

High-throughput developments at BM14

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MRC-France – BM14, EMBL, ESRF, MAAETEL



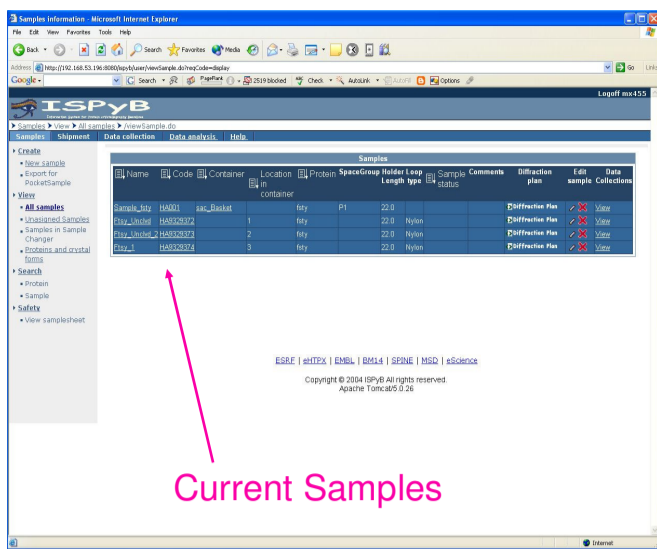
ISPyB Information System for Protein Crystallography Beamlines

Joint project of BM14 eHTPX, and ESRF: S. Delageniere, R. Leal, L. Launer, D. Spruce

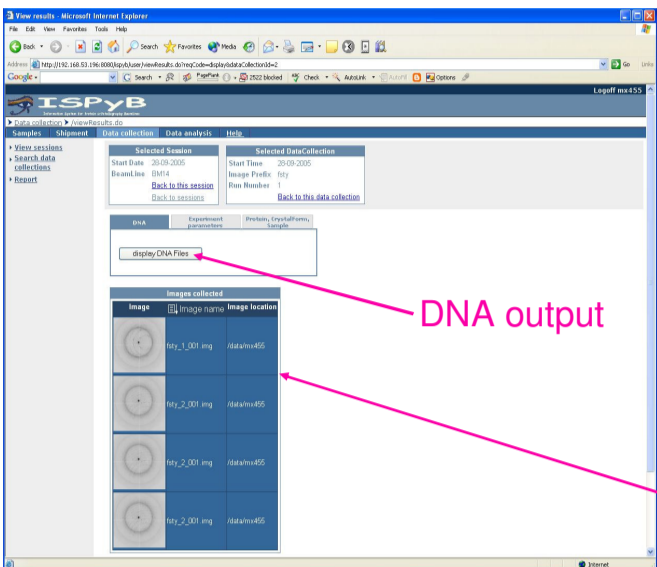
Creation of an automated pipeline for data collection allowing a high-throughput approach to macromolecular data collection and structure solution changes the way a typical experiment can be performed. These changes cover many aspects of the structure determination process. Management of the data and tracking the progress of an experiment through the pipeline becomes a critical part of the process. Provision of an information system for MX beamlines provides the user with the ability to track and manage the progress of his/her experiment. In particular use of an information system allows one to:

- Receive, store, manage and retrieve information from an all encompassing, intuitive and easily accessible user interface
- Allows integration/use of Webservices (industry proven standard based on "firewall friendly" XML communication over HTTP) providing a seamless data exchange between home labs and a synchrotron (e.g. shipment, crystal and sample details, diffraction plan etc)
- Information is available through a web based user interface, and automatically submitted to the appropriate programs (i.e. Beamline control software, DNA).
- During data collection, ISPyB stores all of the meaningful meta-data (exposure time, resolution, type of experiment etc), jpeg generation of diffraction images and links to the original data files. This allows remote users/crystallographers to monitor the progress from his/her home lab and real-time interaction with team on the beamline.
- Data can be exported into various formats and imported back into either the home lab information system, or a local copy of ISPyB.

This overview of the different steps covered by ISPyB shows that it provides for a continuous information flow of data from crystallization (e.g. by use of PIMS) to deposition of the solved structure in the PDB. Moreover, it provides the framework for the management of data received and acquired at a typical MX beamline.

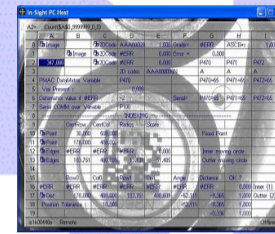


Current Samples



DNA output

Jpeg version of diffraction images



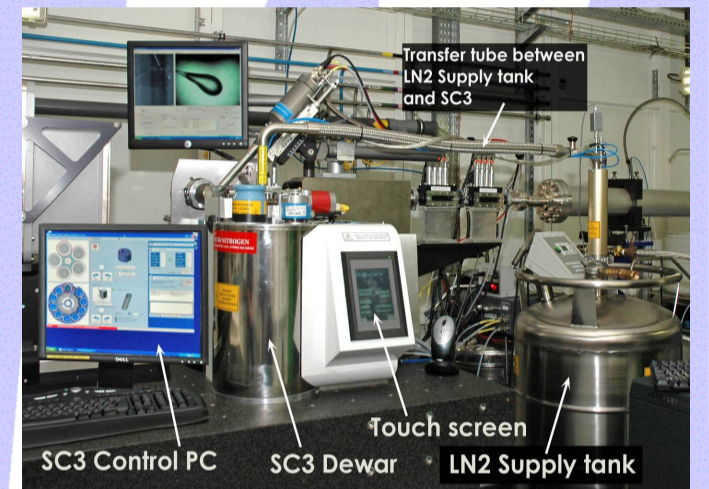
Adaptive datamatrix detection

Automatic Sample Changer*

Joint BM14, EMBL, ESRF initiative

User friendly, intuitive user interface, TANGO Device Server for remote use and interactions with other devices or programs.

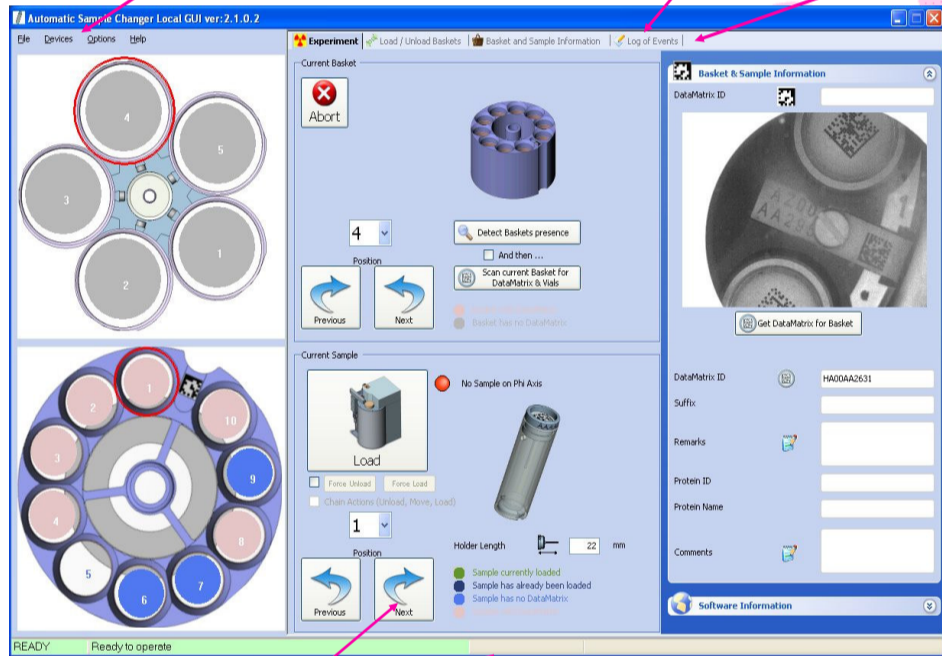
- Smart and adaptive Datamatrix detection algorithm
- Real-time online statistics on use
- Monitoring of cryo. system preventing loss of sample
- Automatic update of software to benefit from latest developments



TANGO Device Server

Log of Events

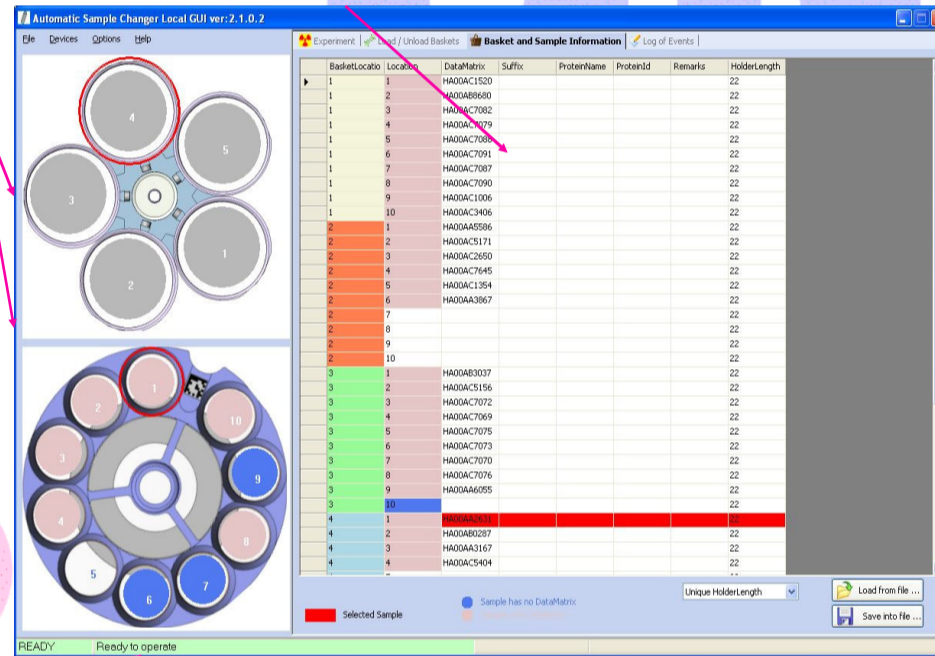
Tuning tools



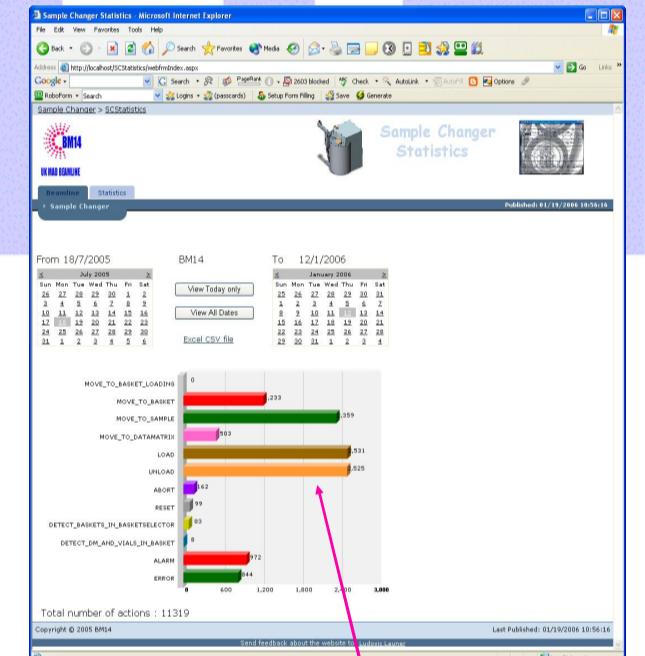
Graphical view of Baskets & Samples

Camera view Inside SC

Datamatrix identification of Samples



Hardware Status



Real time statistics

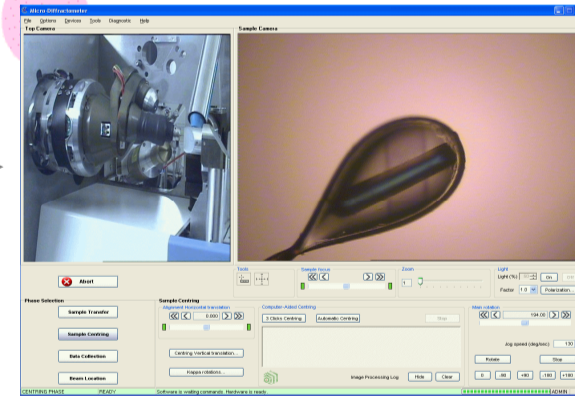
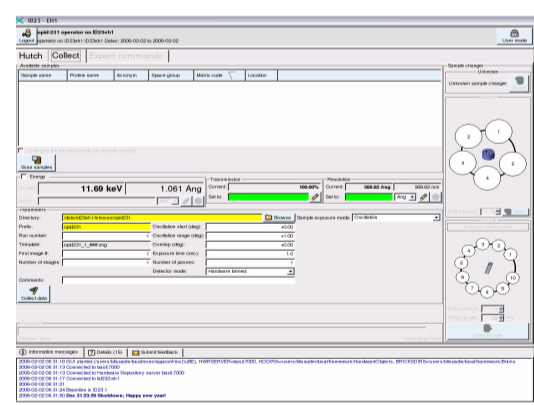
Change current position

Alarm notification by sound, email, ...

MD2 Microdiffractometer and C3D auto centering*

BM14, ESRF, EMBL

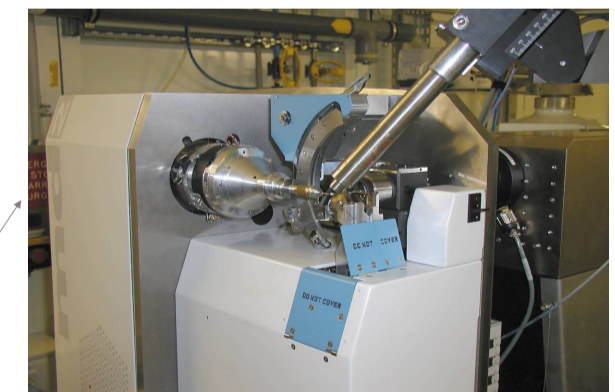
- MicroDiffractometer with mini-Kappa
- 3 clicks or fully automated crystal centring algorithm (C3D)



Video Server

C3D Auto-Centering

Pmac controller



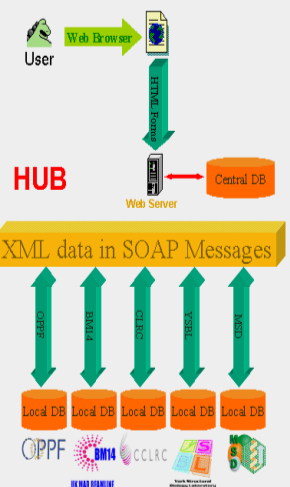
eHTPX project

David Stuart, Robert Esnouf Oxford, Colin Nave, Rob Allan Daresbury, Kim Hennick EBI, Kevin Cowtan York, Martin Walsh Grenoble, Chris Mayo Oxford, Graeme Winter, Ronan Keegan, David Meredith Daresbury, Joel Fillon EBI, Paul Young York, Ludovic Launer Grenoble

An easy-to-use resource for protein crystallographic structure determination. The aim is to unify the procedures of protein structure determination into a single all encompassing interface from which users can initiate, plan, direct and document their experiment either locally or remotely from a desktop computer.

- Develop Grid-enabled UI to allow structural biologists to interact easily with all the required resources for PX
- Portals enabling access to all facilities over the internet
- Develop systems for controlling the diffraction data collection and analysis directly transferable to any synchrotron facility.
- Extend and develop structure determination software to take advantage of low-cost, highly parallel computing facilities.
- Develop a Grid-based application allowing the user to manage flow of data from the initial stages of target selection to the automated deposition of the final refined model in the public databases.

www.e-htpx.ac.uk



Current developments and Future Goals

- Storage Dewar management software and integration into ISPyB
- Data-mining on results produced by processing software and DNA
- Improved communication between SC and ISPyB (datamatrix, ...)
- Improved User reports submission (email notification, keywords, ...)
- Complete automated pipeline predicted for first release in early 2006

www.bm14.ac.uk

*Publications

^a ESRF, ^b EMBL, ^c MRC-France, ^d LURE, ^e OPPF

Automation of macromolecular crystallography beamlines (Progress in Biophysics & Molecular Biology 89 (2005) 124–152)

Steffi Arzti^a, Antonia Beteva^a, Florent Cipriani^b, Solange Delageniere^a, Franck Felissaz^a, Gabriele Foerster^a, Elspeth Gordon^a, Ludovic Launer^a, Bernard Lavault^a, Gordon Leonard^d, Trevor Mairs^a, Andrew McCarthy^a, Joanne McCarthy^a, Sean McSweeney^a, Jens Meyer^a, Edward Mitchell^a, Stephanie Monaco^a, Didier Nurizzo^a, Raimond Ravelli^b, Vicente Rey^a, William Shephard^a, Darren Spruce^a, Olof Svensson^a, Pascal Theveneau^a

Automation Instrumentation for High Throughput Macromolecular X-ray beamlines (Submitted for publication in Acta Cryst D)

Florent Cipriani^b, Franck Felissaz^a, Ludovic Launer^a, Jean-Sebastien Aksoy^a, Hugo Caserotto^a, Stephen Cusack^c, Maximilien Dallery^a, Franck di-Chiaro^a, Matias Gujarro^a, Julien Hue^a, Sine Larsen^a, Mario Lentini^a, Joanne McCarthy^a, Sean McSweeney^a, Raimond Ravelli^b, Michel Renier^a, Christophe Taffut^a, Andrew Thompson^a, Gordon Leonard^d and Martin A. Walsh^e

High throughput sample handling and data collection at synchrotrons: embedding the ESRF into the high throughput gene to structure pipeline. (Submitted for publication in Acta Cryst D)

A. Beteva^a, F. Cipriani^b, S. Cusack^c, S. Delageniere^a, J. Gabadinho^a, E.J. Gordon^a, M. Gujarro^a, D.R. Hall^a, S. Larsen^a, L. Launer^a, B. Lavault^a, G.A. Leonard^d, T. Mairs^a, A. McCarthy^a, J. McCarthy^a, J. Meyer^a, E. Mitchell^a, S. Monaco^a, D. Nurizzo^a, P. Pernoy^a, R. Pieritz^a, R.G.B. Ravelli^b, V. Rey^a, W. Shephard^a, D. Spruce^a, D.I. Stuart^a, O. Svensson^a, P. Theveneau^a, X. Thibault^a, J. Turkenburg^a, M. Walsh^e and S.M. McSweeney^a

