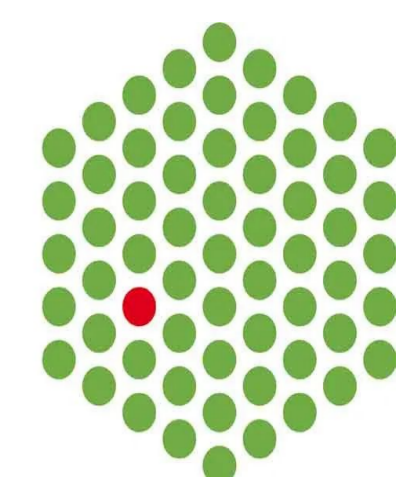# A WEB APPLICATION FOR BIOSAXS HIGH-THROUGHPUT DATA COLLECTION AND EXPERIMENTAL CONTROL

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ESRF The European Synchrotron

EMBL European Molecular Biology Laboratory

The ESRF extremely brilliant source (EBS), Europe's first high energy 4th generation synchrotron, started user operation in August 2020. To benefit from the exceptional high quality X-rays produced by the ESRF-EBS all the experimental control and data analysis pipelines have been significantly upgraded on all the EMBL-ESRF Joint Structural Biology Group (JSBG) beamlines. On the biological X-ray scattering beamline, BM29, a new web-based user interface, BioSAXS Customized Beamline Environment (BSXCuBE3), was developed to simplify and automate bioSAXS data collection on BM29. In 2022 BSXCuBE3 was used by over 277 users during more than 107 individual experiments on BM29. It has been tested on a wide range of biological samples and is constantly being optimized, extended and enhanced to suit the specific needs of bioSAXS users. The user feedback has been positive and found to be instrumental in simplifying bioSAXS data collection.
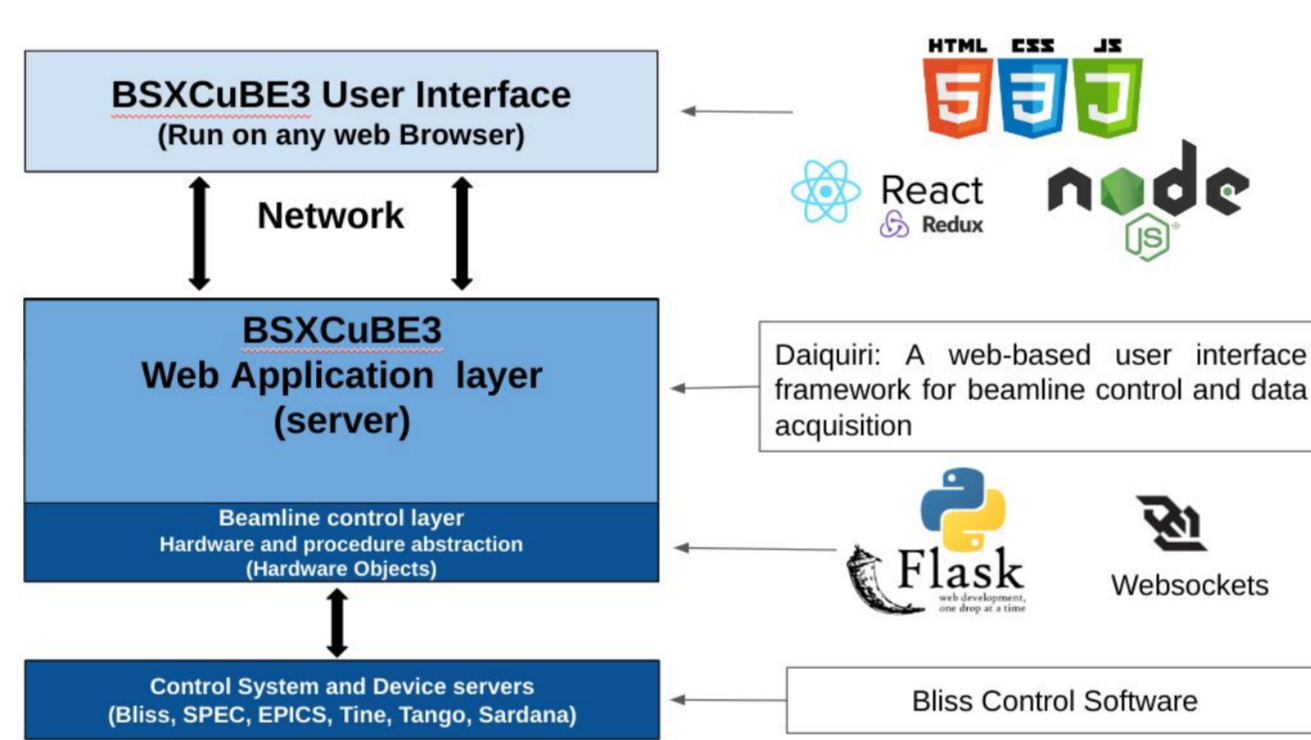
Introduction

BSXCuBE is the older version of BSXCuBE3, it was built on the framework4 a control-oriented graphical interfaces for beamlines, build with Python and Qt. Framework4 was a library with MVC architecture and a set of tools using bricks instead of widgets for ESRF staff to deliver graphical applications on beamlines for data acquisition and experiment control. As the framework4 was no longer maintained at ESRF, a new version of the data collection software based on new technology supported by the ESRF was essentially needed.

BSXCuBE3

BSXCuBE3 is developed by a collaboration between EMBL and ESRF to fully control BioSAXS experiments on BM29, the ESRF Extremely Brilliant Source beamline for BioSAXS. It is currently capable of running full data collections using either of two data collection modes; Sample Changer and/or SEC-SAXS. By successfully complementing the development of MXCuBE3 (Macromolecular Crystallography Customized Beamline Environment version 3), soon mxcube-web 4 the latest generation of beamline control application for MX experiments based on web technology, the ESRF has started a new concept of web based technology for beamline experimental control applications development.

Technology Stack

Other applications based on web technology that inherit the same technology stack as MXCuBE3 have been developed at ESRF. The new BSXCuBE3 application follows these development guidelines and also share some key features with MXCuBE3.

BSXCuBE3 User Interface (Run on any web Browser)

Network

BSXCuBE3 Web Application layer (server)

Daiquiri: A web-based user interface framework for beamline control and data acquisition

Beamline control layer Hardware and procedure abstraction (Hardware Objects)

Flask, Websockets

Control System and Device servers (Bliss, SPEC, EPICS, Tine, Tango, Sardana)

Bliss Control Software

User interface

The interface was designed to be user-friendly, for expert and non-expert users alike, to easily define and run bioSAXS experiments, as well as to visualize both raw and processed data. Initiating an experiment and adding it to the queue can be accomplished with just three mouse clicks, this simplifying the process significantly.
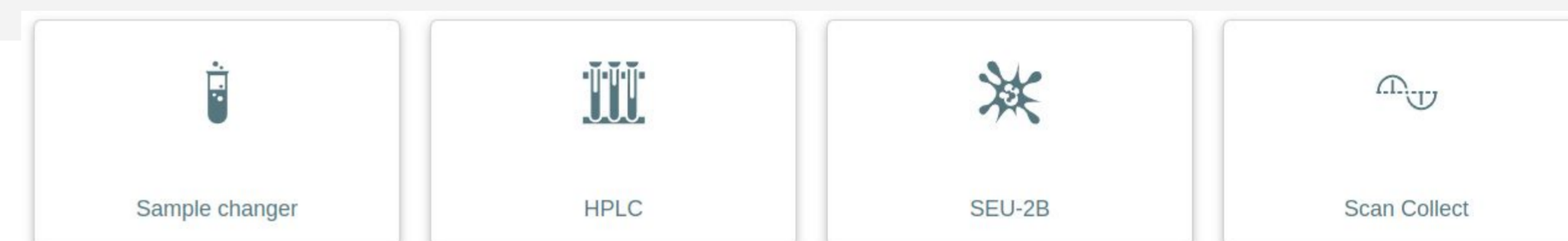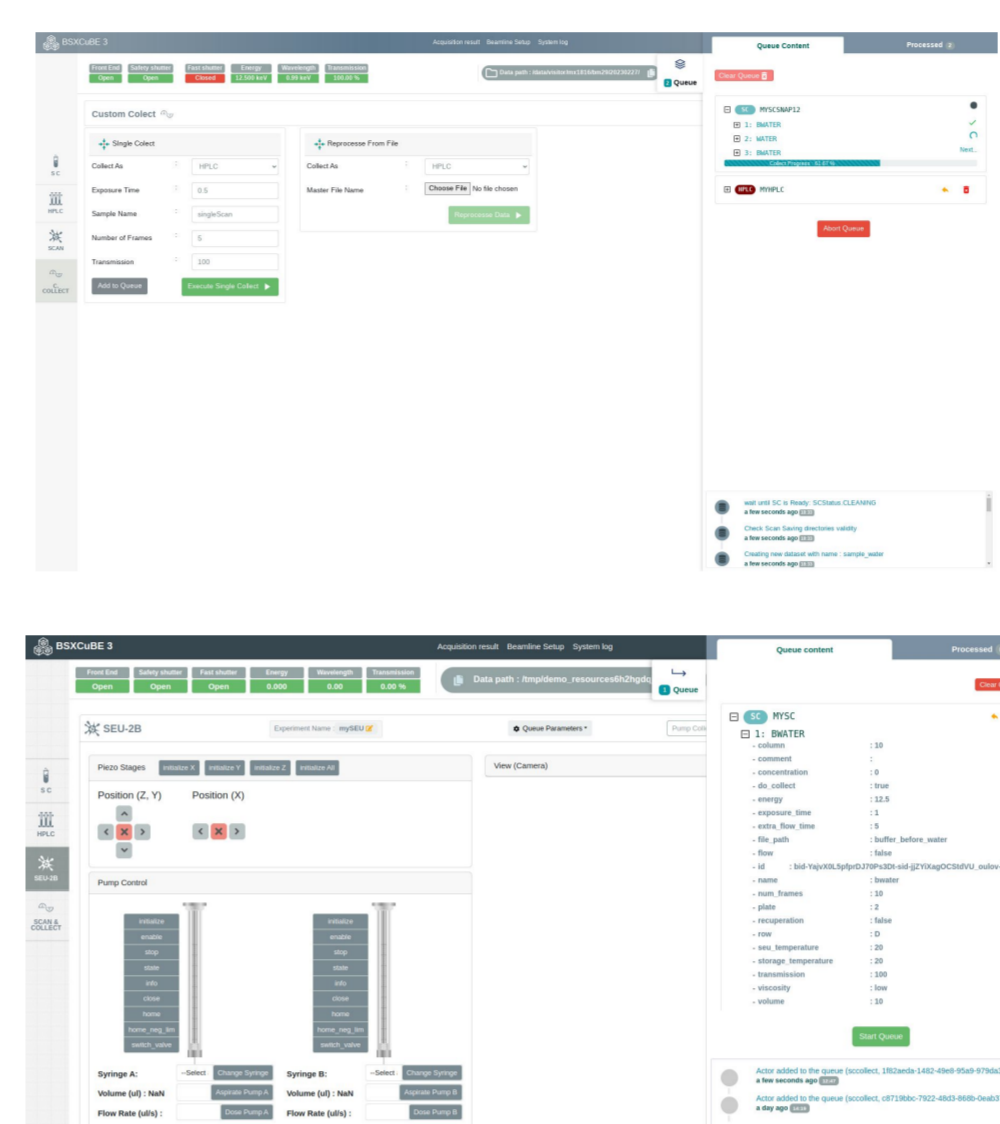
Interface for preparing data collection in Sample Changer Mode
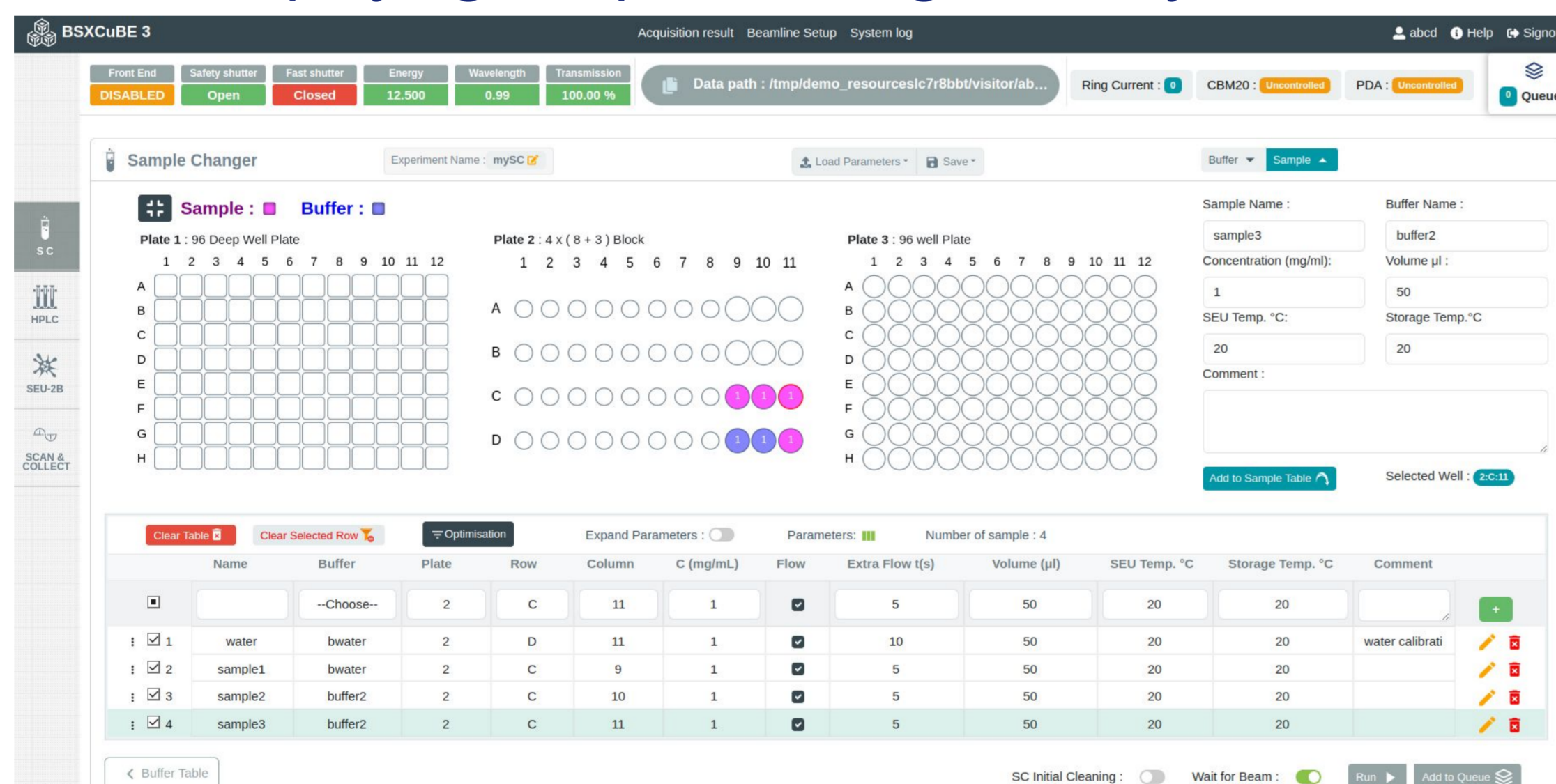
Interface for preparing data collection setup in SEC-SAXS mode.
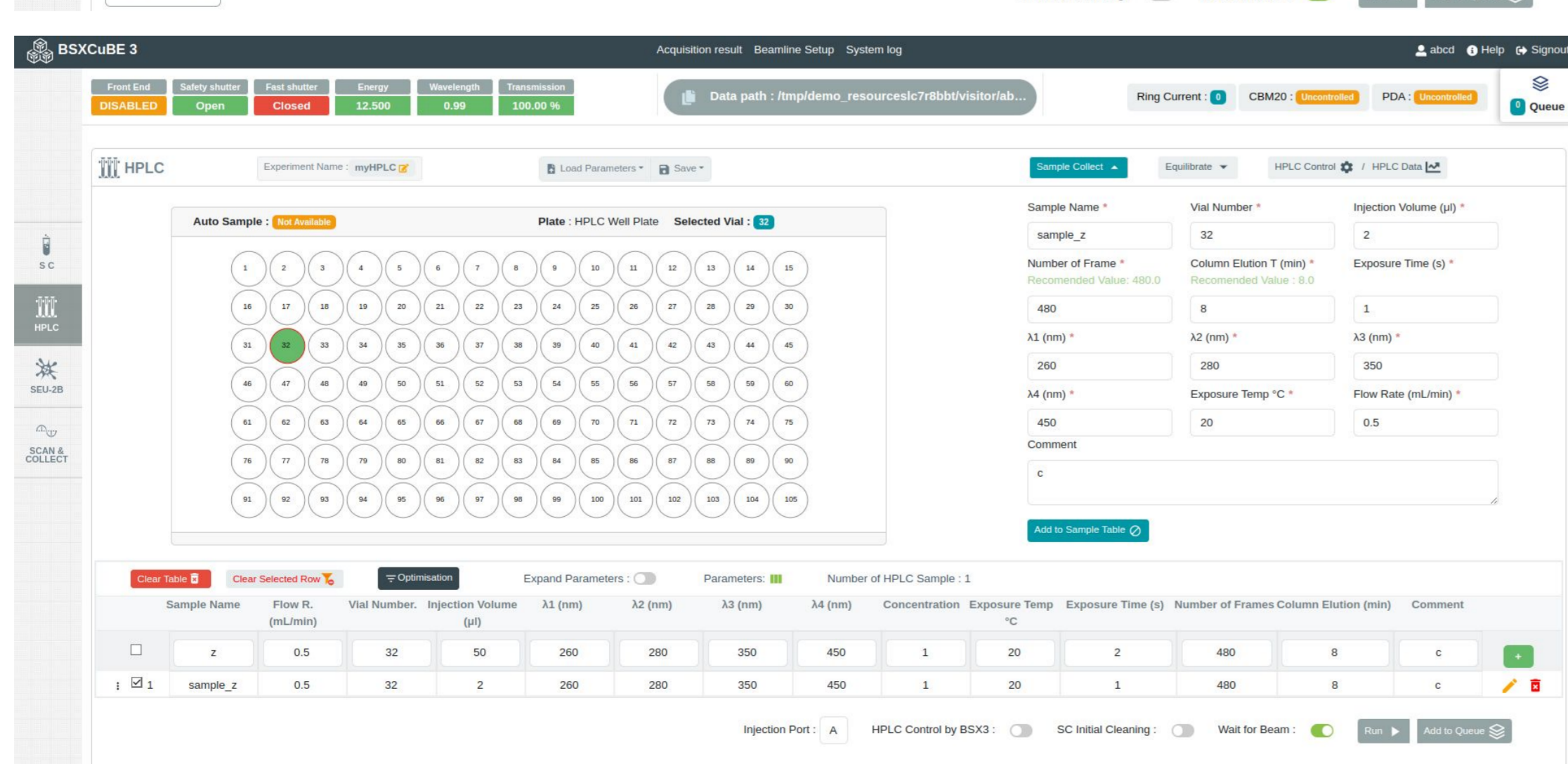
Collect process

- Sample Changer : Experiments using an EMBL designed BioSAXS sample changer (Round et al. 2015).

- HPLC : Experiments using a High-performance liquid chromatography (HPLC) device.

- SEU Scan : Scans on points or regions of interest, for instance, microfluidic chips.

- Workflow : A way to create a custom collection sequence by queuing various predefined scripts in combination with the experiment types above.

Backend

BSXCuBE3, controls the sample stage, detector, Sample Changer robot, HPLC, SEU, and data collection through BLISS (Guijarro et al., 2020) and a Daiquiri backend (Fisher et al., 2021).
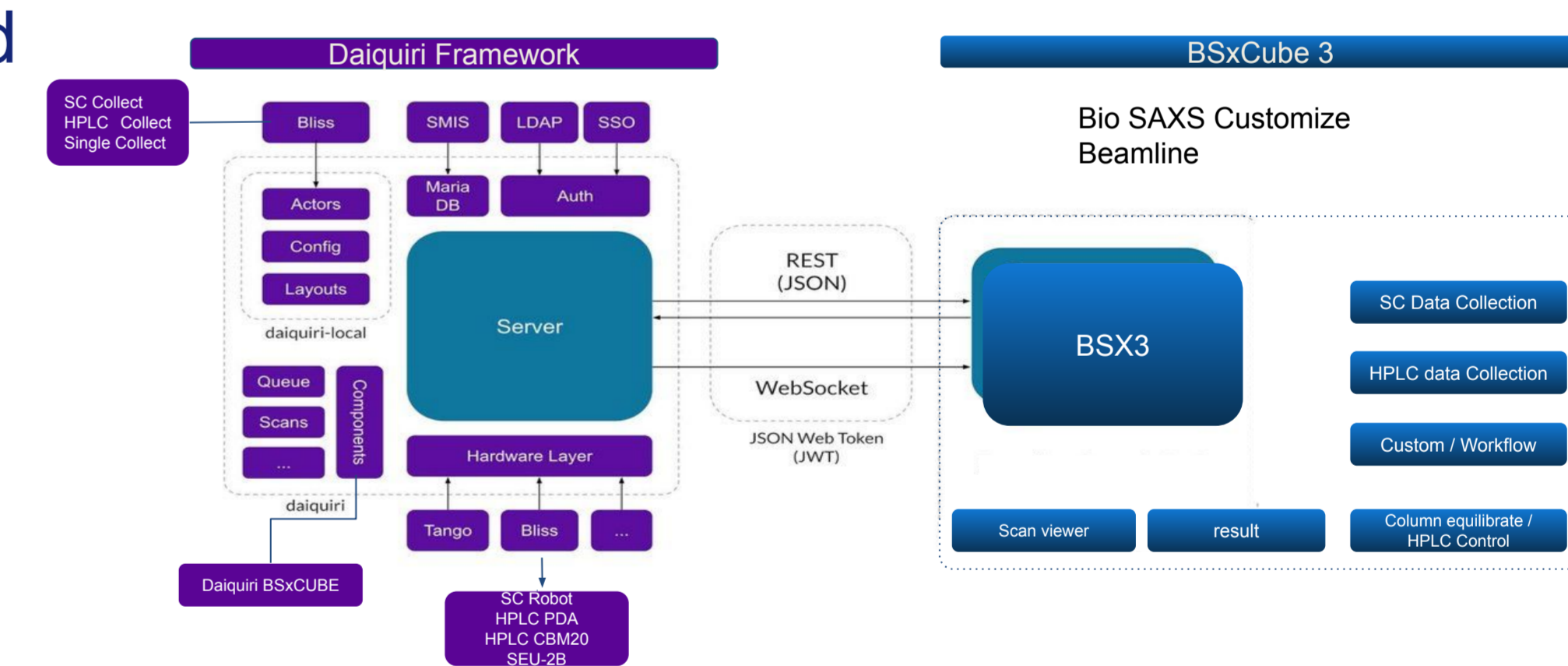
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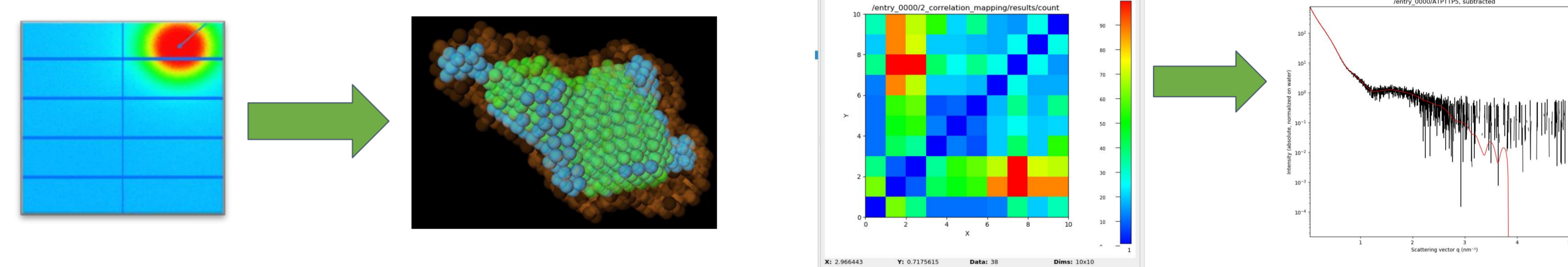$nm^{-1}\ q = 4\pi sin\ \theta/\lambda$
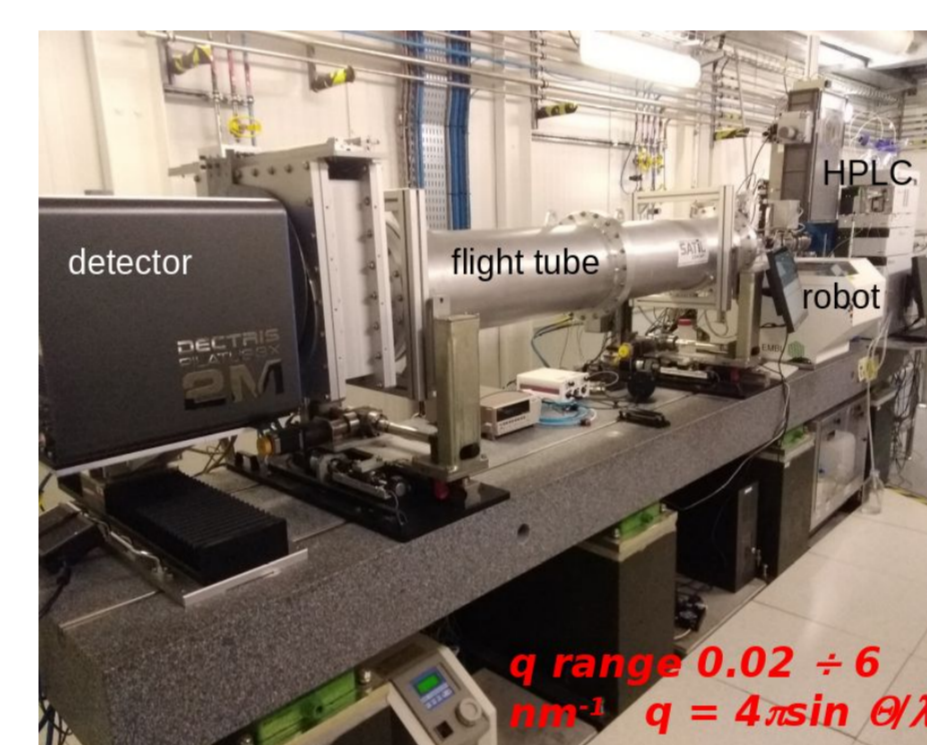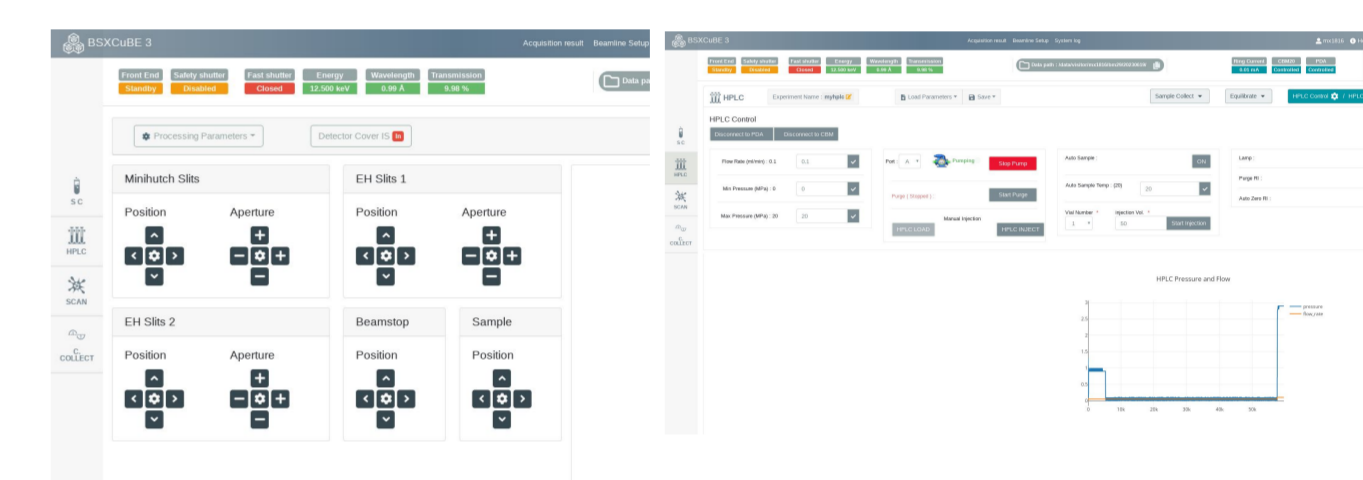
(Tully et al., 2023)   (Round et al.,2015)

General application architecture

Daiquiri : a web-based user interface framework for system control monitoring, hardware and data acquisition designed for synchrotron beamlines.

Daiquiri Framework

BSxCube 3 — Bio SAXS Customize Beamline

REST (JSON) / WebSocket / JSON Web Token (JWT)

BSX3 — SC Data Collection, HPLC data Collection, Custom / Workflow, Column equilibrate / HPLC Control

Scan viewer, result

Data Analysis

The entire data analysis software has been completely rewritten so BSXCuBE3 can send an amplified flow of data collected to a data-processing pipeline designed for diverse data acquisition modes, involving either a Sample Changer for homogeneous batch samples or SEC-SAXS. It is based on FreeSAS, a freely available set of algorithms essential for reducing and analyzing BioSAXS data, along with Dahu (Kieffer et al 2022).

Conclusion and future work

Further enhancements and automation on BM29 at ESRF are foreseen the integration and testing of new sample setups, such as microfluidics and CHIP-SAXS. That means adding new experimental control features in BSXCuBE3. Improvements of the Scan Viewer, Result Display and the application robustness are also foreseen.