

eHTPX at BM14

European
Molecular
Biology
Laboratory
Grenoble Outstation



Ludovic Launer & Martin Walsh

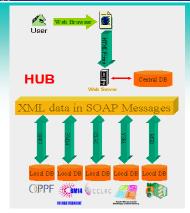
eHTPX www.e-htpx.ac.uk

David Stuart, Robert Esnouf Oxford, Colin Nave, Rob Allan Daresbury, Kim Henrick EBI, Kevin Cowtan York, Martin Walsh Grenoble
Chris Mayo Oxford, Graeme Winter, Ropan Keenan, David Meredith Daresbury, Paul Young York, Ludovic Launer Grenoble

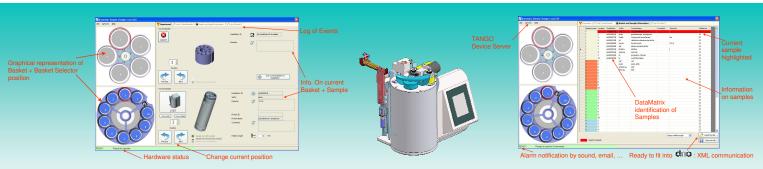
An easy-to-use resource for protein crystallographic structure determination.

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. www.e-htpx.ac.uk

- Develop a 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.



Sample Changer Software Joint project of eHTPX, EMBL and ESRF



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Sean McSweeney Gordon Leonard Joanne McCarthy Jose Faria Jens Meyer

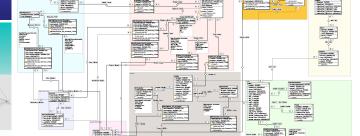
PX Laboratory Information System (LIMS) www.bm14.ac.uk

UML Model developed

Draft UML model for PX beamline LIMS

Presented and validated at joint e-HTPX/ESRF/ EMBL workshop in Grenoble (19/09/03)

- Use-case (Planned functionalities)
- Data Model (Database implementation)



High level of genericity allows easy + fast deployment on any PX Beamline !!

Future Goals

- Improve Sample Changer software after user feedback
- LIMS + WebServices Development
- Beamline Automation methods development

Time Plan

- Mid April 2004: WebService for Safety, Shipping and Data collection Strategy information.
- Mid June 2004: First version of web based portal, giving general philosophy and look & feel.

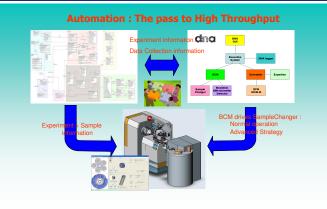
Links

eHTPX : <u>www.e-htpx.ac.uk</u>

BM14 : www.bm14.ac.uk then browse to eScience section

BM14 : Martin Walsh, Hassan Belrahli, Gavin Fox, Francois Fihman, Ludovic Launer, Hugo Caserotto

Integration with other projects



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