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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.*
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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

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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.*
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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

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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.*
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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-