

LABWEB – LNLS BEAMLINES REMOTE OPERATION SYSTEM*

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Abstract

LabWeb is a project of the Brazilian Synchrotron Light Source (LNLS) aimed at allowing remote operation of its beamlines by the user community. Being the only light source in Latin America, LNLS receives several users from Brazil and other South American countries. The implementation of LabWeb will allow researchers to use the laboratory structure through a web browser, without leaving their research centers, reducing time and travel costs in a continental country like Brazil.

LABWEB

In 2010, the LabWeb project was in its first phase in which tests were conducted using a beta version. Two years later, a new phase of the project began with the main goal of giving the operation scale for the remote access project to LNLS users. In this new version, a partnership was established to use the open source platform Science Studio developed and applied at the Canadian Light Source (CLS). So far the project provided remote operation of three LNLS beamlines: SAXS1 (Small Angle X-Ray Scattering), XAFS1 (X-Ray Absorption and Fluorescence Spectroscopy) and XRD1 (X-Ray Diffraction). The expectation is to provide this remote way of performing experiments to all the other LNLS beamlines. Here this tool is described in its main components and features.

SCIENCE STUDIO

After the first prototype software for remote beamline operation on LabWeb has been created, it was concluded that the Science Studio platform from the Canadian Light Source, as a web portal, provided all the features necessary in the LabWeb project and thus, instead of developing a new software for the same purpose, we decided to join the open source project of Science Studio (SS) [1].

Science Studio provides a unified working environment all the way through to the data analysis and retrieval of experimental data and met all the requisites for LabWeb. More importantly, like the first LabWeb prototype, SS only requires a web browser on the client side to perform a complete synchrotron experiment. Since LNLS joined the development of SS many additions were made from the core to the application part of the software which we describe in the following.

Project Structure

Science Studio is built on a Service-Oriented Architecture (SOA) framework where business functions are treated as services.

Using the core application users can access informations about scheduled sessions and navigate through past sessions to recover their experimental data and even go into an active session.

From the Science Studio software point of view, each beamline is divided into four projects:

- WebApp: Web application divided between administration page, where all the experimental setup can be registered, and beamline page, where all the user interfaces for remote experiment are located;
- Service: This is part of the WebApp project and contains the controllers where the messages between equipments and user interfaces are exchanged;
- Data: Creates an exclusive visualization tool for the specific data generated by each beamline;
- BCM or Beamline Control Module: This module is responsible for the experiment execution and devices communication by a high-level interface to a low-level control system, in our case, EPICS using a Java implementation of the Channel Access protocol.

More information about Science Studio architecture and code can be found in the project website <http://sciencestudioproject.com/>.

SCIENCE STUDIO AT LNLS

Infrastructure

Initially, the idea was to have 18 Beamline Control Module (BCM) servers (one for each beamline) but maintenance and upgrades on servers and software would become unviable and service availability could become compromised by single machines without redundancy. Therefore we opted for a centralized solution with the creation of a datacenter where two virtual machines were installed relying on features like backup and high-availability system.

With a focus on integrity and capacity of data storage, a SAN / NAS storage with redundant processing and 20 TB of space on Near Line SAS drives and 512GB on SSD is being used with the NFS protocol and counts with redundancy of four discs parity and two spare disks using RAID-DP features, deduplication for efficient use of space and backup.

LNLS Beamlines Using Science Studio

The first LNLS beamline ported to Science Studio was SAXS1 (Small Angle X-Ray Scattering). The experiment

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consists in sample change, scattering image acquisition (with a Pilatus 300k detector) and data pre-processing, like background subtraction and azimuthal integrations. Sample change in this beamline is carried out through an automated sample holder with space for 144 film and/or powder samples. The beamline staff is working on an automated sample holder for liquids to increase even more the number of remote users.

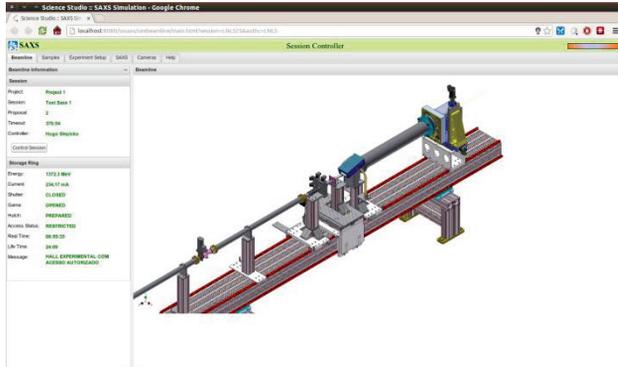


Figure 1: Screenshot of SAXS1 beamline first page showing informations about the storage ring, current session and experimental hutch

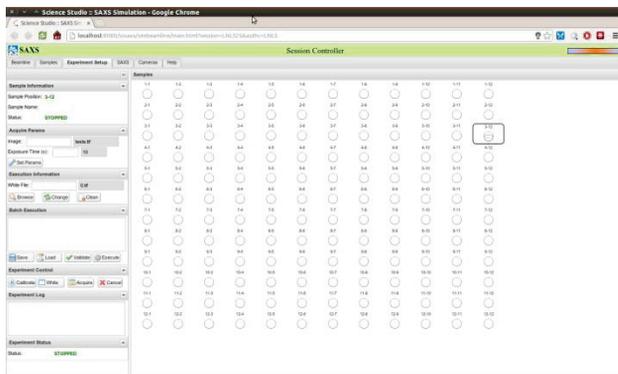


Figure 2: Screenshot of SAXS1 beamline experimental setup page showing on the right side the sample holder where the user can click to move to a sample and at the left the acquire parameters.

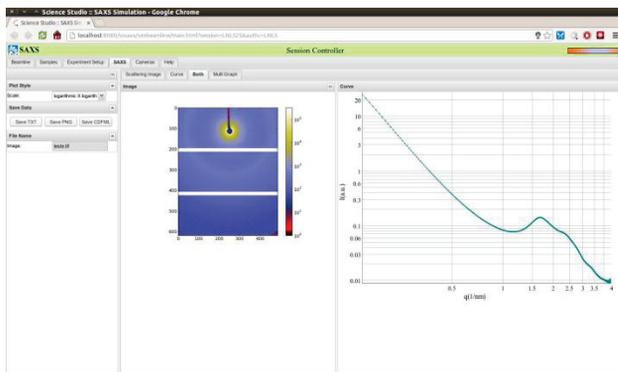


Figure 3: Screenshot of SAXS1 beamline data page where users can see the scattering image and graph.

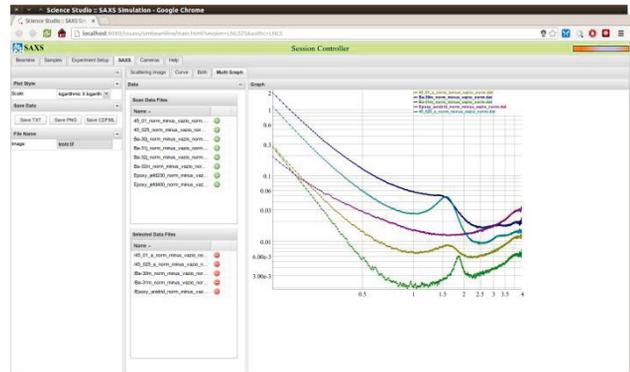


Figure 4: Screenshot of SAXS1 beamline data comparison page.

At XAFS1 (X-Ray Absorption and Fluorescence Spectroscopy) the remote experiment is an x-ray absorption spectroscopy. For each sample the user can specify a maximum of five energy ranges to launch scans. The user can also define optimization strategies for the ion chambers and specify wetter wave-vector or energy steps are required. Once all parameters for the scans are set, the software starts to acquire data that can be visualized almost “on-flight” at the “Current Scan” tab inside Data browser tab.

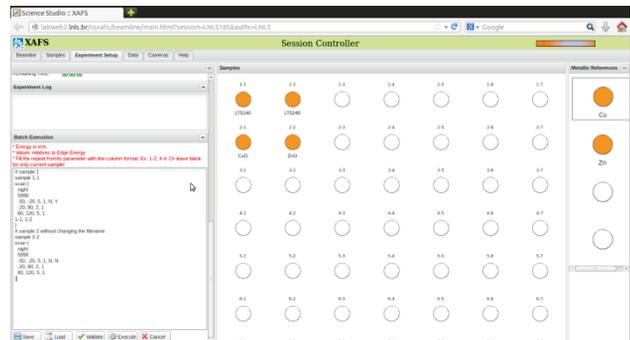


Figure 5: Screenshot of XAFS1 beamline experimental setup page showing on the right side the metallic references holder where the user can click to move to a desired reference, at center the sample holder and at the left the acquire parameters.



Figure 6: Screenshot of XAFS1 live data page with capability of choose displays fields.

Another beamline working with remote experiments is the XRD1 (X-Ray Diffraction) where a scan with a DECTRIS Mythen 24K is made generating a large amount of data per step. At this beamline the samples are changed using a robotic arm capable of positioning, heating and cooling samples. After the end of acquisition the collected data is pre-processed using python scripts.

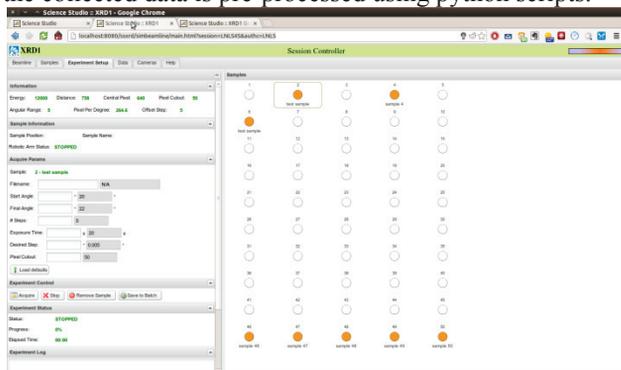


Figure 7: Screenshot of XRD1 experimental setup page.

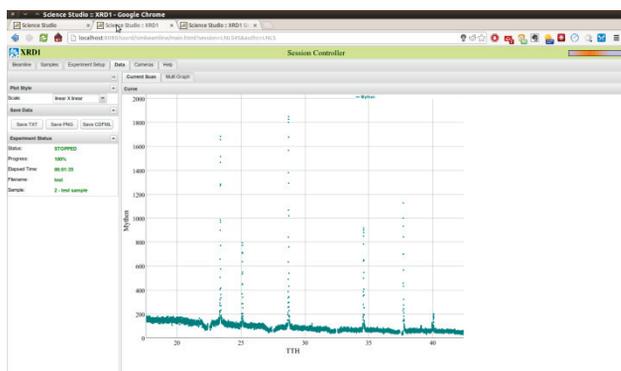


Figure 8: Screenshot of XRD1 live data page.

All beamline portal homepages have six main tabs:

- Beamline: Storage Ring and Session information, Fig. 1.
- Samples: sample registering and parameters, Fig. 2.
- Experimental Setup: data acquisition parameters, progress and sample selection, Fig. 7.
- Data: live data and data comparison, Fig. 3, 8.
- Cameras: live view of PZT cameras looking at different places of the beamline.
- Help: help of all functionalities of the remote operation.

New Implementations under Science Studio

The Science Studio itself is a very complete suite with a large set of functionalities already implemented. New functionalities have been added to SS to improve the remote experiment experience by gathering requirements from beamline scientists and users. They include: New data format for storage, simultaneous live data comparison of collected data, Fig. 4, execution of batch

commands in scripts with an intuitive and simple language, Fig. 5 and a data plotting interface where user can select which data fields are displayed into the graphs, Fig. 6.

At Canadian Light Source (CLS) the Beamline Control Module (BCM) is responsible for the communication with beamline devices such as motors, detectors and others but is not directly responsible for the data acquisition. Instead of holding the logic of the experiments it calls another software that already has the scan commands reusing existing scan configurations and saving development time. At LNLS, besides the devices communication, we decided to code the data acquisition and pre-treatment processes into BCM mainly to avoid problems with external programs and scripts, improve the communication speed and ensure data integrity. The results so far showed us that the BCM code written in Java can do the experiments without compromising the acquisition and equipment response time.

EXPERIMENTAL DATA

A major concern in this new version of the LabWeb project was the file format to be used to store and organize all the experimental data generated by users. This data format should have the following characteristics:

1. Free and Open Source project.
2. Active Project with a large community and support.
3. Solid data model.
4. Support fast I/O operations.
5. Single file to store all informations in a organized way.
6. API for the most common programming languages (C/Python/Java/Matlab, etc.).
7. Support for very large data.
8. Support features of high performance computing.

Based on these requirements we decided to use NeXus Scientific Data Format (NeXus) as standard data format for storage. The data format is divided into six levels: underlying physical file format, in this case HDF-5, file organisation, programming interface (API) for data access, rules for data storage and collections of definitions. [2]

HDF Viewer

Since HDF is a binary format, in order to avoid the need to install third party software for data browsing, a web application for opening NeXus/HDF files and plotting graphs and images online was created and integrated into SS.

The user interface of this application is as simple as possible counting with a treeview on the left side to browse the file and a panel on the right where graphs, images and informations are displayed, Fig. 9.

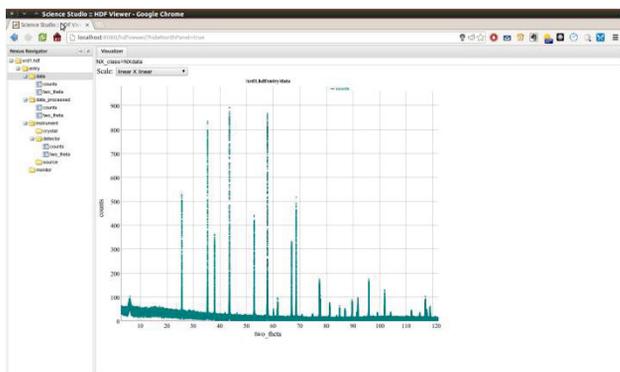


Figure 9: Graph of a HDF file generated with LabWeb at XRD1 beamline at LNLs.

This web application is implemented in Java using Spring MVC for the model and control layers and ExtJS for the view layer. The main flow of the application consists of three steps, Fig. 10:

1. Load HDF file from a local storage or remote submission.
2. Open the file using the native HDF API.
3. Association between the native HDF entities (groups and datasets) and the javascript treeview object that will be displayed on the screen.

Foreseeing the evolution of this application without the need of rewriting everything for new types of data such as 2D and 3D graphs, images, and other possible data, all the communication from the main application with the native HDF API is made with the help of plugins implemented according to the necessity of the task at hand. Currently there are already plugins for plotting data and rendering images.

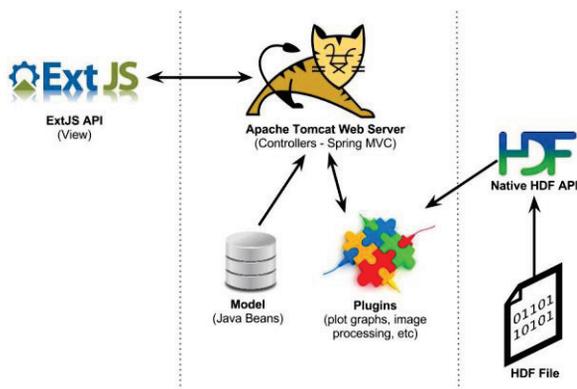


Figure 10: HDF Viewer Workflow.

CONCLUSION

Almost 15% of the SAXS1 beamline users are already using only LabWeb to run experiments and the other beamlines will start remote operations for users in the next months. The next beamlines already on sight for remote operation are IMX (X-Ray Tomography) and XRF (X-Ray Fluorescence). Finally, the software was effective not only for controlling the experiments remotely, but it

was also shown to be useful for the beamline staff as a remote assistance tool to users during presential experiments. All remote measurements were carried out successfully and the quality of the scattering curves, absorption spectra and diffractograms obtained were as good as those by obtained by local beamline operation, showing that the remote communication and interface did not introduce any interference on the experiments. In the future we intend to implement upgrades to perform more complex experiments, controlling temperature and gas devices, to increase the range of remote measurements.

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