometer rotation axis.

X-ray camera: allows automatic (and dynamic) focussing of X-ray beam (ongoing)

Automating the MX 'experiment'



Automation implies standardisation and monitoring

MX Beamline Sample Environment

High precision mini-diffractometer

Fast CCD Detector

Backlight & Beamstop/Collimator

Sample Changer Robot



Oxford Cryostream

Fluorescence Detector

Evacuated Slitbox & Attenuators

On-axis Camera

Micro- and Mini-diffractometers



Microdiffractometer specs

- Handle crystals down to 10 μm size
- High Precision <u>air bearing</u> PHI axis ($2\mu m$)
- On beam axis viewing video microscope
- Integrated beam shaping
- Assisted and automatic crystal alignment
- <u>and more...</u>

Why Do We Need Robotic Sample Changers?



Inside the SC3



How does the SC3 load/unload samples?



SPINE Standard Sample Holders & Vials

European SPINE standard

Full specifications at <u>http://www.spineurope.org</u>, protocols menu

- Design based on Hampton Magnetic Crystal Cap™ and Vial System
- 22 mm fixed sample holder length (18mm pins)
- IO Characters identification code:
 - DataMatrix on the base of Caps
 - Clear code near the DatatMatrix







Automatic sample loading/unloading & centering in X-ray beam





Automatic absorption edge scans - I



Automatic absorption edge scans -II





Metal ions in crystals: fluorescence analysis





Metal ions in crystals: fluorescence analysis

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10		КМЗ	2.7031e+01	2.32e+00	2.816	0.10426	0.137	3.38								
11		KL3 Si_KM3esc	9.0997e-02	7.80e-03	0.785	0.00039	0.105	0.00								
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26		KL3 Si_KL3esc	4.6901e-01	7.13e-02	1.951	0.00903	0.124	1.40								
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Automatic sample screening & characterisation





DNA (automate<u>D</u> collectio<u>N</u> of dat<u>A</u>), Collaborative project involving the ESRF, CCLRC Daresbury Laboratory, MRC-Cambridge, Diamond Light Source; EMBL (both Grenoble an Hamburg outstations); Global Phasing Ltd, MRC - France (BM14) and SOLEIL.

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Automatic data collection, reduction & scaling

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ISpyB (http://ispyb.esrf.fr)

Communication of information concerning individual samples (description, bar-code, location, known unit cell dimensions, space group, 'diffraction plans') from crystallographers in the home lab to those performing the experiments at the ESRF. Real time monitoring of data collections: diffraction images, crystal snapshots, harvesting of output from DNA

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The Data Collection Pipeline (DCP) strings automated procedures together



What the DCP does

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• Scans of the contents of SC3 robot, compares these to ISpyB LIMS, displays the data matrices, associated sample information, postion of the sample in the SC3. Then for <u>each</u> sample selected

- Mount the sample
- Centres the sample in the X-ray beam.
- \cdot Takes two diffraction images at 90° in phi to each other for use by DNA
- · Carries out the DNA characterisation of the crystal mounted

•Writes the results to IspyB.

- Attempts to rank the crystal and suggest an order for data collection for crystals of the same type
 - Dismounts the crystals from the goniometer head.

MxCuBE & DNA together

Process	Results									
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EMBL/ESRF Mini-Kappa





Thaumatin - tetragonal (ESRF; ID23-1)

