CMCF Software Requirements Specification

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1.0 INTRODUCTION

1.1 PURPOSE

This Software Requirements Specification (SRS) document specifies the software requirements for the CMCF Beamline Operating System (BOS). The goal of the specification is to provide a functional tool for guiding the development of the system in a manner consistent with the goals of operation of the CMCF. It establishes both general criteria and specific functional requirements for software and controls design.

This document is oriented toward developers of the CMCF BOS.

1.2 SCOPE

The subject of this document is the *CMCF Beamline Operating System*, which will provide all software components required to operate the CMCF beamlines at the Canadian Light Source. The system will provide a highly integrated solution for interactive and automated control of all beamline hardware, as well as provide all functionality required for scientific data acquisition accessible both on-site and remotely *via* the internet.

CMCF BOS is all software directly involved in the control and use of CMCF Beamline systems, including commercial or third-party software packages used for that purpose. However, only the non-third-party portions of this software are addressed in detail here, along with the interfaces to those third-party packages.

1.3 DEFINITIONS, ACRONYMS AND ABBREVIATIONS

SRS – Software Requirements Specification

CMCF – Canadian Macromolecular Crystallography Facility

BOS – Beamline Operating System

1.4 OVERVIEW

Section 2 presents the overall description of the CMCF BOS. It describes the general factors that affect the CMCF BOS and its requirements, thus serving as a general background to the specific requirements outlined in section 3.

In section 2, the CMCF BOS is placed into perspective with other related products, hardware, software and human interfaces are introduced, the major functions expected of the CMCF BOS will be summarized and the users of the system and their characteristics identified. This section also describes general constraints that will limit the design of the CMCF BOS Software, as well as assumptions that affect the specifications outlined in Section 3. This section concludes by apportioning requirements into functional groups, and prioritizing them.

In section 3, all software requirements are presented in detail. Inputs, and outputs are identified, as well as the functions which must be performed by the system in response to inputs and in support of an output. Performance, reliability, availability, maintainability, portability and security requirements are also described in this section.

2.0 GENERAL DESCRIPTION

2.1 OPERATIONAL CONCEPTS

2.1.1 Operating Modes

Several modes of data acquisition will be supported by the CMCF facility.

(a) *Interactive data acquisition:* This mode provides direct access to the beamline for the collection of science data. In this mode, the 'client' scientist makes all control decisions during the data acquisition period. In this mode, the 'scientist' is the 'operator'.

(b) *Assisted data acquisition:* This is a special type of interactive acquisition mode, in which direct access to beamline minimized. This mode provides simple and safe access to the system for selection of experiment parameters, and 'quick-look' data analysis. In this mode, the system will make most control decisions but giving the operator the possibility of overriding them before their execution.

(c) *Automatic data acquisition*: This implies a significant automation of the decision making process, with as little human input as possible. In this mode, various data-collection requests are kept in a dynamic queue from which tasks are selected in some order in order to maximize utilization of the beamline. In this mode, there is no 'operator'.

(d) *Remote data acquisition*: This mode provides similar functionality to both assisted and automated data acquisition except that the 'operator' is situated off-site.

2.1.2 Operational Actions

Regardless of the mode of data acquisition, every data acquisition sequence involves the following classes of action:

(e) *Pre-data acquisition* – these are actions that take place well before the scheduled data acquisition period. These actions include experiment planning, where the scientists develops an experimental plan, is assigned beam time, prepares and either ships the samples to the facility or brings them in person.

(f) *Beamline setup actions* – These activities are done prior to the data acquisition period. These are typically system operation checks, instrument configuration checks, optimizations and some calibrations.

(g) *Data acquisition setup* – these actions take place immediately prior to data acquisition and include beamline configuration, sample mounting and some instrument parameter selections.

(h) *Sample screening/characterization* – This is a data acquisition process in which preliminary data is collected on a sample and used for parameter optimization and sample scoring resulting in improved parameters for full data acquisition. This step can be skipped if it has previously been performed on the sample or if current sample parameters are already fully optimized.

(i) *Data acquisition* – The period of actual scientific data acquisition. During this process, scientists may carry out actions such as 'quick-look' verification of data quality, minimal parameter modifications and system operation monitoring.

(j) *Data Storage* – Actions and procedures that allow the scientist to access, transfer and/or back-up their data

(k) *System security actions* – On-going actions designed to protect the functionality of the beamline. These actions take place throughout the data acquisition process and are designed to protect both humans and beamline equipment.

(l) *Data integrity* – Actions that assist in validating and preserving scientific data. These include automatic logging of experimental actions, commands, operator comments and beamline states.

2.2 PRODUCT PERSPECTIVE

The growing impact of macromolecular structural analysis to pharmaceutical, academic and industrial research has resulted in a growing demand for access to protein crystallography beamlines. This demand is also reflected in the number scientists of different fields now wanting to use structural information in their research. To achieve the goal of seamless access to, and use of the facility, the CMCF BOS software will need to interact with several external components to completely perform its function. These components include beamline hardware, crystallographic data analysis packages, user-office services, and other CLS facility services such as Stores.

2.2.1 Software Interfaces

The Crystallographic community has already made a significant investment in developing software systems to accomplish specific analysis tasks such as diffraction image analysis, data reduction and crystallography toolkits. The CMCF BOS Software will integrate the services of these tools where required.

- XDS, MOSFLM, HKL2000 – The system will provide automated data processing functionality by interfacing with these third-party software packages. The interfaces of these packages are described in their respective scientific publications [1, 2, 11]
- LABELIT – The system will provide auto-indexing functionality by interfacing with XDS, MOSFLM, and/or LABELIT [3].
- SpotFinder/DISTL – The system will provide automated diffraction image analysis and crystal screening by interfacing with SpotFinder/DISTL [4].
- XREC – The system shall provide automated loop and crystal centering using the XREC software package [12].
- BEST – The system will provide automated data-acquisition strategy and dosage determination by interfacing with the BEST and RADDOSE packages [5, 6, 7].
- CHOOCH – The system will provide automated fluorescence scan analysis and MAD energy selection using CHOOCH [8].
- Third Party databases – The system will store experimental parameters and results in third party databases such as xml databases or relational databases.

2.2.2 Hardware Interfaces

The system will provide instrument control by interfacing with beamline hardware. Beamline hardware will normally be of the following classes:

- Motors
- Beam position monitors

- Intensity detectors
- Multi-channel analyzers
- Beam Viewers
- CCD Detectors
- Robotic Sample Changers
- Cryogenic cooling systems

The specific hardware interfaces for each hardware type, are documented in the relevant hardware manuals.

2.2.3 User Interfaces

Different types of user interfaces will be available depending on the user-class and operation mode. Users will interact with the system through the following interfaces

- Web User Portal – This interface is the first point of contact between Scientist and the Beamline Operating System. It enables the user to prepare and submit experimental proposals, setup experiments, prepare samples, view experimental results, modify experimental parameters, make experimental requests, download results, and submit usage reports. There shall be no direct instrument control through this interface. This interface shall be accessible in a secure manner from anywhere in the world through the world-wide web, and require no extra software than a standards compliant web-browser. It shall be intuitive, experiment focused.   The web portal shall integrate with user office and accounting systems for user time tracking, safety review, user time billing and run-permit generation.
- Interactive Data Acquisition Interface – This is the interface through which Scientists and operators will operate the beamline in the interactive and assisted-interactive modes of data acquisition. There shall be as little direct interaction between this interface and beamline instruments as possible. As much as possible, any instrument control shall be achieved indirectly through instrument control subsystems. The interface shall emphasize the experiment rather instrument control to reduce the learning curve and enable scientists to focus on their experiment. Only decisions impacting the experiments shall be deferred to the Scientist/Operator. All functionality provided by this interface, shall be within a single integrated application.
- Beamline Administration Web Portal – This is the interface through which Beamline Staff schedule tasks and beam time, manage shifts, review shifts, inspect logs, prepare shift reports and communicate with Scientists. This interface shall be securely accessible via the www.
- Beamline Control Panel – This interface enables direct access to each subsystem of the beamline, for setup, diagnostics and monitoring. It shall be a beamline focused interface rather than an experiment focused interface. Access to the Beamline Control Panel for monitoring purposes shall not adversely affect the performance of functionality of any on-going data acquisition activities under normal circumstances.
- Subsystem User Interfaces – Each subsystem shall provide a user interface for testing, and maintenance independent of all other subsystems within the CMCF Control system.

2.2.4 Site Adaptation Requirements

The CMCF will have more than one beamline running essentially the same software. However, the details of specific hardware at each beamline will vary. Even within a single beamline, the specific hardware components may vary in type over a length of time. Therefore the system shall be designed to be easily deployed on a beamline with different underlying hardware in each hardware category identified under Hardware interface above. In such a case, only directly affected subsystems shall be required to be reconfigured.

2.3 PRODUCT FUNCTIONS

The CMCF BOS Software shall provide the following functions. These functions are organized in functional groups for the sake of clarity.

1. Web portal functions

(a) Assist users to prepare and code samples for shipment to the facility

(b) Collect and convey experimental plans from scientists to the facility

(c) Collect and convey experimental reports from scientists to the facility

(d) Present experimental results and assist users in analyzing the results

(e) Enable data retrieval by users.

2. Data Management functions

(f) Store and keep track of all samples related information.

(g) Keep an electronic log of all beamline commands, events and operator notes

(h) Store, preserve, secure and dispose of scientific data and sample parameters as required.

(i) Keep track of beamline and beam time usage.

3. Beamline Control functions

(j) Enable interactive and automated control of all beamline hardware.

(k) Enable scheduling of a series of data acquisition tasks to be carried out at a later time.

(l) Carry out Automatic and interactive initialization, calibration, alignment and optimization of beamline hardware and other parameters.

(m) Carry out Automatic and interactive data acquisition.

(n) Facilitate the automation of sequences of tasks through an easy to use scripting interface

4. Data Analysis functions

(o) Harness the services of external software to perform interactive and automated data validation and analysis.

5. Other functions

(p) Protect the functionality and safety of the beamline instruments during use

(q) Alert users on experiment status, failures and errors.

(r) Control user access and authentication for the BOS

2.4 USER CLASSES AND CHARACTERISTICS

The users of the CMCF BOS Software are classified into the following classes.

(a) *Scientist*. Any person using the CMCF BOS for the acquisition of science data. In a very real sense, the scientist is the customer for the services provided by the beamline. Whatever their level of experience, scientists will wish to concentrate on the efficient acquisition of crystallographic data and on-line assessment of the data quality rather than on the details of controlling beamline instruments.

(b) *Operator*. This is the on-site person responsible for controlling the beamline instruments for acquisition of science data. In most but not all cases, the 'Scientist' and the 'Operator' will be the same individual.

(c) *Beamline Staff*. On-site person responsible for monitoring and fine-tuning the beamline instruments. This person is responsible for ensuring the integrity of the system and for keeping the system functioning accurately during measurements. The beamline Staff works with the 'Scientist' to ensure that the 'Scientist' obtains as good data as is possible.

(d) *Support Personnel*. On-site (or near-site) support personnel are responsible for the real-time maintenance of the system hardware and software. They are the first point of contact during failures and ensure that smooth operation resumes as soon as possible after a failure.

(e) *Developer*. Developers are responsible for the designing, testing, installation, configuring, and upgrading of subsystems.

(f) *Administrative Personnel* – This includes User Office personnel responsible for the evaluation of proposals, beam-time allocation, user-permit generation and creation of user accounts, Health and safety personnel.Stores (Shipping/Receiving) personnel, and Finance/Accounting personnel who may need access to the system for other administrative functions

2.5 CONSTRAINTS

The CMCF BOS Software shall be designed under the following constraints.

(a) The deployment of all CMCF BOS Software across beamlines shall be free from proprietary restrictions. As such, open-source and off-the-shelf public domain software and standards shall be used whenever feasible.

(b) All CMCF Software is to be fully documented, internally and externally.

(c) All CMCF Software must be version labeled both in source and binary form. The version information shall be retrievable from the existing software at run time via control commands.

(d) The syntax of control flow commands shall be consistent across the system.

(e) User interfaces shall be focused on the tasks being carried out, and be intuitive such that the target audience can learn to use it within 1 hour of training.

(f) The use of controls in Stand-alone user interfaces shall conform to the GNOME Human Interface Guide, version 2.0 or later [9] and CLS Human Factors Engineering Standards [14].

(g) Browser based user interfaces shall conform to the guidelines outlined by Wroblewski and Rantanen [10, 11].

(h) All user data shall be treated as confidential, and access restricted.

(i) Access to all user interfaces shall be through controlled user accounts during normal operation.

2.6 ASSUMPTIONS

(a) It is assumed that proposal submission and review is a separate process

(b) It is assumed that once the experimental proposal is approved, the user-office staff or other delegated person will set up an account in the CMCF BOS.

(c) It is assumed that a shipment is defined as a single Dewar. Multiple Dewars shall be considered as multiple shipments even if they are shipped together.

2.7 APPORTIONING OF REQUIREMENTS

Since the CMCF BOS is a large and complex system, it is envisioned that the following order will be followed for deploying the system. It should be noted however that a functional system requires deployment of all components and the following suggestions are based on likely functional dependencies between subsystems

(a) The hardware abstraction layer consisting of all hardware control subsystems should be deployed first together with their associated test and configuration screens

(b) Interactive data acquisition functionality should be deployed next

(c) Followed by automatic data acquisition and the web-based user interfaces

(d) Finally automatic data processing should be integrated.

3.0 SPECIFIC REQUIREMENTS

3.1 SYSTEM FUNCTIONS

3.1.1 Sample Information Management

3.1.1.1 *Purpose*

The purpose of this function is to capture as accurately and completely as possible detailed information about each sample that enters the system, and how the sample is to be treated within the system.

3.1.1.2 *Inputs*

The input for sample information management consists of the following data to be provided by the user. When users do not provide optional parameters, sensible defaults shall be substituted based on values to be determined:

- Sample ID – A unique identifier for each sample
- Sample name (a string)
- Puck ID – A pointer to the puck containing the sample
- Location within Puck – (a string)
- Pin length – The length of the pin in mm (floating point number >15 and < 22)

- Loop size – Size of the loop in mm (floating point number >0 and < 2)
- Spacegroup (a string)
- Cell parameters (vector of 6 floating point numbers)
- Diffraction Plan – Information about how the sample should be handled, which includes
    - Type of experiments (MAD, SAD or single wavelength)
    - Ideal required resolution (floating point number >0 and <20)
    - Optional: Minimum acceptable resolution (floating point number >0 and <20)
    - Optional: Exposure time (floating point number > 0)
    - Optional: Oscillation range (floating point number)
- Shipment ID (a unique identifier of the dewar, initially empty until shipments are completed)
- Comments (text)

3.1.1.3 *Processing*

a) The system shall store the sample information in an appropriate persistent database when the user submits it.

b) The system shall retrieve the stored information for each sample as requested.

c) The system shall allow users to edit and resubmit the previously stored information

d) The system shall delete sample information on request, provided the sample has not been shipped, in which case only editing shall be permitted.

3.1.1.4 *User Interface Requirements*

a) Sample information shall be entered through a web-based HTML form.

b) A list of all samples entered shall be available to the user on request, and permit access to the associated sample information through a single click of the mouse.

c) All actions that will potentially lead to loss of information shall require confirmation from the user

d) Information entry shall be validated on input according to the specified input requirements.

3.1.2 Sample Shipment Preparation

3.1.2.1 *Purpose*

The goal of this function is to keep track of which samples are included in a particular shipment sent to the facility, when they are sent, and how they are sent. These requirements are not intented to supersede facility wide requirements for shipping and handling samples. Rather, they are meant to emphasize aspects of specific importance to macromolecular crystallography.

3.1.2.2 *Inputs, Outputs and Processing Requirements*

a) The input to the sample shipment functionality shall include at least the following information. More detailed requirements such as additional fields and field types will be specified as part of the design process.

- List of sample IDs.
- Dewar type
- Carrier information
- Shipment date
- Estimated Time of Arrival

b) On receiving the input, the system shall generate a unique shipment identifier, update the sample information for each of the samples to include the shipment identifier, and create a waybill which the users will include in the shipment. This waybill should not be confused with the waybill generated by carriers.

c) The system shall create a shipment record in a persistent database with fields corresponding to the contents of the waybill.

d) The system shall generate a bar-code on the waybill corresponding to the generated shipment identifier.

e) The user shall be presented with the final waybill in Portable Document Format.

f) The system shall send an electronic copy of the waybill in Portable Document Format to a designated e-mail address at the facility.

g) The system shall present the user with further instructions on how to print the waybill and complete the shipment.

3.1.2.3 *User Interface Requirements*

a) Sample information shall be entered through a web-based HTML form.

b) A list of all samples stored shall be presented to the user to permit inclusion of samples by simply selecting a checkbox next to the sample to be included.

c) A summary sheet of the waybill shall be presented to the user for confirmation and permit the user to edit the waybill prior to submission.

3.1.3 Experimental Plan Management

3.1.3.1 *Purpose*

The Purpose of this functionality is to capture as accurately as possible, what exactly the Scientist intends to be done with the samples. As such experimental plans can involve one or more samples, and each shipment can be associated with multiple experimental plans.

3.1.3.2 *Inputs*

The information contained within an experimental plan shall be provided by the user including at least the following information:

- Experimental plan ID
- List of sample IDs

- Type of experiment - one of
    - Screen all collect on best one
    - Screen all collect on all good ones
    - Collect on all without screening

3.1.3.3 *Other Requirements*

(a) On receiving experimental information input from the user, the system shall store the information in a persistent database.

(b) The system shall present a list of experimental plan associated with the currently active experimental program to the user on request.

(c) The system shall retrieve information associated with an experimental plan on request and permit editing and resubmission.

(d) The system shall allow experimental plans to be deleted or edited provided they have not already been performed by the system.

(e) The system shall allow the user to create a new experimental plan, using a previously defined experimental plan as template.

3.1.4 Dewar Reception and Storage Management

3.1.4.1 *Purpose*

The purpose of this functionality is to record when a shipment arrives at the facility, and where it is stored within the facility, and when it is sent back to the users. The goal is to keep track at all times which samples are available at the beamline, and where they are located at the beamline.

3.1.4.2 *Inputs, Outputs and Processing*

a) On receiving a shipment, a beamline staff shall provide as input, the shipment identifier from the waybill.

b) On receiving the input, the system shall create a Dewar record in a persistent database. The Dewar record shall contain the same information as a shipment record, in addition to the following fields
    - Dewar ID
    - Storage Location
    - Status
    - Time of last Status
    - Comments

c) The system shall update the sample records within the persistent database, to reflect the Dewar ID.

d) Before sending back a Dewar, beamline staff will provide as input the shipment identifier from the waybill.

e) On receiving the request, the system shall update the status field of the Dewar record in the persistent database.

f) A History shall be maintained of Dewar records.

3.1.4.3 *User interfaces*

a) Shipment and Dewar storage information entry by the beamline staff shall be through an HTML web form and will be assisted by a bar-code reader device.

3.1.5 Beamline Control Functions

3.1.5.1 *Motor Control*

a) Motor positions shall be maintained in at least two coordinate systems. Where a motor driven system is fitted with encoders, a third *Encoder coordinate* system shall be required
b) The *Dial* coordinate system shall be set to correspond to the physical dial settings of the instrument where applicable and have the same engineering units as the *User* coordinate system.
c) The User coordinate system shall be related to the *Dial* coordinates by a simple linear relation, determined by a calibration procedure for each motor. Dial, User and Encoder coordinates shall be related by the following equations.

   - *User = Sign x Dial + user-offset*
   - *Dial = motor-steps / motor-resolution*
   - *Encoder = (encoder-pulses / encoder-resolution) + encoder-offset*

   Where *motor-steps* is the motor step count reported by the motor controller and *encoder-steps* is the encoder step count reported by the encoder hardware.
d) Motor settings shall include at minimum the following:
   - *acceleration*
   - *steady-state speed*
   - *backlash distance*
   - *dial high-limit* and *low-limit*: Also known as soft-limits These shall enable motion to be restricted within certain ranges of the dial coordinate system.
   - *Sign* : shall be positive (+1) if *User* coordinates change in the same direction as *Dial* coordinates and negative (-1) otherwise
   - *Motor-resolution*: the number of steps or pulses per unit of the dial/user coordinates.
   - *Encoder-resolution:* The number of encoder pulses per unit of the dial/user coordinates. For encoded motions only.
   - *User-offset*: This is the offset required to bring the user coordinate system in register with the dial coordinate system.
   - *Encoder-offset*: This is the offset required to bring the encoder coordinate system into register with the dial coordinate system. The encoder coordinate system shall always be in register with the user coordinate system.
   - *Encoder-sign*: shall be positive (+1) if *Encoder* coordinates change in the same direction as *Dial* coordinates and negative (-1) otherwise.
   - *Engineering units*: the units for dial and user coordinates. The Engineering units shall be the same for dial and User coordinates.

e) Each motor shall have a calibration sequence which fixes the dial coordinates within the absolute frame of reference of the range of motion of the motor.

f) Motor positions and settings shall be persistent across software and hardware restarts.

g) The system shall verify on restart if stored motor positions are valid, and restore them from a persistent storage without moving any motors. In the event that motor positions are not reliable, only a calibration of the dial coordinate shall be required.

h) The system shall support *pseudo-motors* otherwise known as compound motors. These are positioning systems requiring combinations of more than one physical motor.

i) Pseudo motor functionality shall be a sub-set of normal motor functionality with at minimum the following parameters
   - *dial high-limit* and *low-limit*: These shall enable motion to be restricted within certain ranges of the dial coordinate system.
   - *Sign* : shall be positive (+1) if *User* coordinates change in the same direction as *Dial* coordinates and negative (-1) otherwise
   - *Motor-resolution*: The motor steps and/or resolution shall be calculated values based on the real motors and a predefined equation to be determined by the specific application.
   - *Encoder-resolution:* The number of encoder pulses per unit of the dial/user coordinates. For encoded motions only.
   - *User-offset*: This is the offset required to bring the user coordinate system in register with the dial coordinate system.
   - *Encoder-offset*: This is the offset required to bring the encoder coordinate system into register with the dial coordinate system. The encoder coordinate system shall always be in register with the user coordinate system with no offset required.
   - *Encoder-sign*: shall be positive (+1) if *Encoder* coordinates change in the same direction as *Dial* coordinates and negative (-1) otherwise.
   - *Engineering units*: the units for dial and user coordinates. The Engineering units shall be the same for dial and User coordinates.

j) The individual motors forming part of a pseudo motor shall be independently supported.

k) Motor parameters shall be determined and stored to a precision higher than 10% of the tolerance of the application in question. For example a motor driving a distance where error-tolerances of 0.1% of an engineering unit or less are required, will require all motor parameters affecting position calculations (such as offsets, resolutions, positions) to be determined to at least 4 significant digits (not decimal places).

l) The motor/pseudo-motor control interface shall support a least two types of motion request commands for each motor or pseudo-motor

   - Absolute motion shall have the User coordinate system as the fixed reference
   - Relative motion shall have the current motor position as reference.

m) Each motor shall provide status information on whether the motor is stationary, in motion, calibrated, or needs calibration, at a soft-limit, at a hard-limit.

n) Each motor/Pseudo-motor shall respond to a STOP command at all times. On receiving a STOP command, the motor shall immediately decelerate to a full stop.

o) Motors shall be indistinguishable from pseudo motors, to applications requiring only the common standard interfaces for

   - Reading the current position
   - Setting the target position and initiating a move
   - Stopping a move

- Checking the status of a motor/pseudo motor (moving, starting or stopping, stopped, at soft limit, at hard limit)
- Enabling and setting the values of soft limits.

3.1.5.2 *Beam Position Monitors*

Beam position monitors (BPMs) provide horizontal and/or vertical positional diagnostic information at various points along the beamline. In some cases, Beam Position Monitors double as intensity monitors or ionization detectors, in which case the requested functionality in those modes will be guided by specifications under "Intensity Monitors" below. Beam Position monitoring functionality for each BPM shall be governed by the following specifications:

a) The system shall provide horizontal and vertical displacement value pair for each BPM. For BPMs which only measure position in one dimension, the value of the displacement in the other dimension shall be zero.

b) The Engineering units for beam positions shall be millimetres.

c) The processing for converting hardware signals to positional values shall be governed by the hardware manuals on a case by case basis.

d) Positional information shall not be lost between updates. For example if the system updates positional information at a frequency of 2 Hz, each data point must be determined by using all the information available to the system within the 0.5 second gap between updates.

e) The actual frequency of update for each BPM is dependent on the specific hardware and can not be specified in detail here. It shall therefore be governed by the hardware manuals on a case by case basis. However, the update frequency shall be configurable for each BPM.

3.1.5.3 *Intensity Monitors*

Support for Intensity Monitors shall be governed by the following specifications:

a) The system shall provide a single intensity value for each intensity monitor.

b) At least two interfaces shall be available for each intensity monitor. In the "continuous update" mode, no input is required and the system updates the intensity value at a specified frequency (default 1 Hz).

c) In the "timed update" mode, the system shall accept a time value in seconds as input and return the integrated intensity value for the specified duration starting at the moment of request.

d) Both modes shall be able to be used simultaneously without adversely affecting the results.

e) The engineering units for intensity values shall be photons/second or counts/second.

3.1.5.4 *Multi-Channel Analyzers*

A multi-Channel analyzer (MCA) simultaneously measures intensity data in thousands of individual channels. Support for multi-channel analyzers shall be governed by the following specifications:

a) Each channel within an MCA shall be treated as an “Intensity monitor” and governed by the specifications above, with the exception that the “continuous update” mode shall not be provided.

b) The system shall permit a group of contiguous channels also known as a Region of Interest (ROI) to be accessed in the same manner as a single channel. In this case, the returned intensity value shall be a sum of the individual values in the ROI.

c) The system shall provide commands for setting up the MCA parameters such as temperature, mode, detector range, ROI in preparation for data acquisition.

d) The system shall provide at least two modes or data acquisition. In the first mode, intensity data shall be a single value, acquired in the same manner as specified for “timed update” intensity monitoring above. In the second mode, the full array of values for all channels or ROI shall be returned rather than a single value.

3.1.5.5 *Beam Viewers and Video Cameras*

a) A video feed shall be provided for each beam viewer and video Camera.

b) The video feed shall be accessible remotely via the Internet.

c) All video feeds shall support multiple simultaneous clients limited only by bandwidth. However local clients shall have bandwidth priority where bandwidth is limited.

d) The system must allow for close to real-time flow of video information. This may be assisted by data-loss compression techniques.

e) In some cases such as for beam viewers, data loss is not desirable. As such data loss-less compression techniques will be preferred. This choice can only be made on a case by case basis therefore, the system should be designed such that the mode of transmission of each video stream is configurable.

3.1.5.6 *CCD Detectors*

These detectors enable the acquisition of crystallographic diffraction data. The Beamline Operating System shall provide the following commands for controlling the detector

a) ‘acquire background’ – take a zero beam image for use in background correction

b) ‘Start’ – start taking an image

c) ‘Set parameters’ – set image file names and image header parameters

d) ‘Stop and Save’ – stop acquiring, readout the image, correct it and write it out

e) ‘Stop and read section’ – collect one section of a multi-sectioned image. When this command has been used to collect multiple sections, the final ‘stop and save’ command must combine all sections in a dezingering correction operation prior to saving.

f) `Abort’ – Stop all operations immediately, and reset to initial state.

g) ‘Setup’ – this command configures the detector system prior to acquisition permitting CCD binning to be configured where available.

h) `Status’ – returns the current detector configuration (binning) and status (idle, acquiring, reading, correcting, writing or error)

3.1.5.7 *Robotic Sample Auto-mounters*

The robotic automounter picks up samples from a sample holding Dewar and positions them on the goniometer head in preparation for sample acquisition. The following commands shall be provided by the system for controlling robotic sample mounters. This list is aimed to represent the minimum of users' expectated functionality.

a) 'mount' – this command takes as input the sample coordinate within the Dewar. On receiving this command the robot shall mount the sample on the goniometer, provided there is no sample already mounted. If a sample is already mounted, a mount command shall 'unmount' the currently mounted sample prior to mounting the new sample.

b) The coordinate shall include all information required to identify the sample position within the dewar The sample coordinate shall be either an absolute address such as 'LA90' or a relative address such as 'next', 'previous', 'first' or 'last'.

c) Only valid coordinates shall be mountable. A valid coordinate is one that is occupied and has been determined to be problem-free through a 'probe' operation. Relative coordinates shall also take into consideration the validity and occupancy of addresses, such that only valid addresses are visited.

d) 'probe' – This command takes as parameter a cassette location, and determines if the address is occupied, and can be accessed normally. A probe operation is required everytime a new cassette has been placed inside the dewar.

e) 'unmount' – on receiving the command, the robot shall un-mount the sample from the goniometer and transfer it back to it's location within the Dewar.

f) Additional commands shall be provided for maintenance purposes such as 'configure', 'calibrate', 'probe', 'reset', etc, shall also be implemented according to the automounter operating manual.

3.1.5.8 *Beamline Scripting Environment*

The goal of the beamline scripting environment is to allow for implementing procedures spanning all of the hardware resources supported by the hardware control layer at a beamline. The scripting environment will enable the implementation of sophisticated beamline automation features in an easy to use scripting language. The requirements for the scripting environment shall be as follows:

a) The syntax of the scripting language shall be easy to learn and should be based on, an existing open-source scripting environment.

b) It shall support the control structures for decision-making, comparisons, loops, definition of procedures and procedure calls with parameter passing.

c) The environment must provide access to all hardware resources supported by the underlying beamline hardware control layer

d) The scripting environment must provide a similar level of functionality and simplicity as illustrated in the following pseudo code example:

```
# comment: scan the DCM pitch and move to the peak. If peak is not found
# run the predefined 'optimize_slits' procedure.

detector = beamline.bpm['dcm_bpm']
positioner = beamline.motor['c2_pitch']
old_position = positioner.get_position()
myscan = scan(positioner, from=1.50, to=1.53, steps=50, detector, count_time=1)

midp, fwhm, success = myscan.gausian_fit()
if success:
        actuator.move_to(midp)
else:
        positioner.move_to(old_position)
        beamline.scripts.optimize_slits()
```

3.1.6 Interactive Data Acquisition Functions

3.1.6.1 *Experimental Setup*

The purpose of this functionality is to allow the users to adjust various parameters, mount and align their samples in preparation for data collection.

(a) The system shall allow the user to visualize current positions and set new positions for the following beamline parameters and motors

- Photon Energy
- Percentage transmission or attenuation
- Beam size at sample (width and height)
- Goniometer angle position
- Beam-stop distance
- Detector distance
- Detector 2-Theta angle

(b) For each controllable parameter, only values within the limits configured for the underlying hardware control layer shall be considered valid, and no motion shall be able to be initiated from this interface unless the underlying hardware is calibrated.

(c) To prevent confusion over parameter names, parameters shall be presented to users in clear terminology relevant to the experiment and familiar to scientists in the field of interest. For example, low level parameter names such as 'GV6K1608-001:deg' shall never be presented to users. Rather, names such as 'omega' shall be used instead. Additionally, a schematic layout of the beamline with the parameters clearly labelled shall be presented to users.

(d) The system shall enable users to see the effects of requested motion by presenting video streams of the area immediately around the sample, an overview of the hutch such that detector motion is visible and an overview of the sample automounter. Additionally, a video stream of the instrument panel shall also be provided. Special care should be taken to comply with Canadian privacy laws as concerns the transmission of imagines of people without written consent.

(e) The system shall present to the user the predicted resolution distribution on the surface of the detector based on the current selected parameters. This 'Resolution Predictor' information must be updated as soon as parameters are changed.

(f) The system shall allow users to open/close the front-end and end-station photon shutters.

(g) The system must allow some previously defined scripted commands to be presented to users for execution.

(h) A command to prepare the sample environment for mounting a sample shall be provided. Specifically, when the system receives a command to prepare for mounting, it shall move the detector beam-stop and other equipment around the sample position to a safe distance. The specific distances will be determined on a case by case basis and may be different for different beamlines. Therefore it must be configurable, post-deployment.

3.1.6.2 *Sample Mounting and Alignment*

The purpose of this functionality is to enable users to visually position the sample at the beam position.

(a) A live video stream of the sample shall be presented to the user.

(b) The system shall overlay on the live video stream, clear markings for the beam position and size at all times.

(c) Users shall be presented with commands to increase, decrease the zoom-level or return to a default zoom level

(d) Similarly, the system shall provide commands to rotate the sample in steps of +/-90 degrees and +/180 degrees

(e) Commands shall be provided for fine-adjusting the sample position vertically and horizontally.

(f) Additionally, a home command shall be available which positions the sample holder to a predefined position. The target position of this command will vary from one beamline to another and should therefore be configurable.

(g) At least three types of sample positioning commands shall be supported: 'click centring', 'loop centring' and 'crystal centring'. 'Loop' and 'Crystal' centring commands will require rotating the sample, capturing images at various angles and processing the images to locate the loop or crystal. All three commands will require accurate calibration of the video microscope at all accessible zoom levels.

- 'Click centring': In this mode, when a user clicks on a position on the sample video display, the system shall move the sample such that, the selected position coincides with beam centre marked on the display.
- 'Loop centring': On receiving a 'loop centring' command the system moves the sample such that the centre of the loop holding the sample coincides with the beam centre marked on the display.
- 'Crystal centring': On receiving a 'crystal centring' command the system moves the sample such that the centre of the sample crystal coincides with the beam centre.

(h) The system shall provide controls for remotely adjusting the lighting around the sample and the contrast of the video stream displayed.

(i) A schematic view of the available sample coordinates within the sample holding Dewar of the automounter shall be presented to the user. Each address with this view must be clearly marked to reflect its state – whether 'occupied', 'empty' or 'unusable'.

(j) The system shall provide commands for mounting a sample from the automounter by simply entering the sample address within the holding Dewar.

(k) Commands shall also be provided for un-mounting a sample from the Goniometer into the sample holding Dewar. In this case, samples shall be un-mounted to the same address from which they were mounted.

3.1.6.3 *Data Collection*

The purpose of this functionality is to enable users to input data collection parameters, collect test images, and initiate collection of complete SAD, MAD or conventional diffraction images.

(a) The system shall allow users to input the following parameters for collecting diffraction data

- Data Prefix: A text string without any spaces, for identifying the data set.
- Directory: The location where diffraction images will be stored.
- Detector Distance in millimetres
- Goniometer Delta: the rotation range in degrees for a single frame of data
- Exposure Time: The duration of a single exposure in seconds
- Start Frame number: the index number for the first frame in the set
- Start Angle: The starting position of the Goniometer in degrees
- End Frame number: the index number for the last frame in the set
- End Angle: The final position of the goniometer in degrees
- Wedge angle: This is the slice of data collection in degrees to be collected non-stop in the case of multiple energy data collection. The maximum wedge shall be 180 degrees.
- Inverse beam mode: One of two options ‘On’ or ‘Off’
- Energy: This is the energy at which data should be collected. The system shall support up to 5 energies. Each energy entry shall be associated with a label.

(b) The system must perform input validation of entered parameters. The delta, start angle, end angle, start frame and end frame values shall be consistent with each other. Therefore, on changing one of these values, the system shall immediately update the others to maintain consistency, with the least loss of information.

(c) Methods shall be provided to enable users to recover overwritten parameters by undoing changes.

(d) The sequence of images to be collected shall be presented to the users and updated on request.

(e) The system shall provide commands for initiating a data collection based on the selected parameters. On receiving a start command, the system shall verify that previously collected data will not be overwritten and take appropriate actions to prevent data loss.

(f) As data collection proceeds, the list shall be updated to reflect completion status.

(g) At least two methods of interrupting an on-going data collection shall be provided. A ‘Pause’ command shall suspend data collection and permit data collection to resume as required. The system shall permit users to change the resume position within the sequence while data collection is paused. Additionally, an ‘abort’ command shall stop data collection and reset the system to the same state as before data collection was initiated.

(h) A special ‘snapshot’ mode (or ‘Run 0 mode’) of operation shall be the default mode of operation. In this mode, only single frame data collection shall be supported.

Therefore users will not be allowed to change ‘End Frame’, ‘End Angle’, ‘Wedge’, ‘Inverse mode’ and ‘Energy’ parameters. Instead, users shall be presented with ‘Resolution predictor’ functionality in this mode.

(i) The system shall allow for multiple runs of data collection to be defined, each with its own set of parameters prior to initiating data collection, after which the system shall collect the full sequence of images defined in all runs without intervention.

3.1.6.4 *Fluorescence Scans and MAD Parameter Selection*

The purpose of this functionality is to enable users to perform an absorption-edge energy scan on their samples, and determine the optimal wavelengths for MAD or SAD anomalous dispersion experiments. Additionally, an excitation scan allows users to identify or verify the existence of anomalous scatters in the sample.

(a) The system shall allow users to choose the type of scan to be performed, either ‘MAD’ or ‘Excitation’.

(b) The inputs for scans shall include the following parameters:

- Prefix: identifier for naming data files, also used as Prefix for automatically generated runs created as a result of a MAD scan.
- Directory: Data directory
- Edge: The absorption edge around which to scan
- Energy: The energy corresponding to the absorption edge
- Exposure time: This is the counting time for each position during the energy scan.

(c) On receiving input in the MAD mode, the system shall open the shutter and scan the 100 eV region centred on the selected edge, at a step size of at most 1eV. For each point in the scan, the system shall count the multi-channel analyzer for the specified duration.

(d) For each point in the MAD mode, the system shall return the sum of counts within the region of interest defined by the emission energy of the selected absorption edge, normalized to the beam intensity.

(e) At the end of the scan in the MAD mode, the output of the scan shall be used as input to the external CHOOCH software package, and the CHOOCH output processed to extract the energy, f’ and f’’ values for the ‘peak’ and ‘inflection point’. A third energy or ‘remote’ shall be selected in the region above the ‘peak’ where the change in f’’ values is smallest (usually ~200 eV above the inflection point)

(f) All output files shall be saved in the data directory specified during input.

(g) The resulting peak and inflection point and remote parameters shall be used to automatically set up a new data collection Run, with three energies equal to the values selected from the CHOOCH output, and the energies appropriately labelled ‘peak’, ‘infl’, and ‘remo’. The default prefix, and directories shall be the same as those chosen for the scan.

(h) On receiving input in the Excitation mode, the system shall open the shutter, move the energy to the excitation energy (usually ~500 eV above the input edge-energy) and collect a full spectrum from the Multi-channel analyzer for the duration specified.

(i) When the excitation scan is complete, the system shall perform a one-dimensional peak search on the spectrum and output a list of peaks, with each peak consisting of two values, the ‘peak position’ in eV, and the ‘peak height’ or amplitude in counts.

(j) For each peak identified, the system shall also search a database of emission lines and return a list of identified emission lines ordered according to confidence level or likelihood.

3.1.6.5 *Quick-look Data Analysis*

The purpose of this functionality is to allow users to verify the quality of data being collected as it is being collected. The system shall be able to perform the following analysis on request:

(a) Diffraction image analysis using DISTL [4].

(b) Intensity distribution analysis, in which the BOS shall calculate intensity distribution histogram, the mean pixel intensity, and the 5^{th} and 95^{th} percentiles.

(c) The maximum pixel intensity and the corresponding number of pixels

(d) Number of saturated pixels

3.1.6.6 *Sample Screening/Characterization*

The purpose of this functionality is to allow users to characterize a sample in order to determine suitability for successful data collection, initial parameters for data collection and also to be able to compare similar samples in order to obtain the best sample for data collection. The system shall be able to perform the following analysis on request

(a) Collect a predetermined number of frames of data

(b) Auto-Index and integrate the data using XDS and or MOSFLM

(c) Determine the space group

(d) Calculate the recommended data collection strategy for the sample

(e) Diffraction image analysis using DISTL [4].

(f) Calculate an absolute score based on the results of the analysis.

3.1.6.7 *User Interface Requirements*

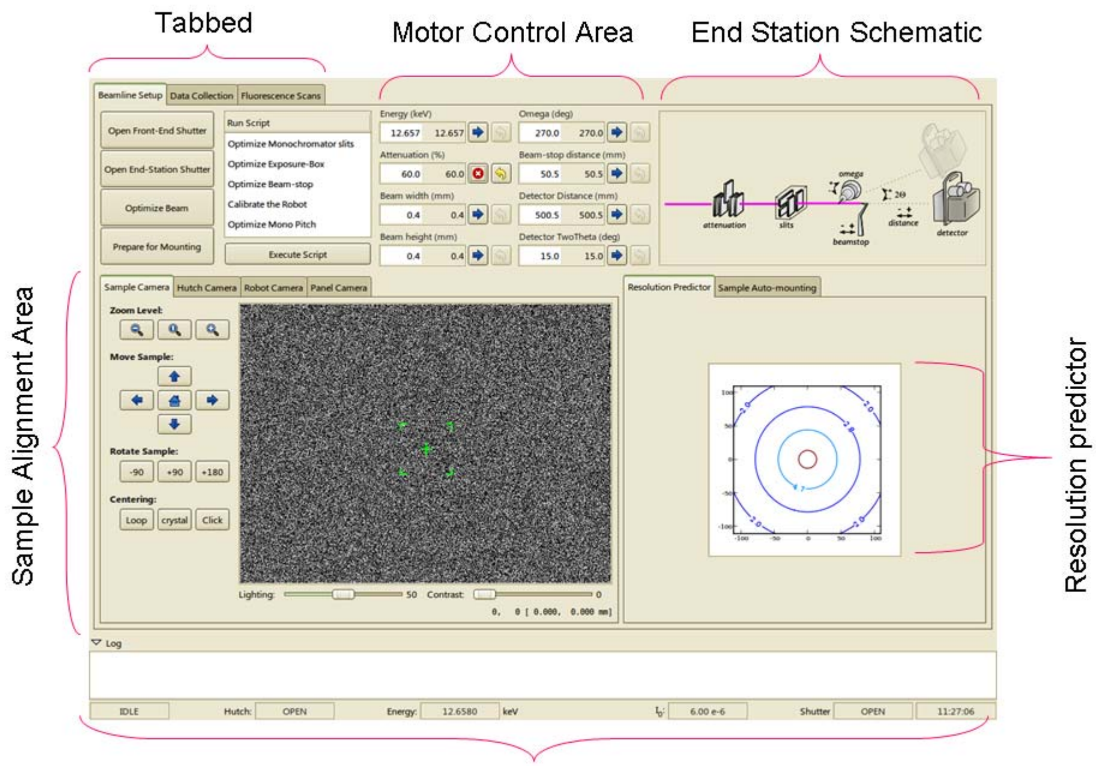
The following user interface layouts and requirements illustrate the level of simplicity and functionality required.

(a) All interactive data collection functionality shall be present within a single tabbed application window.

(b) Status information such as shutter states, intensity readings and motor positions shall be clearly visible.

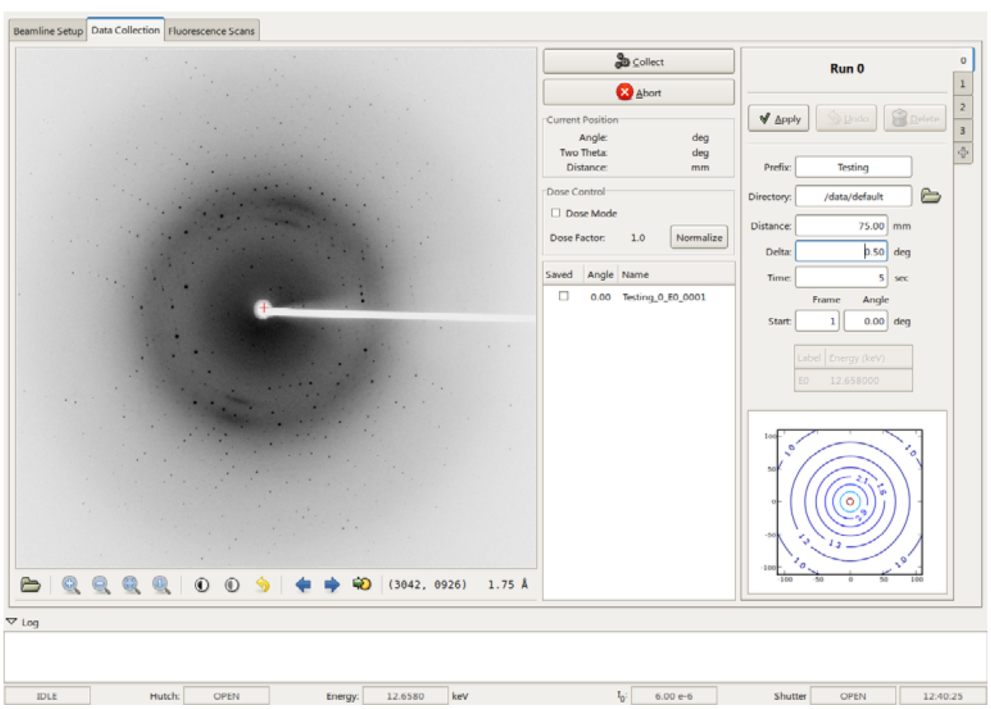
(c) The layout of the screens for interactive data collection should be similar to the following illustrations:

1. The Beamline Setup Screens

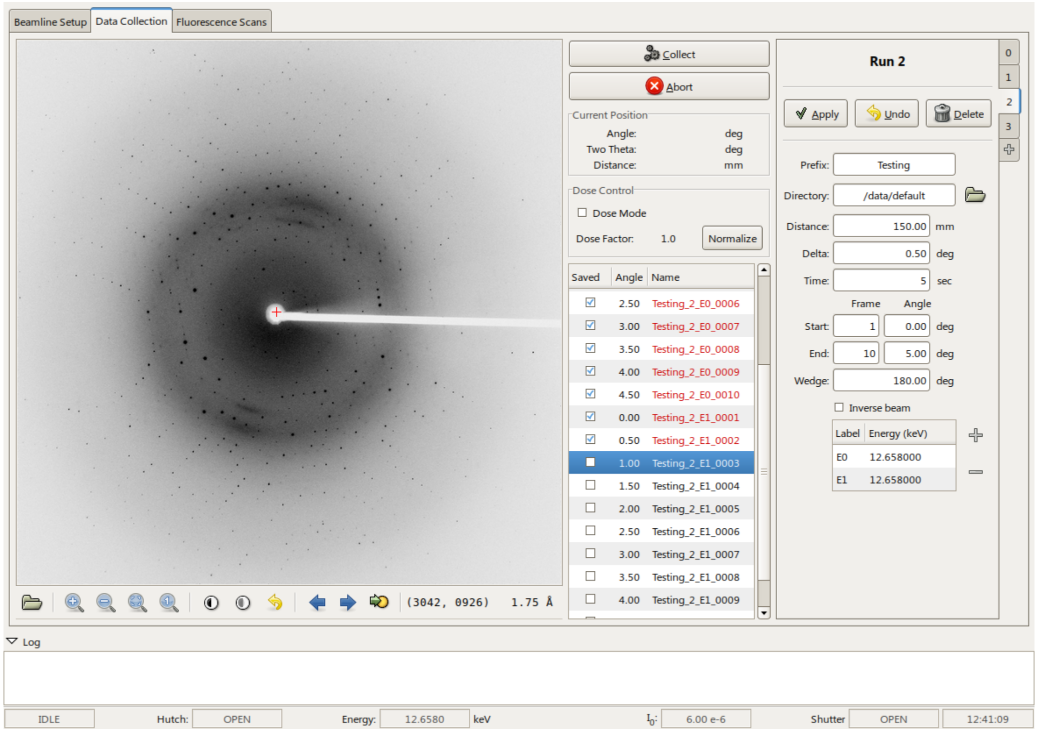


Log and Status area

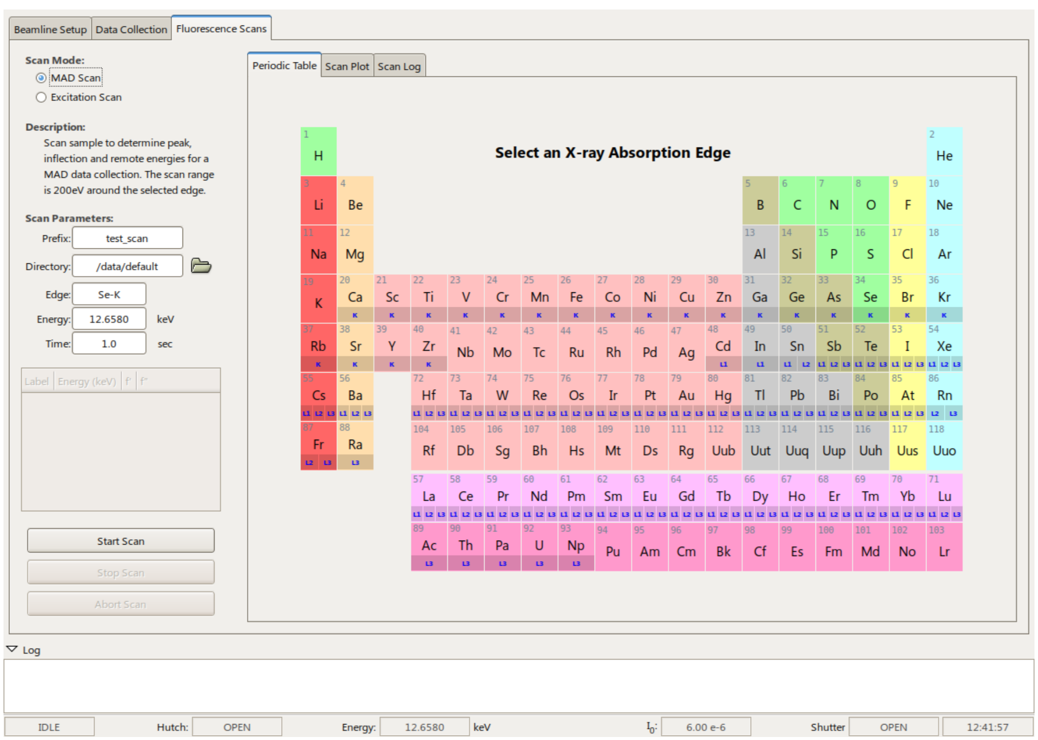
2. The Data collection screens



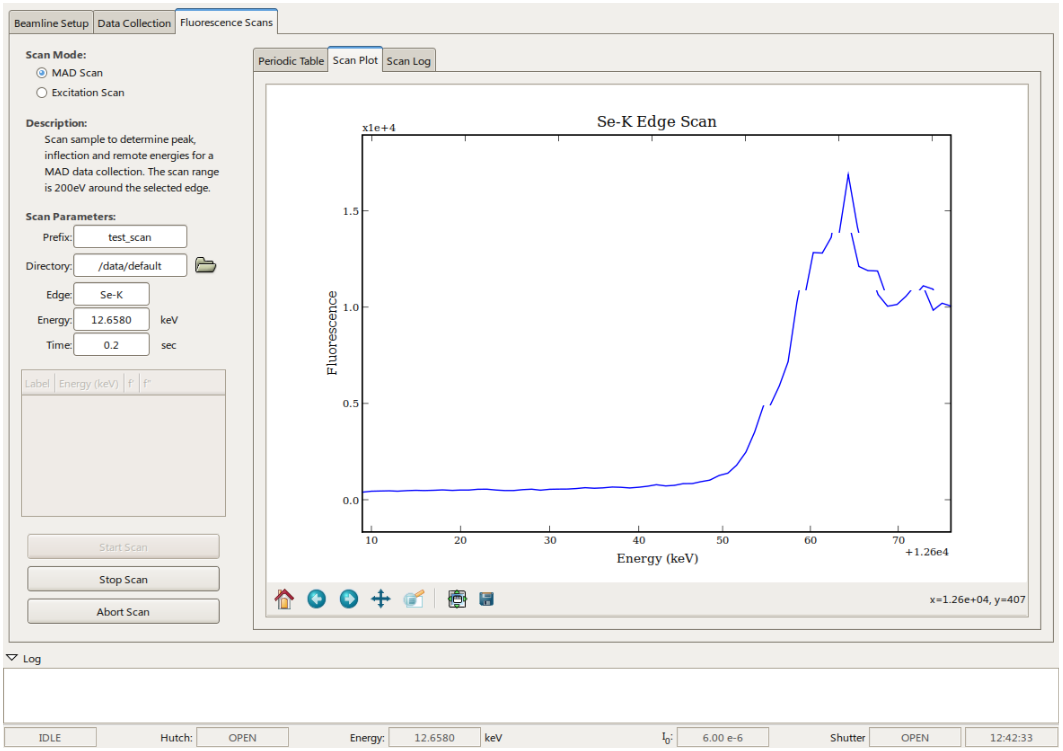
Run 0, ‘snapshot’ mode



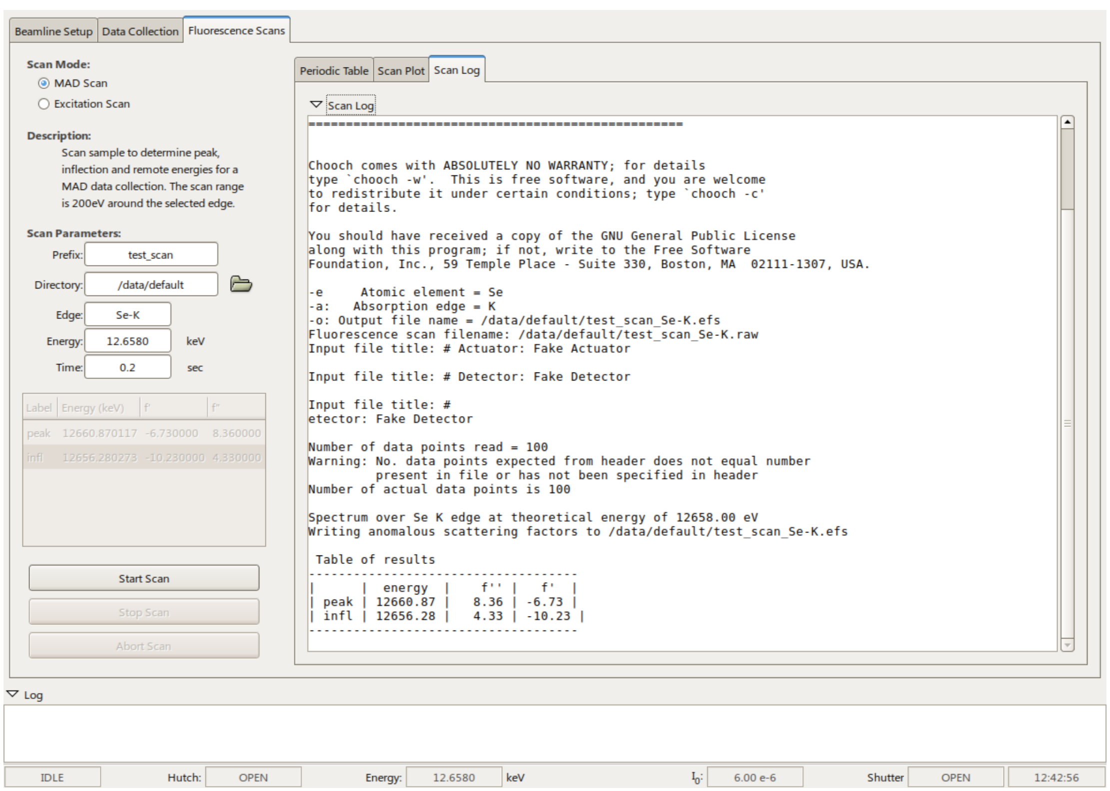
3. Fluorescence and MAD scan screens



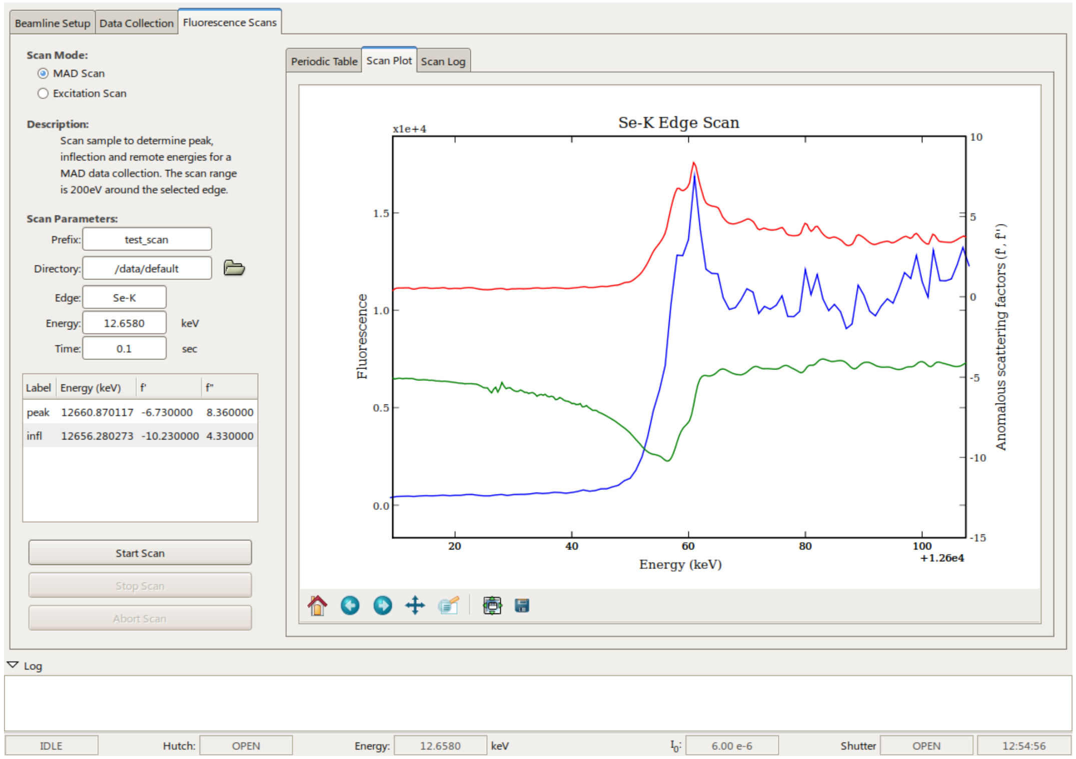
Edge Selection



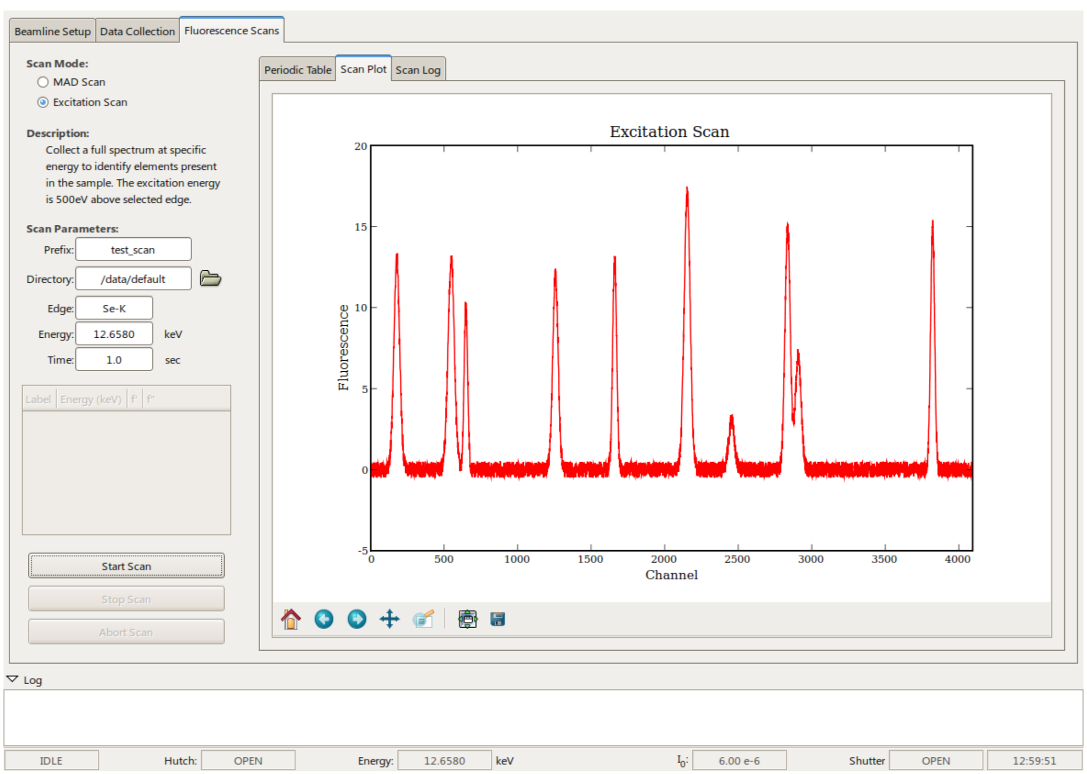
MAD Scan in progress



CHOOCH Output



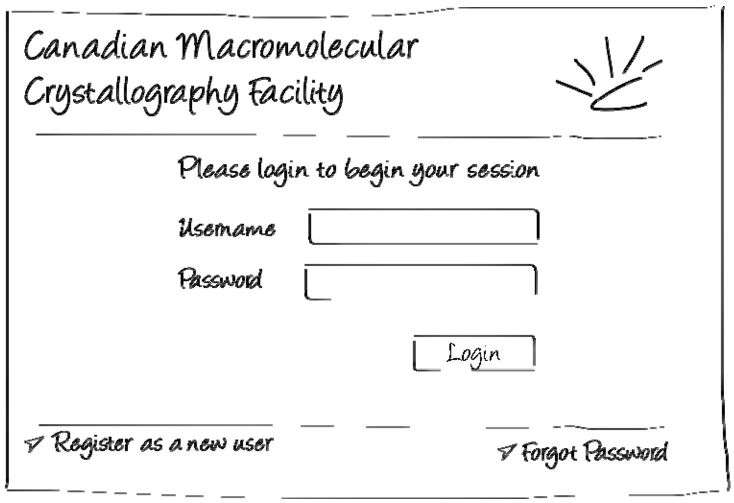
MAD Scan and CHOOCH run complete



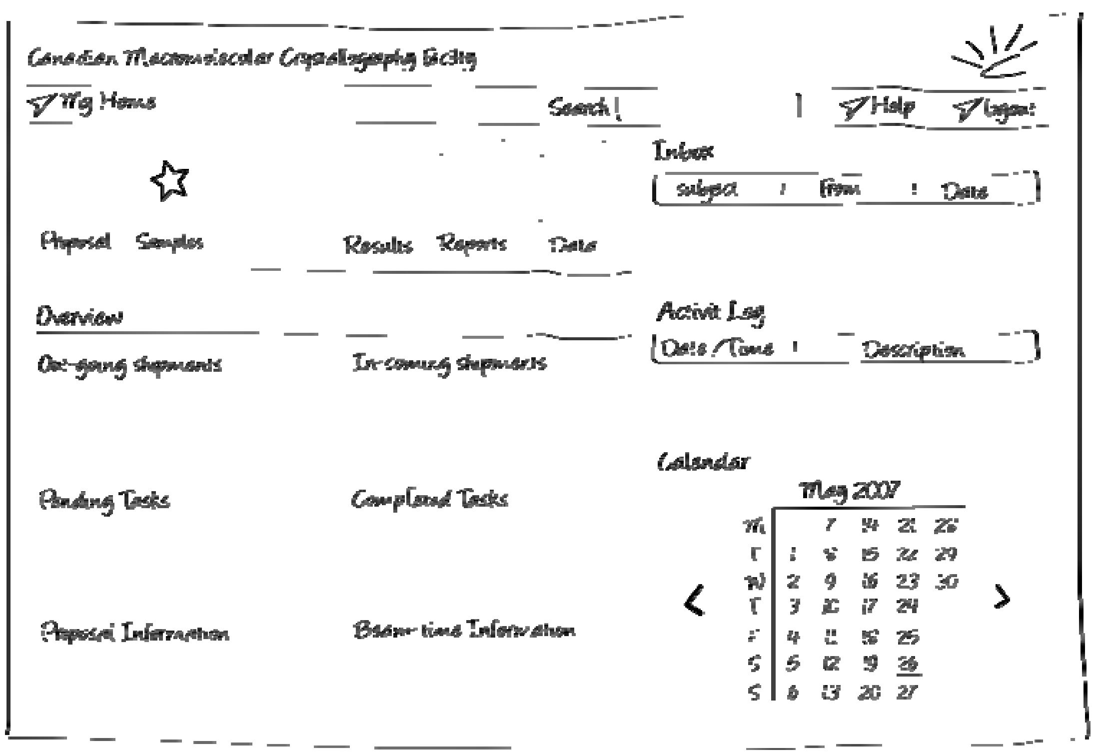
Simulated Excitation scan

(d) The layout of the screens for web portal functionality should be similar to the following illustrations:

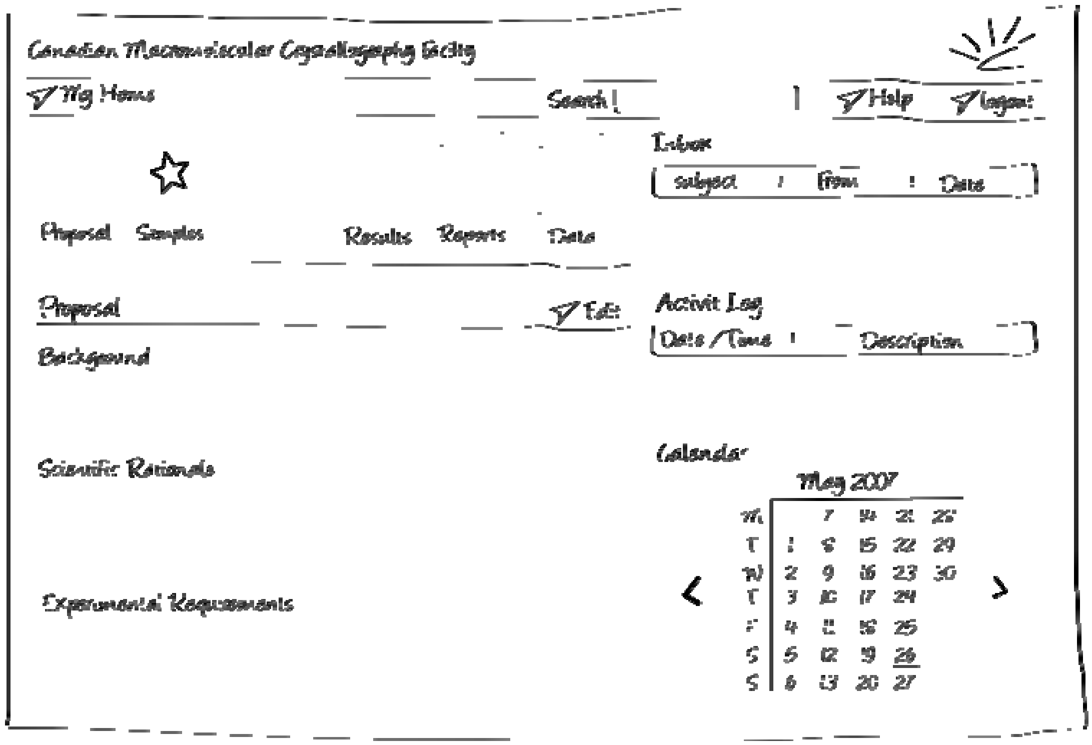
1. Login Screen



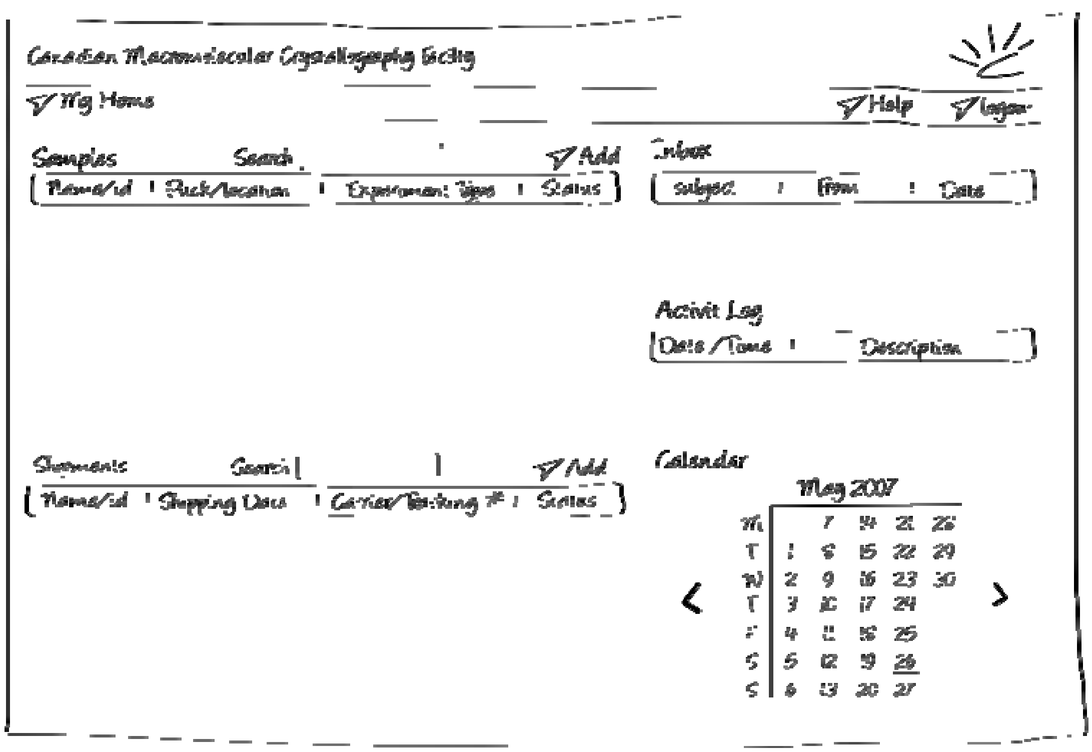
2. Account Overview



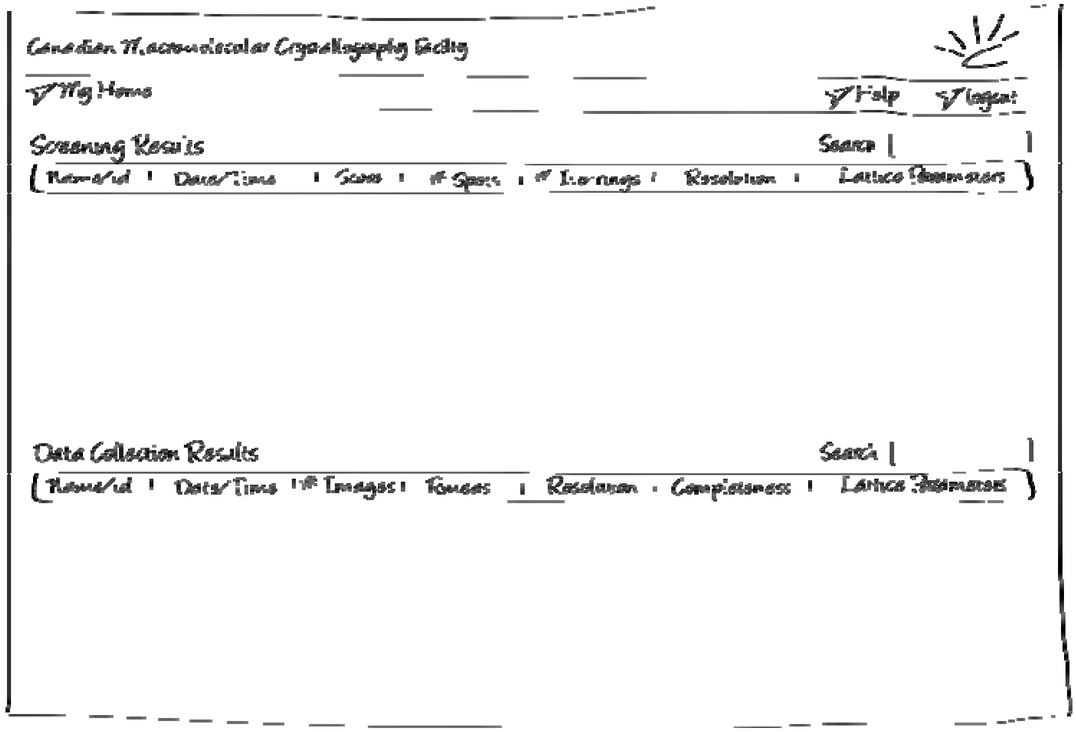
3. Proposal Context



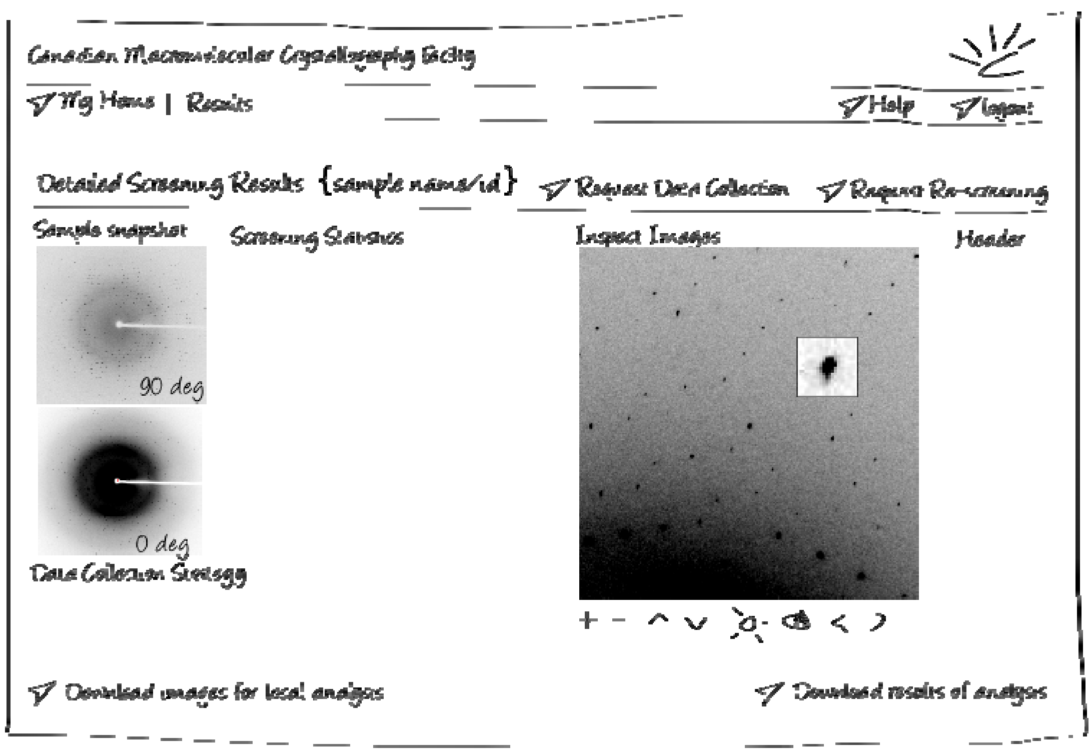
4. Samples Context

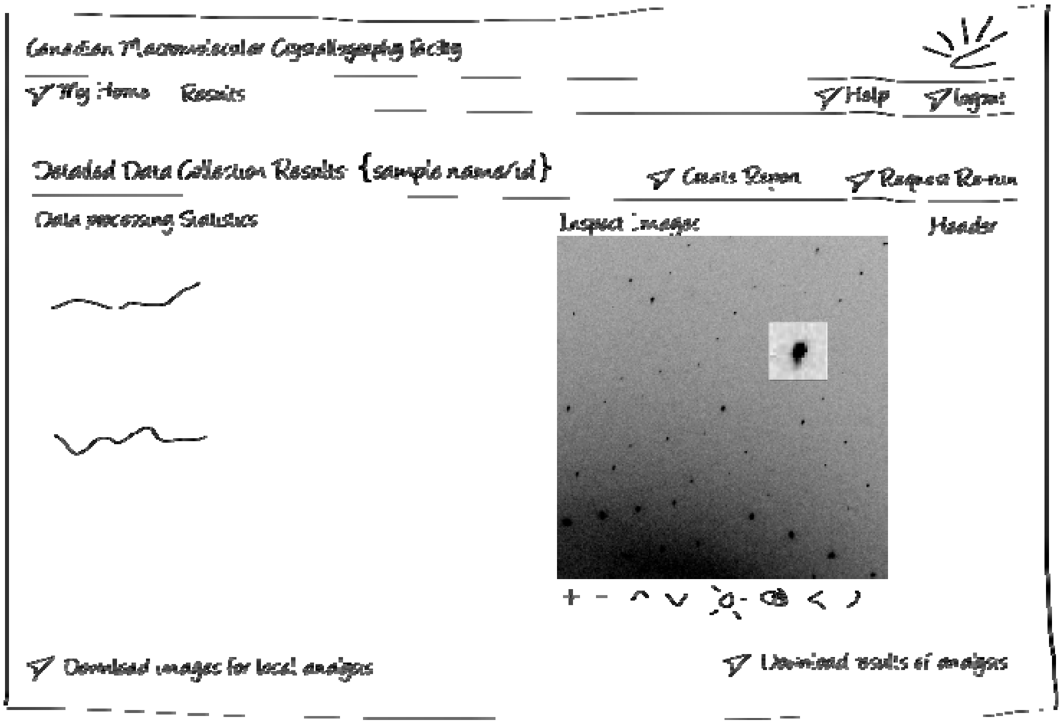


5. Results Context

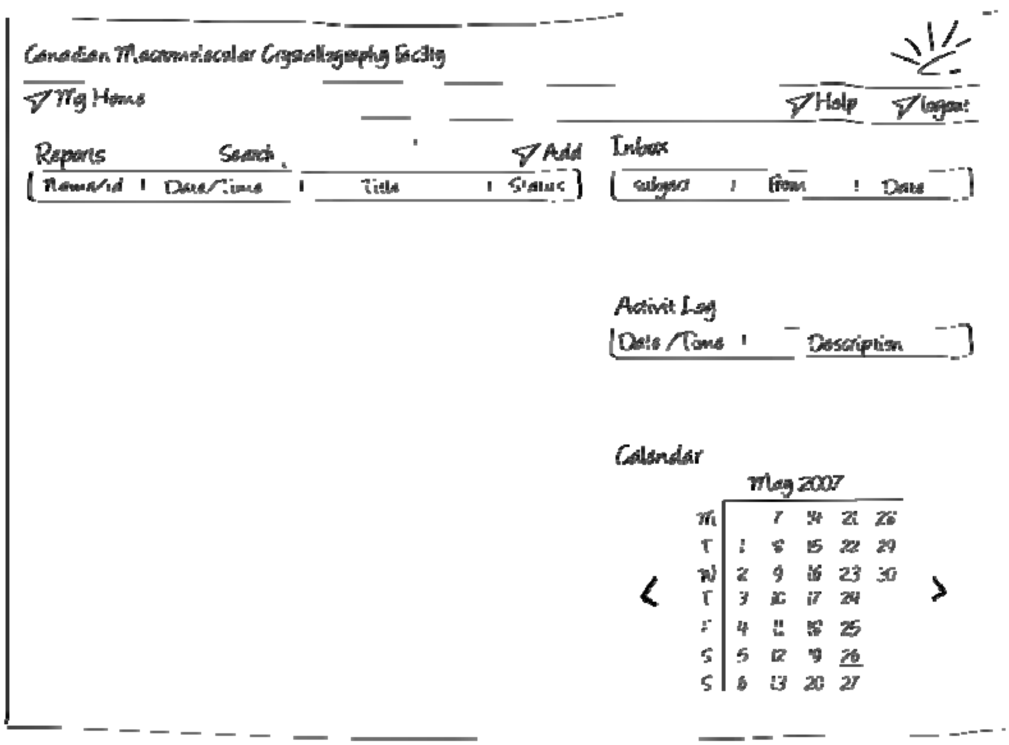


6. Results Details





7. Reports Context



3.1.7 Automatic Data Acquisition Functions

3.1.7.1 *Automatic Beamline Control Functionality*

The purpose of this functionality is to enable automatic control of the beamline without human intervention. Therefore the system shall make it possible for all functionality required for data acquisition to be carried out without human intervention. Specifically, the following functionality shall be implemented.

(a) Automatic beamline alignment and optimization. To achieve this, the system shall implement algorithms for aligning specific relevant beamline optical components, and interpret beamline diagnostics and error states.

(b) Beamline reconfiguration. This involves moving beamline components into a requested state. For example, energy, detector distance, beam size, detector-pitch, etc. in order to achieve a configuration suitable for a required experiment. The exact parameters required for an experiment will be selected from a relational database.

(c) Mounting or dismounting of samples. The system shall automatically mount or dismount a specific sample onto the goniometer.

(d) Automatic sample centering. This will require automatic adjustment of the illumination system, adjustment of the sample microscope, image analysis for determining loop or crystal positions and control of the goniometer head for crystal positioning.

(e) Automatic data collection. The system will manage the sequence of events required for collecting single data frames for screening, or a series of frames for complete data sets. The exact parameters for data collection, such as exposure time, oscillation range and beamline configuration will be read from a relational database.

3.1.7.2 *Beamline Expert Functionality*

The purpose of this functionality is to provide a level of expertise required to substitute an operator for automatic data acquisition. Therefore the system shall be equipped with algorithms for carrying out a full crystallography experiment from start to finish.

(a) The input to the system will be a list of sample identifiers, corresponding to all samples currently loaded into the sample holding dewar.

(b) For each sample, the system shall request specific experiment plans from the relational database and execute the data acquisition as determined by the input parameters.

(c) The system shall then update the relational database to reflect the results of the experiment.

(d) Execution of experiments shall include all the operational actions outlined in section 2.1 of this document. Specifically, the following expert functionality must be supported:

1. *Crystal characterization (screening)*
    - The system shall control the beamline hardware to mount a crystal, automatically center it, and collect a series of images based on parameters to be determined based on the crystal parameters requested experimental plan.

- The images shall be analyzed using DISTL [4], and auto-indexed using LABELIT, XDS and or MOSFLM [1, 2, and 3]. The output of this step will be the cell parameters, crystal orientation, mosaic spread, diffraction quality, resolution and overall diffraction score.

2. *Data acquisition setup*
   - The system shall be able to select one or more samples from a list of characterized samples based on the diffraction score
   - The system shall then retrieve the diffraction plan
   - The system shall configure the beamline hardware as required by the diffraction plan, by selecting the appropriate energy, beam size, detector distance, and optimizing the beam intensity.
   - The system shall then mount the sample, center it and initiate data acquisition.

3. *Data processing.*
   - For each image collected, the BOS shall be capable of performing image analysis using the external program DISTL [4]. The input for the analysis shall be the image file. The output shall include, the total number of diffraction spots present in the image, the total number of overloaded spots, the spot the number of ice rings if any, 'spot quality' and diffraction resolution.
   - Online data processing shall be supported. The images will be processed as they are being collected using MOSFLM or XDS [1,2], and the following data quality statistics shall be extracted as data processing proceeds:
     - Scaling factor
     - The standard deviation of the reflecting range or mosaicity
     - The standard deviation of spot position in pixels
     - The standard deviation of spindle position in degrees
     - The refined beam direct beam position on the detector surface
     - The refined detector origin
     - The number of accepted, and rejected reflections
     - The average spot profile
     - The refined unit cell parameters
     - Completeness of data
     - R-factors
     - I/Sigma

4. *Beamline alignment.* Beamline alignment functionality includes low level alignment of a single parameter of an optical element such as 'mirror angle', 'bending radius', etc. as well as high level alignment of a single optical element such as 'toriodal mirror' or even a complete beamline. During normal operation, the CMCF BOS system must be able to produce optimum intensity at the sample position for any valid set of experimental parameters, without human intervention through automatic beamline alignment. Additionally, during maintenance and operation the system shall provide assisted beamline alignment. Specifically, the following beamline components shall be able to be aligned automatically

- Primary slits
- Monochromator – Energy selection, optimization using crystal pitch and piezo. Where sagittal focusing is available on the second crystal, assisted focusing shall be supported.
- Mirror stripe selection and alignment shall be automated. Where the mirror is fitted with a bender, assisted focusing shall be supported.
- Exposure box and experimental table.

3.1.7.3 *Use Case for Automatic Data Acquisition*

The following illustrates a use case for automatic data acquisition.

(a) Scientist sets up an experimental plan

(b) Scientist prepares and ships samples to CLS

(c) Beamline Staff receives samples

(d) Scientist receives an e-mail with confirmation that samples have been received

(e) Before the beginning of a shift, Beamline staff sets up shift

(f) Samples are automatically screened and scored according to Scientists specifications

(g) At the end of a shift, Beamline staff reviews shift results

(h) Scientists receives an e-mail with confirmation that samples have been screened user

(i) Scientist logs onto website and reviews screening results.

(j) user requests data collection

(k) beamline staff sets up shift

(l) beamline collects data

(m) beamline staff reviews shift

(n) beamline notifies user

(o) user reviews collected data (if rejected return to 14)

(p) user downloads data

3.2 ERROR HANDLING

All run-time errors of the system shall be characterized based on the source and impact:

(a) *Internal* - Errors due to the internal logic of software systems. The system shall be designed to minimize internal errors as much as possible.

(b) *External* – Errors due to events beyond the scope of the program, originating from hardware, external software systems and humans

(c) *Recoverable* – These are errors from which the system is able to recover. Where automatic recovery is possible without adversely affect on-going experiments, recovery should be automatic.

(d) *Non-recoverable* – These errors have no recovery mechanism. However, they should be predictable in advance and encountered at relatively low levels.

The system shall handle errors as follows:

(e) Non-recoverable errors and Recoverable errors requiring human intervention during recovery shall be fatal. This means all on-going activities in the subsystem shall be suspended.

(f) Each subsystem shall be designed such that the suspended mode preserves as much as possible, all equipment, personnel and samples in its proximity.

(g) Some error states which may be fatal include: Automounter errors, hardware failures, beamline-vacuum failure, among others to be determined as the system is developed.

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