



Automation of the Macromolecular Crystallography Beamlines at the Canadian Light Source

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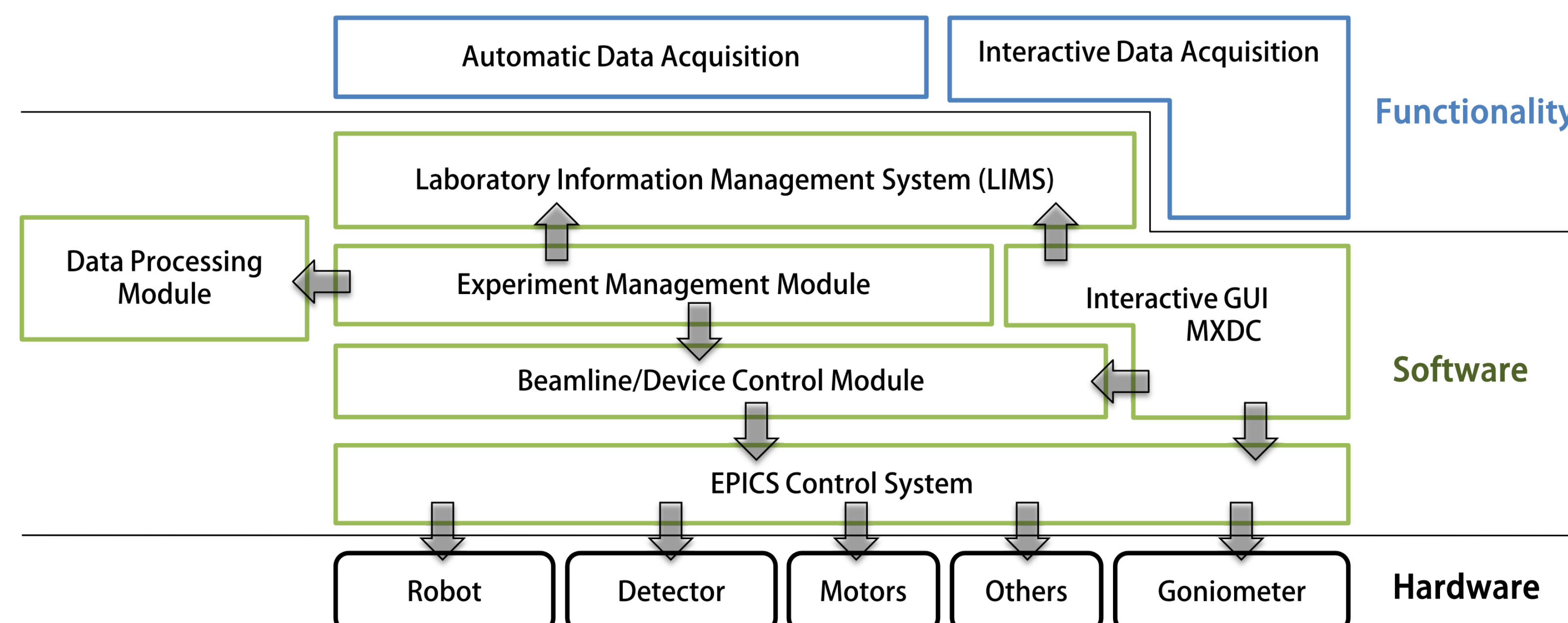
Summary

The Canadian Macromolecular Crystallography Facility (CMCF) is a suite of two beamlines 08ID-1 and 08B1-1. Beamline 08ID-1, is an undulator beamline for studying small crystals and crystals with large unit cells, while beamline 08B1-1 is a bending-magnet beamline for high-throughput macromolecular crystallography with a high level of automation. The primary method of access to CMCF 08B1-1 will be remote, in what is commonly referred to in the field as “Mail-in” crystallography. We are developing a software system for automating both beamlines, with modules for beamline control, experiment control, data analysis, information management, and graphical user interaction. The system is developed using the Python programming language and makes use of popular open-source frameworks such as TWISTED, DJANGO and GTK+. Once completed, the system will allow automation of the macromolecular crystallography experiment from experiment setup to data analysis, thereby increasing the efficiency of the CMCF beamlines and reducing the need for user travel to the synchrotron.

Technologies



The Software System



Laboratory Information Management System (LIMS)

The LIMS is responsible for the storage of information about samples, shipments, experiment requests, results and data sets. It is accessible over the web.

Experiment Management Module (EMM)

This module replaces the human in decision making as concerns the crystallographic experiment. It directs the Beamline Control and Data Processing Modules to successfully perform the experiment without human intervention.

Beamline Control Module (BCM)

The BCM controls and coordinates hardware devices. The capabilities of this module include automatic configuration of the beamline, crystal mounting and centering, measurement of fluorescence spectra and collection of diffraction images.

Data Processing Module (DPM)

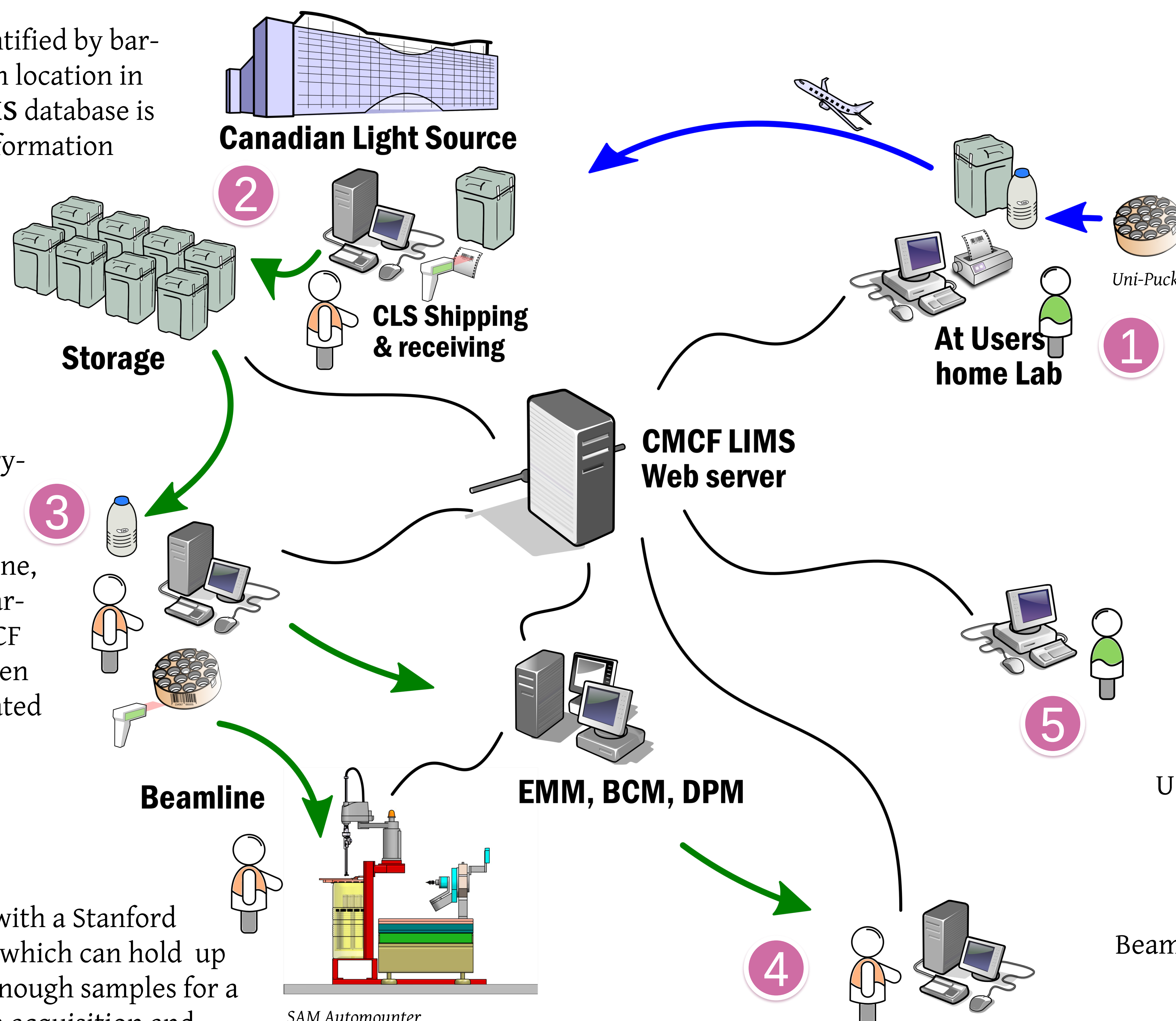
This module performs data analysis tasks required for successful data acquisition, such as sample characterisation, scoring and automatic data processing.

Remote Access and Automation

On arrival shipment is identified by barcode and placed at a known location in the storage. The CMCF LIMS database is updated to contain new information about the storage location.

Beamline Staff retrieves Dry-Shipper from storage and loads Uni-Puck onto the automounter at the beamline, identifying the Pucks by barcode and updating the CMCF LIMS at each step. Staff then initiates a queue of automated data acquisition.

The beamline is equipped with a Stanford Automounter (SAM) robot which can hold up to 192 samples at a time, enough samples for a full shift of automated data acquisition and analysis by the EMM, BCM and DPM.



- User Logs onto their CMCF **LIMS** web account
- Prepares samples and places them in a Uni-Puck sample container. Each Uni-Puck can store 16 samples
- Enters sample information into the CMCF **LIMS** database using a web browser
- Creates experiment requests via the CMCF **LIMS** website and associates them with samples

User Logs in to verify preliminary results, update experiment requests, inspect results and download data. Users can also see the status of their outgoing and incoming shipments.

Beamline Staff verifies results and sends notification to user.

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