SynchLink:

an IOS app for viewing data interactively from synchrotron MX beamlines

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ISPyB[1] (Information System for Protein crystallography Beamlines) is a Laboratory Information Management System (LIMS) developed to manage Synchrotron radiation macromolecular crystallography experiments. ISPyB provides features that allow users to register sample information for a particular experiment, manage the shipment of samples and collate data collection and processing parameters for each experiment providing a portal for users to view current past and future visits to the synchrotron. ISPyB is currently used at the ESRF and Diamond for MX experiments and, at Diamond, currently extends to presenting results of automated processing results from XIA2[2] and FastDP[3]. The system is accessible to the user remotely through a web based interface.

In January 2013 Diamond officially released V1.0 of SynchLink, an iPhone/iPad (iOS v6 onwards) app which allows users of Diamond MX beamlines to monitor, re-visit, and search information on their data collections and automated data processing results recorded in ISPyB[1].

Introduction

Smartphones and tablets have significant advantages for use in a variety of industrial sectors where there is a high level of mobility of workers. For example, the healthcare industry was an early adapter to mobile devices and uptake increased steadily from their introduction in the late nineties[5].

Despite their increased processing, data storage and graphical capabilities few use-cases have thus far allowed us to exploit the technology in the structural biology workflow. There are some lightweight applications for chemical information, 3D molecular graphics viewers and for monitoring synchrotron and beamline status, but due to either the data-heavy nature of processing images or computational intensive nature of structure solution, few applications are yet available.

However, the obvious advantages of using small easily portable mobile devices for MX synchrotron users was clear and the availability of an Information-rich database ISPyB which is populated by data acquisition software and automated data processing and structure solution pipelines brought about the requirement for an app that could exploit these past developments.

Here, we have developed an IOS v6+ app to allow MX users of Diamond to interact with ISPyB. We chose IOS in the first instance to mitigate the number of variables by limiting the number of hardware to support to iPhone/iPad (iOS v6+) and use the native Mac development tools i.e. Objective-C language and the XCode toolset as a development environment.

Methods

As with many software development projects, the user interface is often all a user will see and its reliability, intuitiveness and speed of interaction will determine the success of the project overall. Fortunately, given a populated data source, this initiative was able to focus on the three main components to achieve this: 1) the app itself on the device and how it interacts with 2) the webservices servicing the data and 3) interfacing with the data sources. Moreover, the workflows and the way the data are presented to the user were reassessed and optimised for current expected use.

GUI

The GUI was developed as a series of windows into the data exposing more and more detail on the user request whilst minimising the number of windows to navigate before reaching the data. We worked hard to limit the information displayed to what was necessary, to avoid overloading the user. Figure 1 shows a montage of some of the screens as they would appear on an iPhone, along with a schematic representation of the navigation.

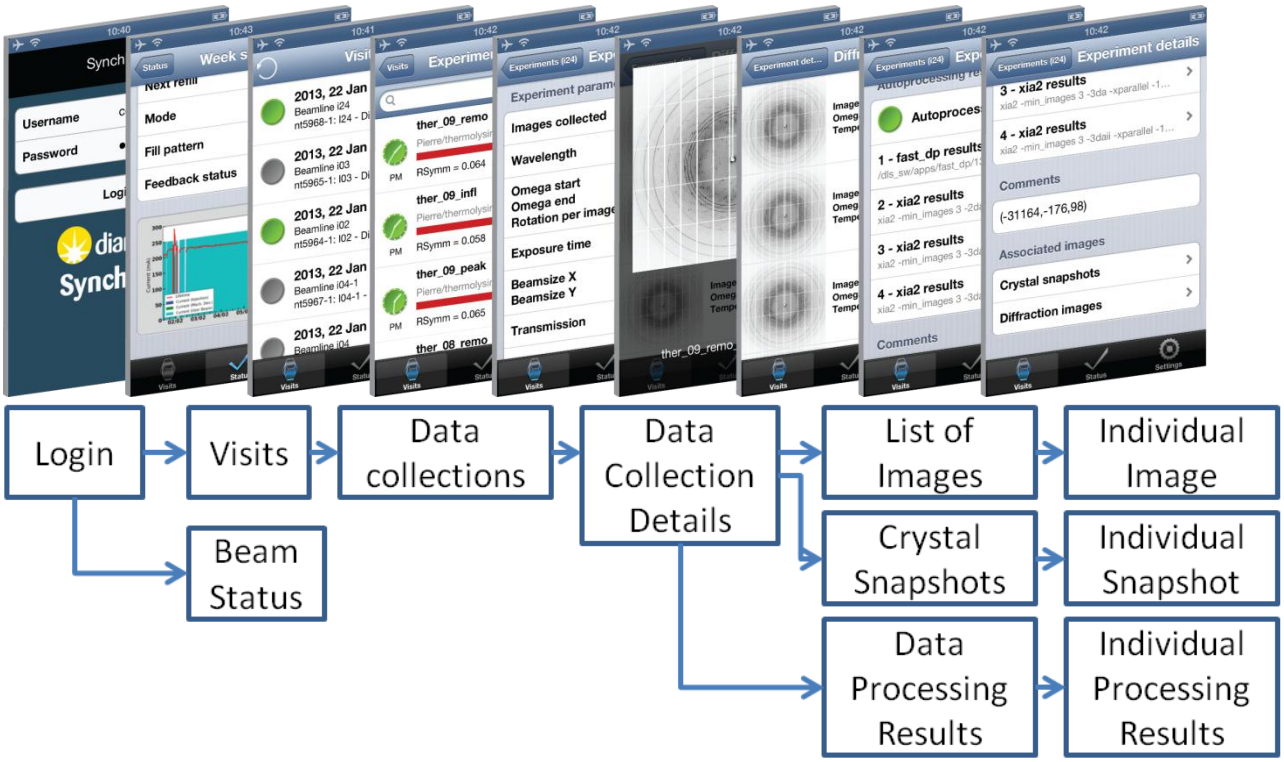

Figure 1; Screenshot's from SynchLink as shown on an iPhone and the main user workflow.

As previously outlined, displaying useful information quickly was vital to distract the operator from potentially longer running data transfers caused by either slow networks or simply volume of data. To this end the GUI was developed to prioritise the display of information for

the current screen before downloading off-screen data (figure 2). Additionally a search option was create to select only visits and data collections matching the search key.

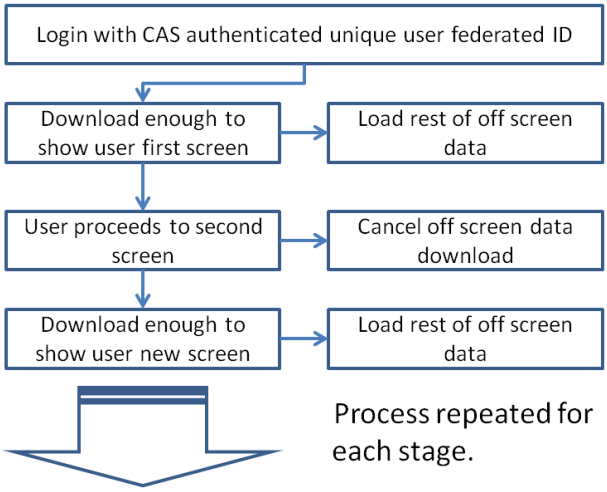

Figure 2; GUI workflow on how the app can remain responsive to user interaction.

WebServices

A number of web service technologies were explored, but eventually a JSON web service developed using Java/Axis2 and running on an Apache Tomcat server was chosen due to its limited data exchange size, thereby increasing the responsiveness of the client app. A generic structure was developed for these webservices based on the database tables and its structural linking as this ensured maximum flexibility to the application developer whilst authentication and authorisation to the data was applied server side. As a continuous session could not be held open with a mobile device (either no support or a draining of battery power) a server side session token is shared with the app upon successful login/authentication. This is valid for 24 hrs and used to authenticate the request from the device without having to fully authenticate against the facility's CAS (Central Authentication Service) mechanism.

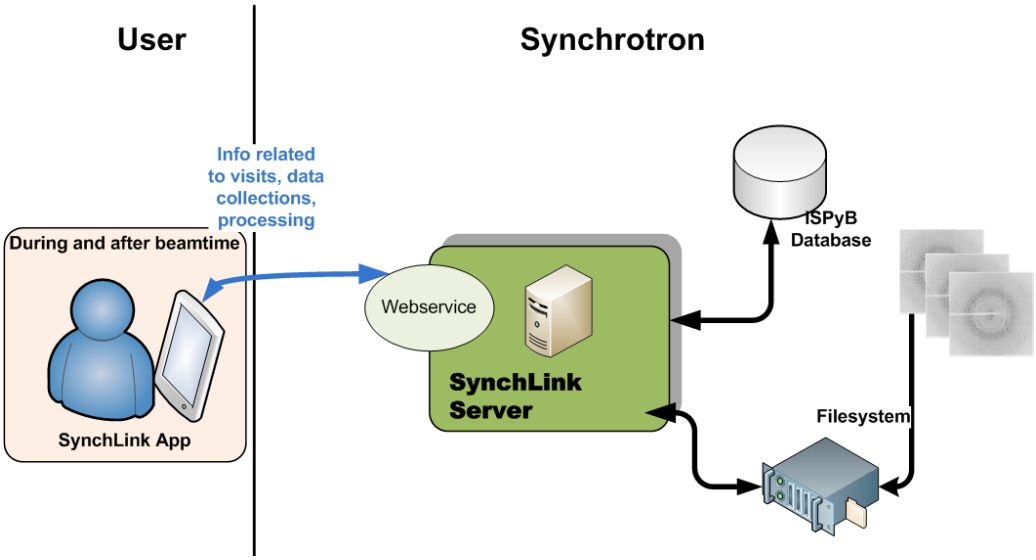

Figure 3: A schematic view of the SynchLink webservice and app Client

Message encryption between the SynchLink webservice and the app is achieved using SSL certificates. The transmission confidentiality is important given the sensitivity of data collected by some synchrotron users.

The webservice is implemented using the Apache Axis2/Java framework and the server is hosted on a machine internal to the synchrotron network. The webservice is accessible through an URL accessible externally that redirects to the internal server machine. This choice, allows more freedom in moving the webservice to other internal machines (for

maintenance or upgrade) but also to limit access to the server only to clients of the webservice.

The webservice has direct access to the ISPyB database and the synchrotron filesystem achieving a perfect encapsulation layer of the synchrotron resources (figure 3).

To aid performance, JSON data-interchange format is used and gzip compression is performed on the exchanged messages in order to reduce the size of data.

Integration with the facility site

Key to the app's success is the ISPyB[1] database (https://forge.epn-campus.eu/projects/ispyb3) and its continuous population from the user office scheduling software, data acquisition software (www.opengda.org) and Diamond's automated data processing pipelines[2,3,4]. The way ISPyB integrates within a facility is outlined elsewhere[1], but the use of Synchlink integrates seamlessly into the user experience as summarized in figure 4 below.

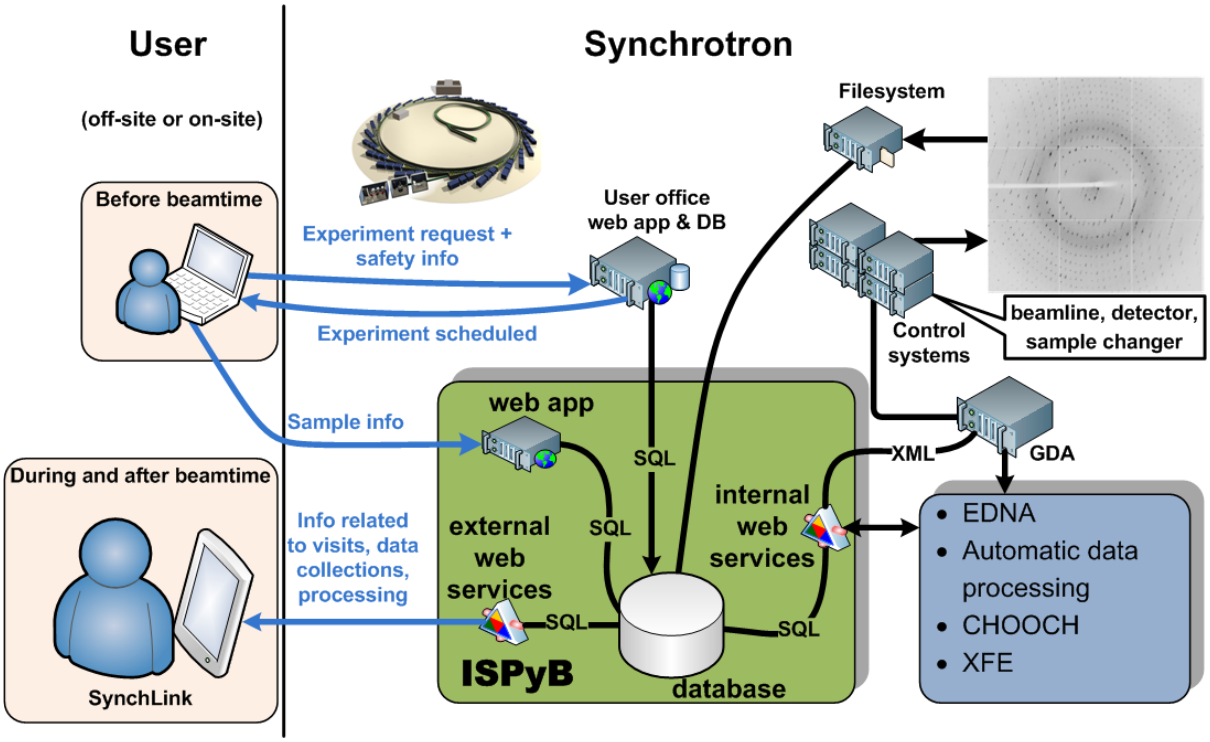

Figure 4; Schematic representation of how SynchLink integrates with facility services.The figure has been modified from Delageniere et al[1]

Availability

The app is available from the App Store and is free to download, though the data charges of your network provider will apply. Nearly 200 downloads have already been recorded. The ISPyB database and frameworks are available to participants of the ISPyB collaboration.

Future

There are many potential developments from V1.0 in increasing the functionality and science coverage of the current app, including support of other devices, such as Android-based.

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