SEVENTH FRAMEWORK PROGRAMME

Research Infrastructures

Deliverable 7.1

A secure Grid portal for remote SAXS experiments

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Section 1: Summary of Deliverable

Background

WeNMR (Worldwide e-Infrastructure for Nuclear Magnetic Resonance and Structural Biology) is a EU FP7 project that brings together research teams in the Structural Biology area into a Virtual Research Community at a worldwide level, focusing on bio-molecular Nuclear Magnetic Resonance (NMR) and Small Angle X-ray Scattering (SAXS).

Work package 7 of the project aims at the development of new computational tools and applications to improve the Grid-based infrastructure and services provided by WeNMR, thereby assuring both implementation as well as the development of the latest techniques as part of the WeNMR virtual research community. An important part is the inclusion of SAXS into the grid technology, including remote access to the SAXS instrumentation.

Goal

This document is the project deliverable D7.1 due by Month 24. It outlines the steps a user of the WeNMR community needs to take in order to access the SAXS instrument P12 at the PETRA III storage ring at EMBL in Hamburg, Germany and describes how remote measurements and data analysis may be conducted.

Section 2: Remote Instrument Access

Most of what is described below was also published in [1].

Applying for Beam Time

Every user who wishes to use SAXS beamline facilities of EMBL Hamburg, from remote or local, has to submit a project proposal using the Virtual User Office [2] where the planned experiments shall be described in detail. Proposals are evaluated and ranked by a review committee, instrument access is granted, and beam time assigned, according to the rank of the proposal.

Sample Preparation

After beam time was assigned, users need to fully prepare their samples in 96 well plates following the Sample Requirements [3] and have them send to EMBL in Hamburg, Germany by courier in time for the experiment.

The physical samples and buffers need to be accompanied by their details, i.e. a human readable description that allows to identify corresponding specimen, a machine usable short code, concentrations and the respective location within the well plate that will be placed in the samplechanger device [4] once the beam time begins.

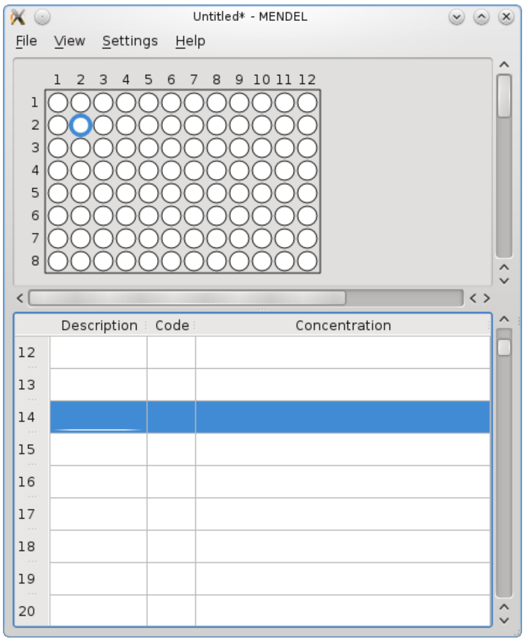

Figure 1 Stand alone user interface with wellplate layout.

To help the users providing this information a platform independent graphical user interface was developed. With this interface, users may conveniently create a sample description file that contains the required details for the beamline control software. This sample description file is meant to be submitted via a secure portal from where it would be associated with the user's proposal and be retrieved by the beamline responsible at the day of the measurement. At present, the portal is being finalized and synchronized with the developments in WP7 of Biostruct-X [5], a FP7 collaboration of EMBL Hamburg, EMBL Grenoble, the ESRF and Diamond. The advantage of the synchronization is the implementation of the SAXS extensions of ISPyB (*Information System for Protein CrystallographY Beamlines)*. ISPyB already provides a web interface to an information database tracking all the available sample information, from preparation in the laboratory to the measurement at the facility and final data analysis. After deployment in early 2013, ISPyB, together with the Virtual User Office (SMIS) and the ATSAS Grid Portals (D7.2), shall share a secure Single Sign On method; the SSO has already been implemented in the VRC and is expected to be rolled out to the various portals early 2013. Then users may either use the stand-alone software to provide the sample details, or use ISPyB and export a similar file for use for data acquisition.

Data Acquisition

At the begin of the assigned beam time, the buffers and samples are loaded into the sample changer by the beamline responsible. Data collection may be conducted interactively from remote by the users themselves or automatically, supervised by the beamline responsible.

In interactive mode, a user may use their EMBL Hamburg Single Sign On credentials to access the remote gateway host using the NX of NoMachine (www.nomachine.com) as a remote desktop solution [6] using a secure shell connection. There the users have the same control over the experiment that they would have at the beamline directly.

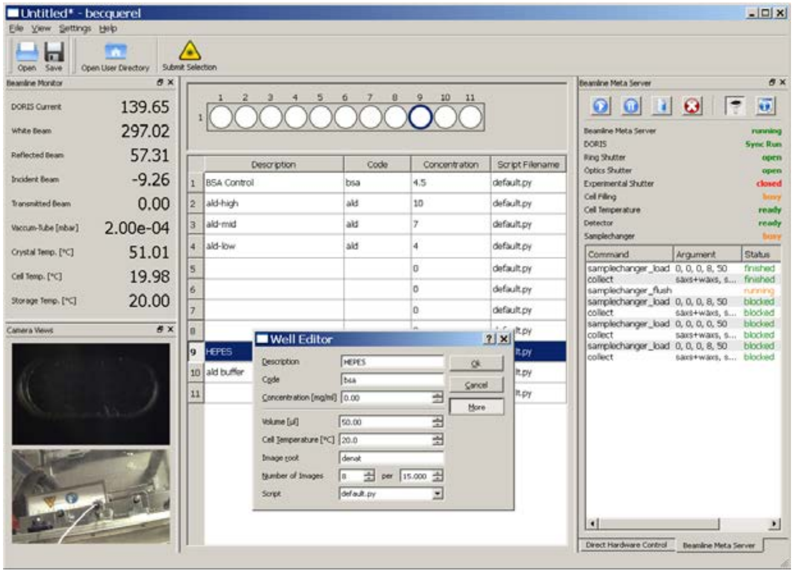

Figure 2 Beamline Experiment Control User Interface. Sample details and wellplate in the center, beamline monitors and cameras to the left, automation control to the right.

Both, an interactive remote user and the local beamline responsible, would control the data collection in the same way by importing the sample description file prepared earlier into an instance of the beamline control software BECQUEREL (Beamline Experiment Control – QUEue and RELax). With the required information available, an experiment is scheduled simply by selecting, i.e. single-clicking, the wells of interest and pressing the Submit Selection button above the well plate. The commands required to conduct the experiment are sent to the Beamline Meta Server (BMS) command queuing system, queued and subsequently executed. Progress may be observed in the BMS panel (lower right), additional experiments may be queued at any time. After radial averaging, the data files are picked up for automated data analysis.

Further, development of the Autonomous Data collection Agent (ADA) for automated and autonomous data collection was initiated. ADA is designed as an intelligent software system to plan and execute experiments in the generally dynamic, stochastic and nondeterministic environment of a modern SAXS beamline. It shall make rational choices by reasoning about its environment and by planning ahead the consequences of possible actions to successfully collect a SAXS data set. After completion, ADA shall support users and the beamline responsible in the routine data collection tasks of non-interactive data collection, supervising the data collection system, notifying the responsible persons if their assistance is needed.

The remote access is now available at the EMBL beamline P12 and the first remote data collection was conducted on 15th of June 2012 by a user group from Salamanca, Spain.

Data Analysis and Storage

The collected data is automatically subjected to an automated analysis procedure. For each specimen measured, one generally needs to (1) radially average the two- dimensional detector images to a one-dimensional scattering curve, (2) subtract the background scattering, (3) determine the overall parameters such as radius of gyration, molecular mass, excluded volume, maximum dimension and, optionally, (4) compute an ab initio three-dimensional model. Additional modeling steps may be performed later if information from complementary methods is available. All this derived information is stored in a hierarchical XML file, ready to be displayed in a web browser.

It is to note that all computations are done on local computing facilities as, besides ab initio modeling, the tasks are completed quickly, i.e. often in less than a second. Users would not benefit from submitting them to the grid, as this would introduce significant latencies during the analysis.

It was foreseen that after collection, the data should be stored in predefined grid locations for easy retrieval by the users. No automatic solution for this was implemented yet, but we expect to achieve this by February 2013.

References

[1] Automated Acquisition and Analysis of Small Angle X-ray Scattering Data. Franke, D., Kikhney, A.G. and Svergun, D.I. *Nuc Inst Meth* A. 2012. 689: 52-59, http://dx.doi.org/10.1016/j.nima.2012.06.008.

[2] http://www.embl-hamburg.de/facilities/access_infrastructures/saxs_2012/index.html

[3] http://www.embl-hamburg.de/biosaxs/sample.html

[4] Instrumental setup for high throughput solution scattering at the X33 beamline of EMBL-Hamburg. Blanchet, C.E., Zozulya, A.V., Kikhney, A.G., Franke, D., Konarev, P.V., Shang, W., Klaering, R., Robrahn, B., Hermes, C., Cipriani, F., Svergun, D.I and Roessle, M. *J Appl Cryst.* 2012. 45:489-495, http://dx.doi.org/10.1107/S0021889812013490.

[5] http://www.biostructx.org/content/automated-sample-handling

[6] New paradigm for macromolecular crystallography experiments at SSRL: automated crystal screening and remote data collection. S.M. Soltis, A.E. Cohen, A. Deacon, T. Eriksson, A. Gonzalez, S. McPhillips, H. Chui, P. Dunten, M. Hollenbeck, I. Mathews, M. Miller, P. Moorhead, R.P. Phizackerley, C.Smith, J. Song,H. van dem Bedem, P. Ellis, P. Kuhn, T. McPhillips, N. Sauter,K. Sharp, I. Tsyba, G. Wolf, *Acta Crystallographica Section D* 64 (2008) 1210, http://dx.doi.org/10.1107/S0907444908030564.