## FA5-MS03-O1

**A Facility Wide Solution to Remote Experimentation and Automation.** Alun Ashton[a], Mark Basham[a], Peter Chang[a], Joachim Diepstraten[a], Karl Levik[a], Duncan Sneddon[a], Graeme Winter[a], Richard Woolliscroft[a]. [a]*Data Acquisition and Scientific Computing Group, Diamond Light Source, UK.*
E-mail: alun.ashton@diamond.ac.uk

It is increasingly expected that we should be able perform not only data collection and evaluation remotely but also to be able to monitor, access and analyze the data collected with a common user interface. This provides us with an important challenge to coordinate potentially disparate and distributed software into a standard interface.
Diamond Light Source, the new UK SR facility, now has 13 operational beamlines and another 5 beamlines being commissioned in 2009. Despite the diverse range of hardware and science being addressed on these beamlines, it has generally been possible to underpin all these instruments with a common, integrated computer hardware and software solution.
Though developments are continuing at pace, this presentation will report the current status of a generic data acquisition, recording, analysis, visualization and data processing framework geared towards optimizing beamline use and user experience. The benefits of collaborating and using the excellent software and some standards already developed and finely tuned by years of use (or debate) will be highlighted but the strength of this solution is in the mix of the implementation. Some of the technologies to highlight are Eclipse [1], GDA [2], EDNA [3], XIA2 [4], jReality [5], Mosflm [6], ICAT [7], and ISPyB [8].

[1] http://www.eclipse.org/ [2] http://www.gda.ac.uk/
[3] http://www.edna-site.org/ [4] http://www.ccp4.ac.uk/xia/
[5] http://www3.math.tu-berlin.de/jreality/
[6] http://www.mrc-lmb.cam.ac.uk/harry/mosflm/
[7] http://sourceforge.net/projects/icatx [8] http://www.ispyb.org

**Keywords: remote access for crystallography; data processing software; software design**

## FA5-MS03-O2

**Remote Access: The Virtual Scientific Instrument and The Web.** Peter Turner[a], Douglas du Boulay[a], Sandor Brockhauser[b], Romain Quilici[a]. [a]*School of Chemistry, The University of Sydney, Sydney, NSW, Australia.* [b]*EMBL Grenoble Outstation, 6 rue Jules Horowitz, 38042 Grenoble, France.*
E-mail: p.turner@chem.usyd.edu.au.

The provision of remote control services for a scientific instrument, such as an X-ray diffractometer, offers an increase in the efficiency of use, research yield and user base of the instrument. Given variable latency in the fabric of the internet, an important consideration in developing remote control services, is to the need to ensure safe operation of the remote instrument. With this in mind, we are incorporating a virtual representation of an instrument within the Web browser driven remote access service for the instrument. In addition to providing a means of training users without risking real instrument or human injury, the use of a virtual model offers a means of safely assessing a data collection strategy. A virtual representation also has the important benefit of providing a low-bandwidth, interactive and immediately interpretable view of the current state of the instrument, that offsets the 'dark lab' problem arising when lighting is switched off, or a web-cam fails. The virtual model can be inspected from all angles and distances, and so provides flexibility not possible with a Web-cam. We are developing a system for a conventional laboratory instrument, and a synchrotron beamline instrument. The use of the virtual model is incorporated as part of a Web services system for remote access that, in effect, makes the instrument available as a Web resource. To this end we have adopted and adapted the Common Instrument Middleware Architecture model (CIMA) as a basis for developing a Web service for remote instrument operation, and the use of the Web browser to access the Web service. Services for data management and distribution are also being developed.

**Keywords: remote access; virtual instrument; web services**

## FA5-MS03-O3

**Auto-Rickshaw: A Tool for Online Validation of X-ray Diffraction Experiment.** Santosh Panjikar[a], Venkatara-man Parthasarathy[a], Victor Lamzin[a], Manfred S. Weiss[a], Paul A. Tucker[a]. [a]*EMBL Hamburg Outstation, Notkestrasse 85, 22603 Hamburg, Germany.*
E-mail: panjikar@embl-hamburg.de

We present an automated crystal structure determination platform, *Auto-Rickshaw.* It contains several distinct computer coded decision-makers, which invoke a variety of macromolecular crystallographic programmes/programme packages during the structure determination process. [1]. A large number of structure solution paths are encoded in the system and the optimal path is selected by the decision-makers as the structure solution evolves. The primary aim of the pipeline is to validate the crystallographic experiment at the synchrotron site while the crystal is still at or near the beamline. Thus, the system has been optimized for speed, so that typically within a few minutes the answer is provided whether the collected data will be of sufficient quality to allow successful structure determination. The pipeline is controlled by a web-based graphical user interface. Important parameters are entered (e.g. space group, number of residues per monomer, number of heavy atoms per monomer, number of monomer(s) in the asymmetric unit) and the desired phasing protocol (SAD, S-SAD, SIRAS, two-, three- or four- wavelength MAD, MR, MRSAD) is chosen based upon the availability of the data sets.
Search model or protein sequence is necessary as input for MR or MRSAD phasing, but optional for experimental phasing. Each procedure of experimental phasing combines data reduction, substructure solution, heavy atom refinement, phase calculation, density modification, non-

crystallographic symmetry (NCS) averaging (if required) and partial/complete model building. Once important parameters are entered, X-ray derivative data are loaded and the process is invoked by pressing the „submit“ button, no further user intervention is needed. The GUI allows the users to follow the progress and provides a tarball of the initial model, electron density, bones and a macro for O/COOT/XFIT to view the model and map on appropriate computer graphics.The platform has been installed on a Linux cluster at EMBL-Hamburg and is remotely accessible to the beamline users via a web-server. The server [2] is accessible from most Internet browsers and allows beamline users and the crystallographic community to validate their X-ray diffraction experiments in the shortest possible time. An overview of *Auto-Rickshaw* with its architecture, functionality, some examples and the way this platform is used as a feedback system for X-ray data collection or validation of the X-ray experiment, will be discussed.

[1] Panjikar S., Parthasarathy V., Lamzin V.S., Weiss M. S. & Tucker, P.A. **2005**. *Acta Cryst.* D61, 449-457. [2] http://www.embl-hamburg.de/Auto-Rickshaw/

**Keywords: automation; phasing; remote access for crystallography**

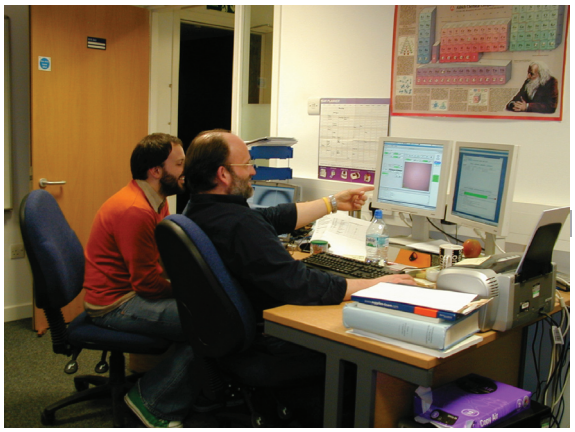
## FA5-MS03-O4

**Automation and Remote Access on the ESRF's Macromolecular Crystallography Beamlines.**

Leonard Gordon. *Macromolecular Crystallography Group, European Synchrotron Radiation Facility, 6 rue Jules Horowitz, F-38043 Grenoble Cedex, France.*
E-mail: leonard@esrf.fr

The end-stations dedicated to Macromolecular Crystallography (MX) at the European Synchrotron Radiation Facility (ESRF) currently welcome over 2600 visitors each year with experimental sessions lasting anything from 4 hours to 2 days. To cope with such a high user throughput and to ensure the beam-lines are reliable and user-friendly, the MX Group at the ESRF has developed a policy of, where possible, standardising hardware and software in both optics and experimental hutches of the beam-lines. Such standardisation, and the fact that MX 'experiments' are essentially repetitive in nature, lends itself to automation. The automation available on the ESRF's MX beam-lines [1-6] will be described.
For several years, a form of remote access to the ESRF'S MX beam-lines has been available to industrial users via the highly successful MxPress data collection service. However, manpower requirements mean that a similar service cannot be offered to academic users. We have therefore, as a direct result of the high levels of automation now in place, developed a system, accessible to industrial and academic users alike, whereby experimenters can control the ESRF's MX beamlines from the comfort of their home laboratories [7]. The remote access protocols used at the ESRF will also be described as will our experiences, both good and bad, with the system currently deployed.

[1] Arzt *et al.*, **2005** *Prog. Biophys. and Mol. Biol.,* 89, 124-152. [2] Cipriani *et al*., **2006**. *Acta Cryst.*, D62, 1251-1259. [3] Beteva *et al.*, **2006**. *Acta Cryst.*, D62, 1162-1169. [4] Leslie *et al*., **2002**. *Acta Cryst.*, D58, 1924-1928. [5] Giraud *et al*., **2009** *J. Appl. Cryst*., 42, 125-128. [6] Leonard *et al.*, **2009** *J. Appl. Cryst.*, 42, 333-335 [7] Gabadinho *et al.*, **2008** *Synchrotron Radiation News*, 21, 24-29.



Academic users controlling their experiment at an ESRF MX beam-line from their offices at the Univeristy of York, UK

**Keywords: automation; remote access; synchrotron facilities**

## FA5-MS03-O5

**Remote Synchrotron Data Collection and Structure Determination Pipeline.**

Miroslaw Gilski. *Department of Crystallography, Faculty of Chemistry A. Mickiewicz University, Poznan and Center for Biocrystallographic Research, Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland.*
E-mail: mirek@amu.edu.pl

The process of determining macromolecular crystal structures may be thought of as a simple sequence of operations: protein production, crystallization, diffraction, phasing, model building, refinement and deposition of coordinates. This sequence is sufficiently understood and all steps of such pipeline may be automated. The yield of the structure determination pipeline depends on many organizational and human factors. One of the ways to speed up this process is to facilitate access to a few synchrotron radiation centers operating worldwide. Beamlines on these facilities have long queues, and increasing the efficiency of utilization of these facilities will help in expediting the structure determination process. Most of the synchrotron centers offer remote data collection capabilities on its macromolecular beamlines. Remote experimenters have access to the same tools as local users, have the capability to manipulate crystalline samples and to collect, analyze, and backup diffraction data. Automation and remote data collection are therefore essential steps in ensuring that macromolecular structure determination becomes a very high throughput process.