WEB APPLICATION FOR BIOSAXS EXPERIMENTAL CONTROL

Marcus Carl Oskarsson, Antonia Beteva, Daniele de Sanctis, Gordon Leonard, Petra Pernot, Mark D Tully, Stuart Fisher (ESRF, Grenoble, France)
Jean Baptiste Florial, Andrew A McCarthy (EMBL, Grenoble, France)

Introduction

A new version of the beamline control application BSXCuBE (BioSAXS Customized Beamline Environment) to control BioSAXS (Small Angle X-ray Scattering on macromolecules in solution) experiments at the new ESRF Extremely Brilliant Source (EBS) is currently being developed. The new application is implemented as a Web application based on MXCuBE3 (Macromolecular Xtallography Customized Beamline Environment version 3) from which inherits the same technology stack and application structure.
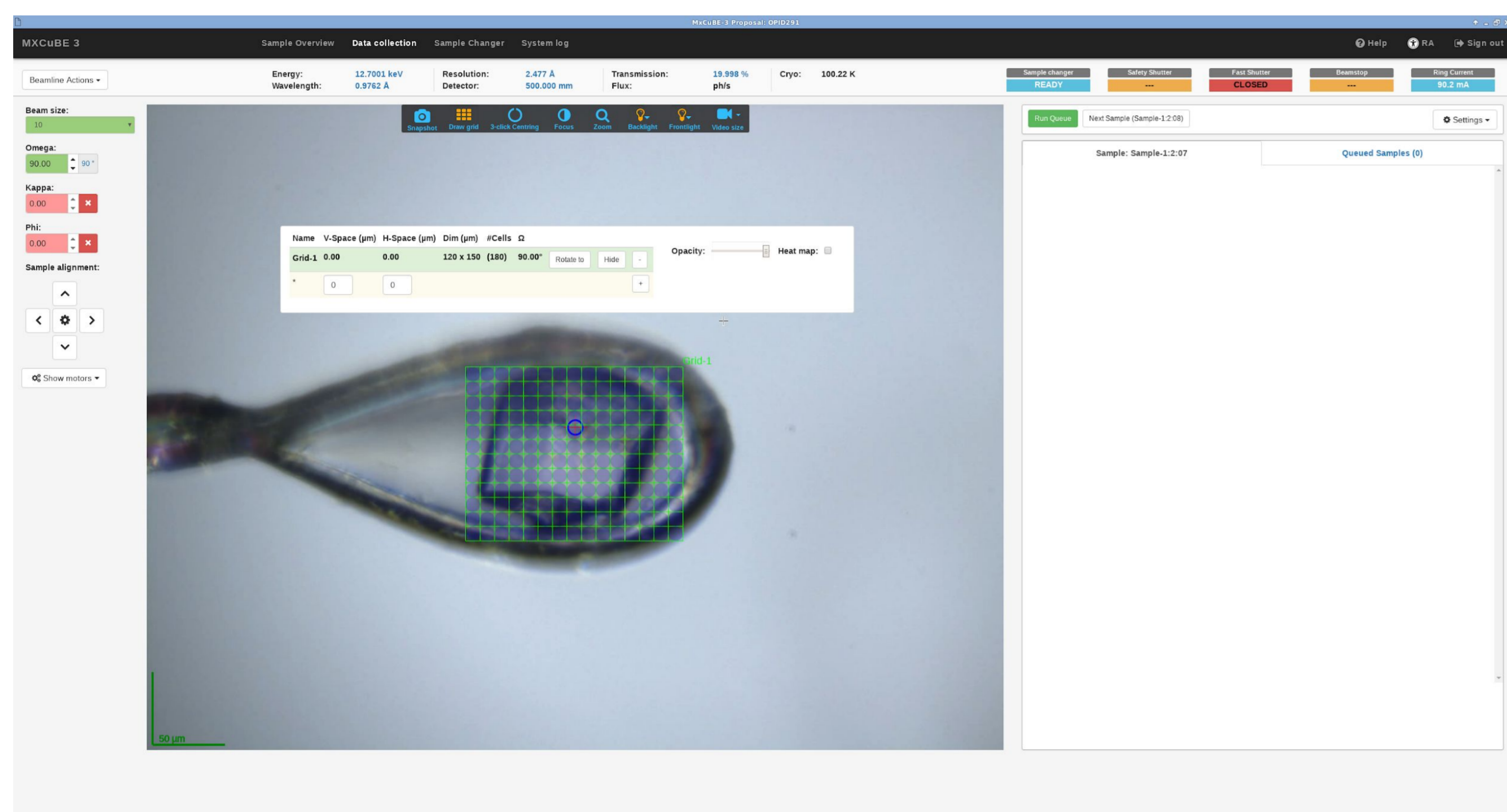

The success of the MXCuBE3 application has inspired and influenced the development of a new general framework for beamline applications, capable of serving both web and Qt front ends. The framework consists of reusable UI components, many already existing in MXCuBE3 and a general purpose backend, that further facilitates good developmental practices by providing patterns and abstractions for both backend and frontend development.

Front end development
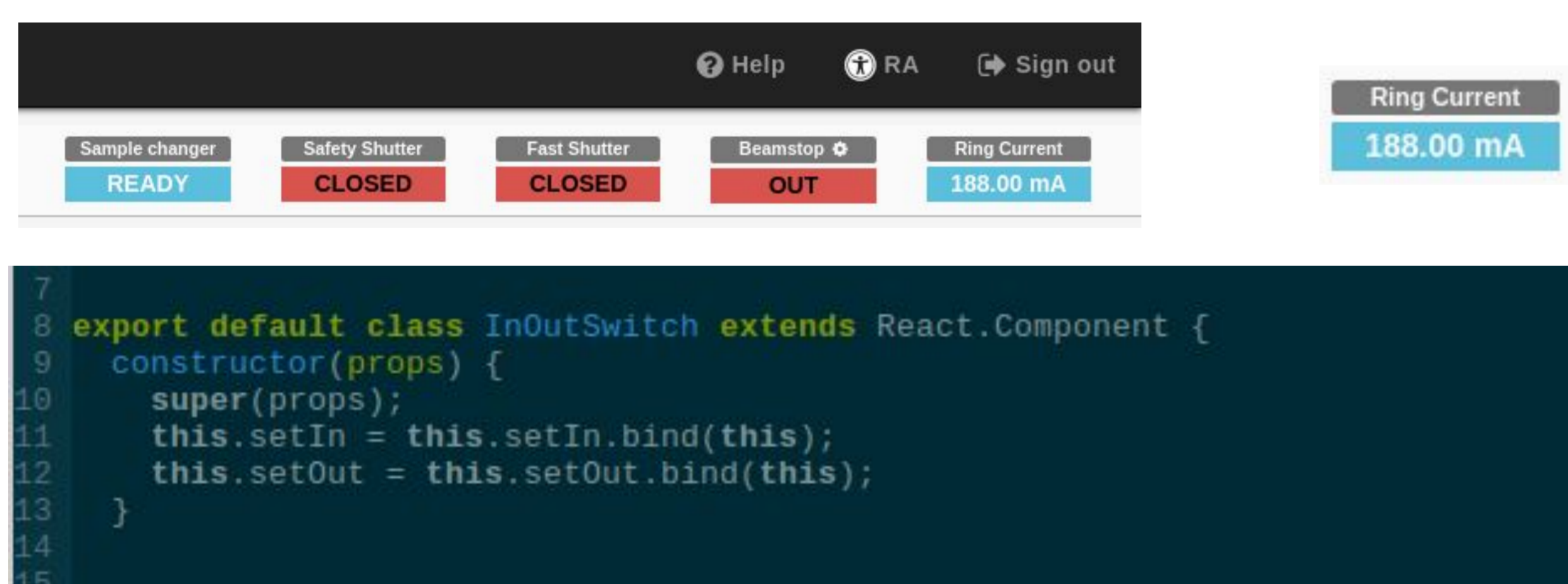
Similarly to MXCuBE3, the BSXCuBE3 user interface is implemented with React, Redux and Bootstrap using HTML5 and ECMAScript 9. React provides means to encapsulate interaction logic and display, to create reusable user interface components.

The data provided to a user interface component is handled with the state management library Redux. Redux keeps the entire application state in what is called a store. The Redux store is an immutable data structure that can only be updated by dispatching a Redux-action
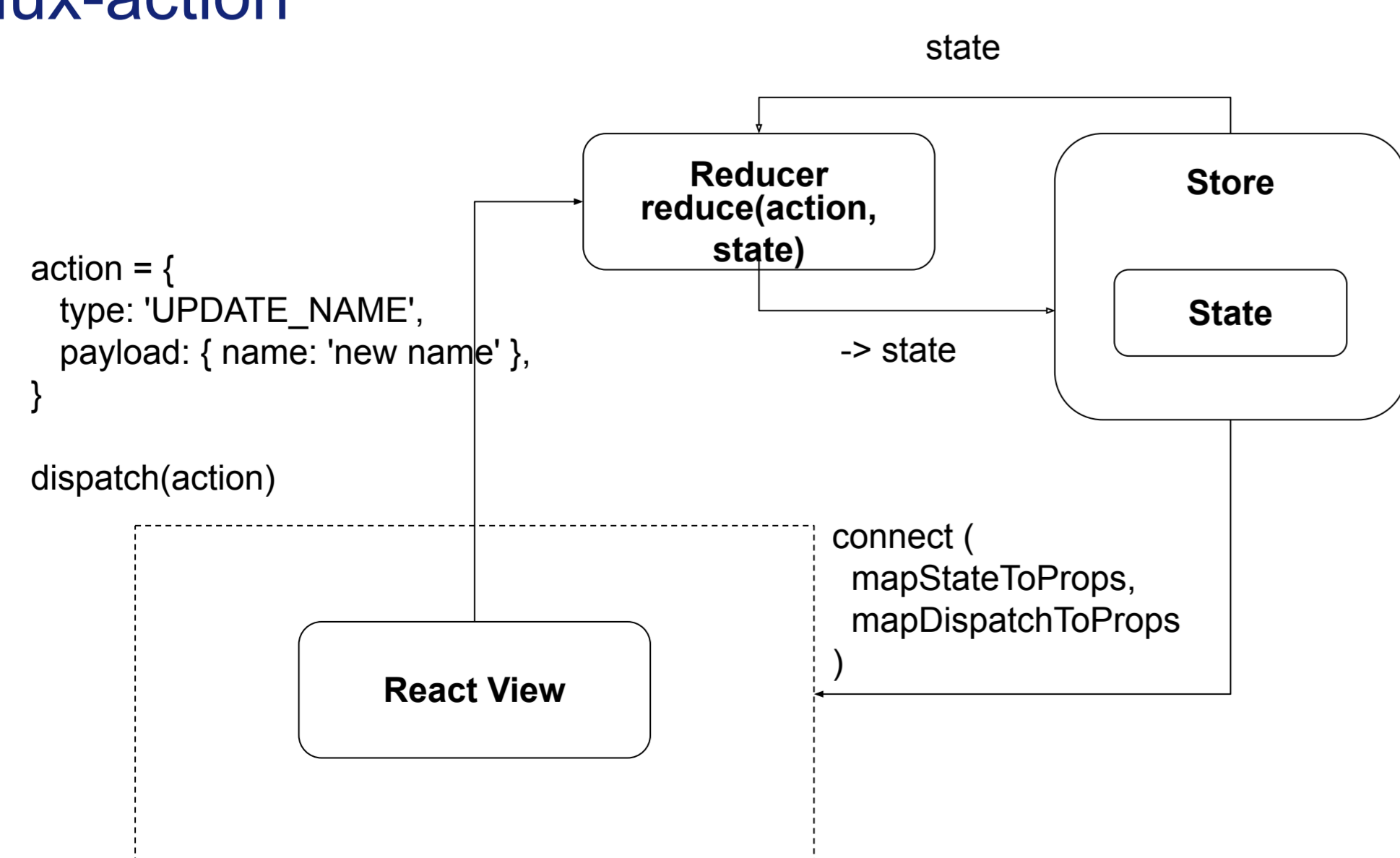

User interface

MXCuBE3 and BSXCuBE3 share the same key concepts such as beamline configuration and calibration, an on axis viewer (OAV), a queuing system, one or more types of sample environment and LIMS integration. Many of the graphical components in MXCuBE3 can be directly reused, making it possible to use the same general look and feel.
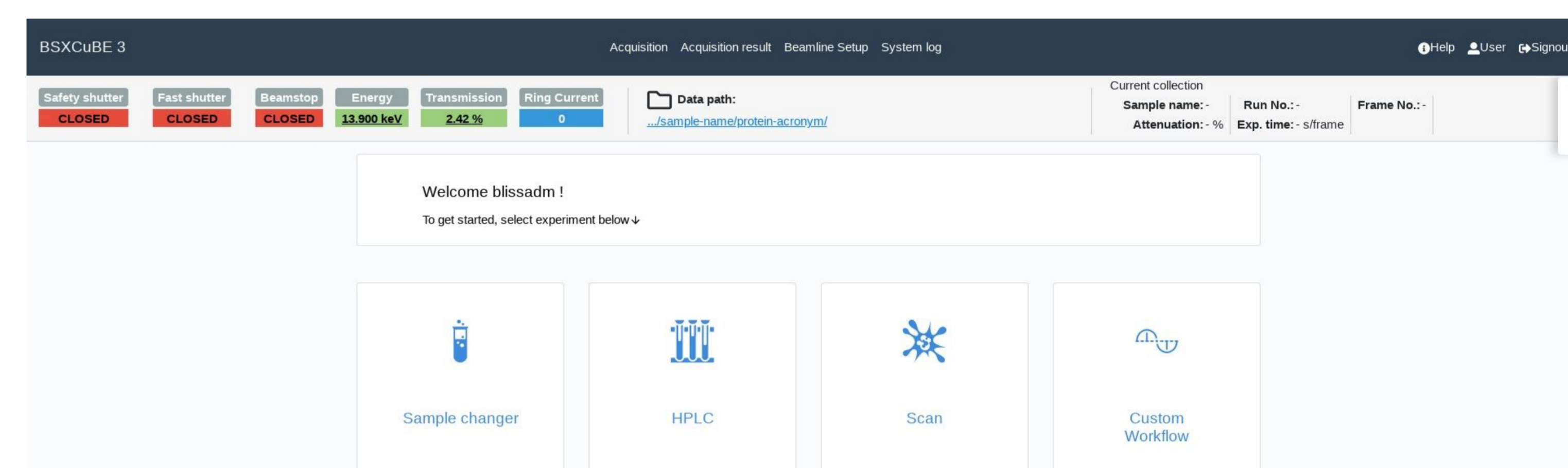
At the time of writing the different experiment types foreseen are: Sample Changer, HPLC, Scan and Workflow.

- Sample Changer - Experiments using an Arinax BioSAXS sample changer (Round et al. 2015)
- HPLC - Experiments using a High-performance liquid chromatography (HPLC) device
- Scan - Scans on points or regions of interest on, 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.
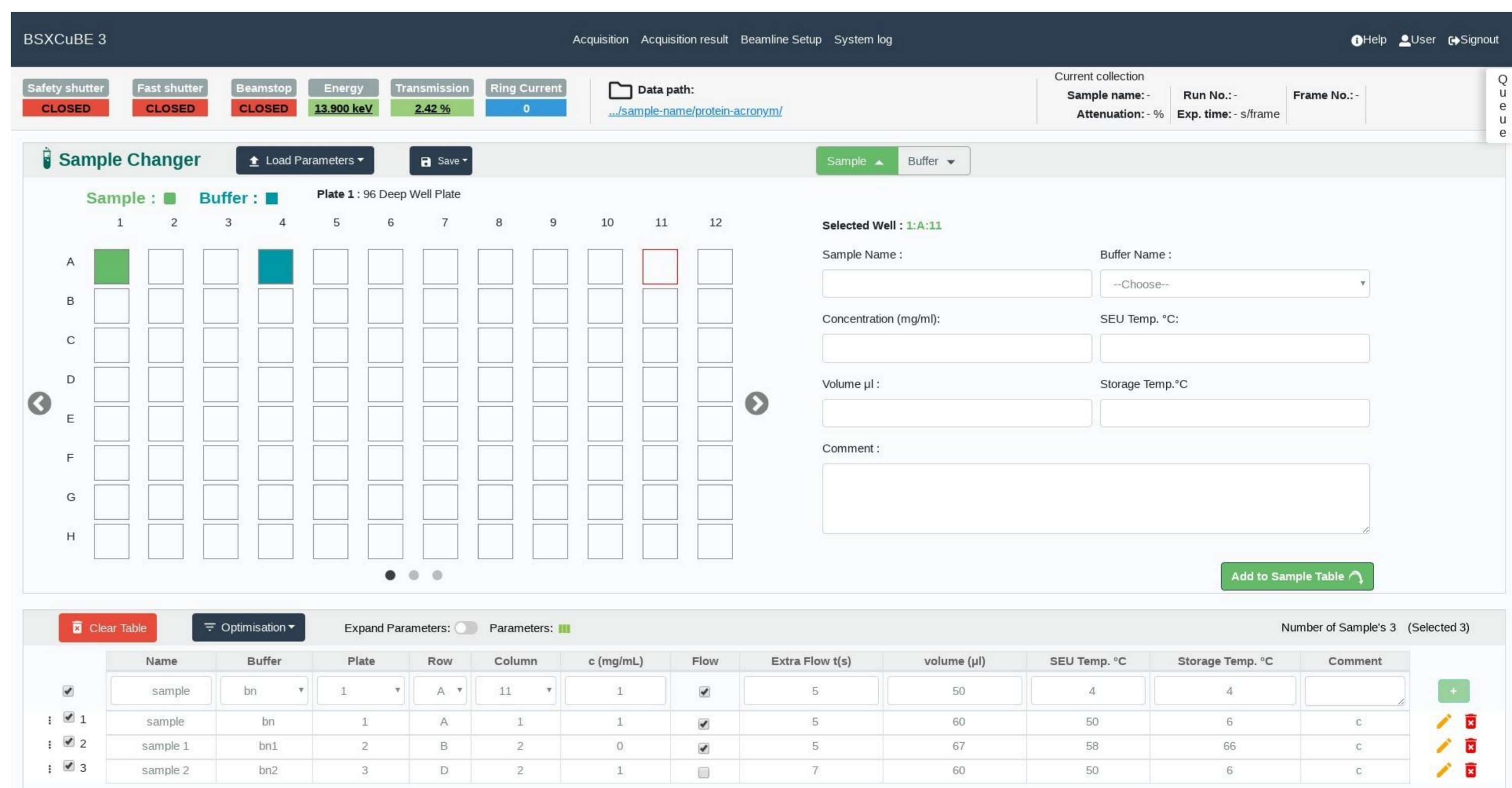
Conclusion and future work

The technology stack and overall application structure is very similar to that of MXCuBE3. MXCuBE3 has, as one of the first web applications for beamline control at ESRF, inspired and influenced the new application framework currently under development at ESRF.