CLS Remote Beamline Access Software Requirements Document

7.4.1.1 Rev. 0

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Revision History

Revision	*Date*	*Description*	*Author*
A	2006-DEC-15	Original Draft	Chris Armstrong
B	2006-DEC-21	Incorporated comments by Marina Suominen Fuller. Some additional material.	Chris Armstrong
0	2006-DEC-31	Issued for use.	Chris Armstrong

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1.0 INTRODUCTION

1.1 PURPOSE

This project is a sub project of the Web Oriented Research for Lightpath Development of eScience (WORLDS) Project (see Background section). Under this sub project Canadian Light Source (CLS) has undertaken to develop a remote access and remote control system framework for CLS Beamlines that will leverage the CANARIE Intelligent Infrastructure (CA*Net4). This phase of the project is to develop the initial Proof of Concept that will validate the overall architecture design and initial architecture decisions.

The purpose of this document is to describe the RBA requirements. It documents the first phase of a longer term vision to development a framework for developing remote access to CLS services, including remote running of beamline experiments. The longer term vision is planned to be realized over 5 years. This document addresses some of the requirements for this longer term vision, as well as specific requirements for a working proof of concept to validate the architectural ideas and decisions.

This document contains the following sections:

- Vision and problem overview – a brief description of the long term vision for the remote beamline access and experimental services
- Glossary of terms – definitions of some of the terms used through out the project's documentation.
- Stakeholder requests – a list of requests made by stakeholders for features, enhancements, and fixes to a proposed new or existing system.
- User story – higher level scenarios in how the different users work with the system
- User roles and use cases – a description of some of roles supported within the system, and examples of how the user would use the system. Contains many of the functional requirements and provides some detail on specific work flows.
- Business model – a description of the business processes and information models – lists and defines many of the business processes, business entities and information organizational hierarchies within the business context and the business rules
- Non-functional requirements – a catch all for requirements and client constraints that are not specifically a functional requirement
- Prototype Requirements – specific requirements for the working prototype due December 2006 including requirements for some of the specific components

This document is still is a living document and it will evolve with the longer term vision.

The intended audience for this document is personnel that will be doing RBA development and anyone has an interest in the system's requirements.

This document restricts its requirements to providing a generic interface into devices. It does not go into the specific requirements to build a CMCF or VESPERS interface, although many of the important requirements are captured.

1.1.1 Vision

The vision provides a high-level basis for the more detailed requirements that are visible to the stakeholders. It captures the "essence" of the envisaged solution in the form of high-level requirements and design constraints that provides an overview of the system to be developed. It communicates the fundamental "why and what" for the project and is one of the gauges against which future decisions are validated.

The vision for this project from the business user's perspective is to move towards *a single User Interface for all End User applications and systems for the CLS,* even systems residing in different locations and organizations. This user interface needs to be responsive, user friendly, useful and intuitive for experienced and novice users both.

The business user could reside in any location and would be able to access the CLS from anywhere on the internet. Some business users would have faster access through the use of the CANERIE lightpath.

The business user would have access to common tools for:

- Collaboration
    - Working on shared business objects, documents and running experiments
    - Online chat, voice over IP, video conferencing
    - Shared work area and organization
- Document and business object management
    - Lifecycle management
    - Versioning and change tracking
    - Simple document and business object searching
- Data services
    - Backup, recovery and file transfers
    - Experimental data storage space
- Basic time, task/activity management
    - Calendaring, reminders, automatic organizational filtering
- Session and Experiment Setup
    - Session scheduling
    - Session and experiment setup to automate experiments
- Experiment data processing analyzing tools
    - Integration in one place of many divergent tools
    - Automating processing tasks

The vision from a project sponsor's and developer's perspective is to move towards a generic development Framework that:

- is flexible
- can integrate internal and external services
- can be used to control and receive feeds a large number of divergent devices including devices that produce very large amounts of data

- is a rich easy to maintain and easy to use client
- that can be open sourced and based on open standards
- is not tied too closely to non open/proprietary development and production solutions

This is a 5 year plan of which this project is just the first step. Please refer to the Background section of this Introduction for more initial scope and vision of this project.

1.2 SCOPE

The scope for this phase of the project includes:

- Requirements Gathering
  - Deliverable: Requirements Document (this document)
- Development of Architecture and Design
  - Deliverable: System Design Document
- Initial Prototyping of:
  - Partial simulated beamline experiment demonstrating UI capability
  - Metadata schema and management
  - Some reusable framework services
- Open source part of the solution

1.2.1 Goals of the System

The primary goal of the system is to provide an infrastructure and framework for developing:

- generic UI's for Scientists to remotely access and control Beamlines
- generic and reusable services around information, people and process integration

The primary goal of the Proof of Concept is to demonstrate a useful UI and development framework for remote access and control of a simple simulated X-Ray source scans and the resulting experimental data. The secondary goal of the Proof of Concept is to demonstrate the capability of remote access and control of a selected number of physical devices.

The critical success factors (business drivers) for the Proof of concept were identified as:

- Develop a framework architecture that can leverage the CANERIE lightpath so that remote scientists can access CLS services, providing the requirements and architecture design documentation
- Develop a working Proof of Concept that validates the requirements and application architecture.

The critical success factors (business drivers) for the final system were identified as:

- Saves users time
- Make more efficient and effective use of Beamlines
- Provides remote access and control of devices

- Based on a Service Oriented Architecture
- Becomes Open Source Software
- Supports multiple Beamlines
- Integrates systems
- provides a development framework for CLS

The final system will make use of a Service Oriented Architecture (SOA) to integrate diverse information systems to effectively meet the needs of researchers. The following are some of the services that must eventually be seamlessly integrated into one unified User Interface[1]:

- user management services
- sample management services
- experimental data storage and access services
- beamline control
- data analysis services

1.2.2 Architecture Goals

The following are the main architecture goals or principles that were explicitly or implicitly followed on this project. See also the section on Development Method for additional goals and principles.

- **Develop a usage-centric system**
  - The system should be modeled the way users perform their work. It should be easy to navigate to related data and transactions based on the current context being displayed.
- **Develop an easy-to-use system**
  - Uses common paradigms and UI standards so that training is reduced.
  - All components have a common look and feel so that the system is more intuitive and productivity is increased.
- **Develop a document-oriented system**
  - Ensure that business objects can be expressed as XML documents to facilitate best-of-breed solutions and leverage current architectural principles. Allows simplified searching, exchanging, and editing of business objects across many technical domains.
- **Develop a component-based system**
  - Allow additional components to be added, modified, or inter-connected without major repercussions throughout the entire system.
- **Use well established vendor-neutral (open) standards**
- **Develop a services-oriented system**
  - Provide services and resources for the users to manipulate data using existing analysis applications from a single interface.

[1] Note, that these services are currently outside the phase I scope.

- **Provide common services**
  - Use a common security (authentication and authorization) model. Have all authorization data managed centrally to ease administration, provide a common information model, and to provide consistent security. Centralize authentication management so that users do not need to log on multiple times to each component in the system. Provide common system services such as logging, transaction auditing and analysis.
- **Create a simple system**
  - By following the KISS ("Keep It Sweet and Simple") principle, the system will be easier to maintain and modify to changing business requirements. Exceptions to general rules should be examined closely and questioned. Features should be applied on a general case such that a required feature for a single function can be applied more globally if appropriate.

1.3 BACKGROUND

This project is a sub project of the Web Oriented Research for Lightpath Development of eScience (WORLDS) project. The goal of the WORLDS project is to develop and demonstrate the use of remote eScience technology for the scheduling and access to synchrotron Beamlines at the CLS over CA*Net4.[2] The expected result is the deployment of a web based system that permits (protein crystallography and VESPERS) scientists to more efficiently and effectively conduct synchrotron science experiments.

The project is innovative because it will result in the first production remote access system of this type in the world utilizing the high bandwidth infrastructure available on the CA*Net4. This infrastructure makes opportunistic access feasible where time can be allocated in smaller and smaller slices, permitting more efficient and timely access to the beamline. Canada will benefit because it will reduce the time needed for conducting medical research. The benefits to the community of interest are associated with reduced travel costs and the wait times for beamline access. This new mode of access provides for more samples being processed on the same scarce beamline resources. This permits expanding the number of samples that can be processed within the same facility.

CLS contracted IBM[3] to assist in helping to build a web based remote access into CLS services. The purpose was to improve access to CLS services, including the submission and access of experiment data to and from the Beamlines.

The goal of this project is to improve access to these facilities by permitting researchers to submit, monitor and review experimental results from their home institutions. As an added benefit this system will permit the introduction of opportunistic access, under this new mode of operation samples will be queued for analysis and then interleaved between different users. This mode of operation will permit faster turn around times for user samples and increased beamline throughput. This will provide more effective use of a scarce national resource.

[2] This background material was taken directly from the WORLDS - Statement of Work Prepared for the CANARIE Intelligent Infrastructure Program CIIP-14 CLS Document Id 7.14.71.2 – Rev. A, 2005-Aug-02

[3] SOW December 2005. All information on the two proposed "projects" taken from this document.

1.4 RELATED DOCUMENTS

The following are a list of documents that either make up the system documentation or are useful references.

RBA System Design Document

Word Document with following sections: High Level Requirements, Architecture Overview, Architecture Component Model, Entity Relationship, Deployment Model. December 2006.

RBA Software Architecture Document

Word Document with following sections: UML Models, Detailed Architecture Decisions, Architecture Principles, Generated Code Diagrams and Documentation. December 2006.

Project Management Templates

(Optional) Word Document with following sections: Status Template, Testing Strategy Template, Defect Tracking Template, Risk and Issue Management Template. December 2006.

RBA Business Case for Next Phase

PowerPoint presentation. December, 2006

RBA Preliminary Requirements, Architecture and Design

PowerPoint Presentation. May 2006

User Group CANARIE Project Status

PowerPoint presentation. June, 2006

CLS Project Overview

PowerPoint presentation. June 2006

Vespers – Wizard Description

Word Document. Stewart McIntyre and Diony Medrano, February 2006

Preliminary Logical Architecture and Design

PowerPoint presentation. May, 2006

CIIP-14 Statement of Work (between CLS and CANARIE)

Word Document. August, 2006

CIIP – Statement of Work (between CLS and IBM)

Word Document, December, 2006

1.5 TEAM

The Project Team was made up of the following:

Main Team

Name	Role
Elder Matias	Project Sponsor/Client Project Manager
Bruce Larsson	Project Manager
Chris Armstrong	Solution Architect
John Haley	Application Architect/Development Team Lead
Marina Suominen Fuller	Functional Authority/Subject Matter Expert
Dionisio (Diony) Medrano	Lead Developer
Daron Chabot	Senior Application Developer
Jason Chan	Application Developer

Support Team

Name	Role
Bob Harvey	Systems Support/Network Administrator
Jason Cyrenne	Systems Support/Systems Administrator/PX Beamline Requirements
Renfei Feng	Beamline Scientist
Pawel Grochulski	Beamline Scientist
Tom Kotzer	Industrial Liaison Scientist
Stewart McIntyre	CLS Client/End User
Russ Berg	Controls Group

1.6 REQUIREMENTS GATHERING PROCESS

The requirements gathering process follows the IBM Rational Unified Process (RUP). See the RUP description in the RBA System Design Document. The requirements discipline is responsible for requirements definition. This requirements discipline explains how to elicit stakeholder requests and transform them into a set of requirements work products that scope the system to be built and provide detailed requirements for what the system must do. The following tasks and resulting work products are recommended in RUP and form the main sections of this document.[4]

Task	Work Product
Develop Vision	Vision User Story[5]
Elicit Stakeholder Requests	Stakeholder Requests, User Story
Capture a Common Vocabulary	Glossary of Terms

[4] From version 7 of RUP. Note: the process of requirements gathering is referred to in RUP as requirements elicitation.

[5] User Story is referred to as a Storyboard in RUP.

Detail a Use Case	Detailed Use Cases
Find Actors and Use Cases	User Role (Actor), Use Case, Use Case Model, and Use Case Summary
Structure the Use-Case Model	Use Case Model, Glossary of Terms, Non Functional Requirements
Develop Supplementary Specifications	Non Functional Requirements
Detail the Software Requirements	This document

The following diagrams describe the relationship between the roles (the who), the tasks (the how) and the work products (the what).

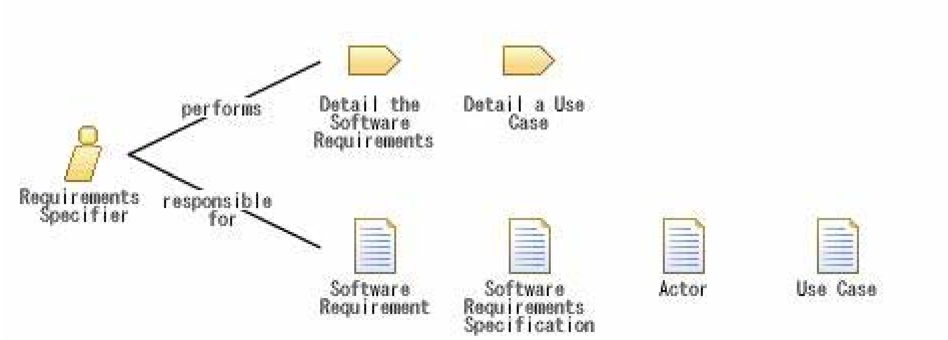

Figure 1: The Requirements Specifier Role

The Requirements Specifier role specifies and maintains the detailed system requirement and well as providing the detailed use cases.

The purpose of the *Detail the Software Requirements* task is to collect, detail and organize the set (package) of work products that completely describe the software requirements of the system. The package of work products is this document.

The purpose of the *Detail a Use Case* task is to:

- Describe one or more of the use case's flow of events in sufficient detail to enable software development to begin on it.
- Detail the use-case to the understanding and satisfaction of the actor representative or client.

Figure 2: System Analyst Role

The system analyst role leads and coordinates requirements elicitation by outlining the system's functionality and delimiting the system.

The purpose of *Develop Vision* task is to:

- Gain agreement on what problems need to be solved.
- Identify stakeholders of the system.
- Define the boundaries of the system.
- Describe primary features of the system.

The purpose of the *Elicit Stakeholder Requests* task is to:

- Understand who are the stakeholders of the project.
- Collect requests on what needs the system should fulfill.
- Prioritize stakeholder requests.

The purpose of the *Capture a Common Vocabulary* Task is to define a common vocabulary that can be used in all textual descriptions of the system, especially the software requirements.

The purpose of the *Define System Context* Task is based on the use case model be able to create a top-level collaboration showing the system (modeled as a top-level subsystem), its interfaces and its relationships with its actors, including the external I/O entities that flow between actor and system.

The purpose of the *Find Actors and Use Cases* Task is to:

- Define the scope of the system - what will be handled by the system and what will be handled outside the system.
- Define who and what will interact with the system.
- Outline the functionality of the system.

The purpose of the *Structure the Use Case Model* Task is to:

- Extract behavior in use cases that need to be considered as abstract use cases. Examples of such behavior includes common behavior, optional behavior, exceptional behavior, and behavior that is to be developed in later iterations.
- Find new abstract actors that define roles that are shared by several actors.

The purpose of the *Develop Supplementary Specification* Task is to capture requirements that are not easily captured in use cases.

2.0 GLOSSARY OF TERMS

A

Absorption Edge (re- X-ray absorption spectroscopy): a sharp step in the absorption cross-section is exhibited at some specific energy as the X-ray energy is increased. This sharp increase is called the absorption edge or edge-jump and is related to the oxidation state of the absorbing atom.

Acquisition Time: time required to collect spectrum

Alloy: a macroscopically homogeneous mixture of two or more metals

Atomic Number: the number of protons in the nucleus of an atom

B

Bandpass (X-ray energy)/Bandwidth: range of frequencies/energies. This could apply to a single spectral line or to the energy range selected by the monochromator/multilayer mirrors, for example.

Beamline: Synchrotron light is carried from its source in the storage ring to the experimental areas (end stations) through high vacuum 'beam lines'. Most of the x-ray beamlines contain focussing optics to concentrate the synchrotron light at the sample - mirrors are used to do this as, x-rays will pass straight through conventional lenses. Often the optics are cooled internally, enabling them to cope with the enormous heat loading of the bright light source without distorting. Some of the experiments use so called 'white' beam - a broad spectrum of wavelengths - whereas others require a single wavelength or 'monochromatic' beam which is isolated by a device known as a monochromator. The beamlines are kept under high vacuum so that the highly polished surfaces of the mirrors inside are not contaminated.

Beamline Scientist: person responsible for looking after the beamline (see beamline)

C

CCD Detector: 2-D charge-coupled x-ray area detector which functions as electronic photographic film

Compound: substance containing more than one element

Concentration: a measure of the relative amounts of a component in the mixture

Core electron: an electron in an inner, complete level

Counts: refer to events recorded by a detector

Crystallography : is the use of X-ray diffraction to determine the structure of crystals of molecules. A single crystal is made up of atoms packed in a repeating three-dimensional arrangement. When such a crystal is placed in a focused beam of x-rays, diffraction of the primary beam occurs. The measurement of the position and intensity of the diffracted x-ray beams produces an x-ray diffraction data set. This information is then used to resolve the structure of the crystal.

D

Density (d): an intensive physical property of a substance at a given temperature and pressure, defined as the ratio of the mass to the volume: d = m/V

Differential-Aperture X-ray Microscopy (DAXM): exploits a knife edge step profiling to provide a micrometre-resolution x-ray slit with high angular acceptance, in connection with a charge-coupled device (CCD) x-ray area detection and computer reconstruction of Laue diffraction patterns from polychromatic x-ray microbeams. Using this method, complete Laue diffraction patterns are extracted as a function of depth along the penetration direction of the microbeam.

Dwell Time (exposure time): the time the detector stays at a setting to collect data (counts/image)

E

Element: a substance whose atoms are all chemically the same, containing a definite number of protons

Energy: a property of a system which can be altered only by exchanging heat or work with the surroundings

Energy level of atoms: energy corresponding to the principal quantum number

Event: a change in the system

Excited State: an electronic state that has a higher energy than the ground state

Experiment: a set of conditions applied to an object or part of an object. For example, applying a technique to a specific sample area.

F

Frequency: the number of complete wave cycles per unit time

FWHM (Full width half maximum): The width of the peak at half the maximum intensity/counts

Filename: project code (3 to 5), session (06nov12), material(7), experiment(7), type of object (4), numerical number up to 9999.

G

Grain: single crystal

Grain Boundary: region between grains/crystals

Graticule: a wire or cross lines in an optical focussing system

Ground State: the electronic configuration of an atom or ion that is lowest in energy

H

I

Ionization energy: the energy that must be absorbed to remove an electron from a species

Information Model: An information model is the abstraction of the business domain into business entities or objects. It can be mapped into data models, object models, XML schemas, organizational hierarchies, UML diagrams, Entity Relationship Diagrams

Insertion Devices: While dipole magnets change the direction of the electrons, thus producing light, multi-magnet insertion devices called undulators and wigglers move the electrons back and forth creating a narrow beam of much more intense light.

Intensity: time averaged energy flux

J

K

L

M

Mass Number: an integer equal to the sum of the number of protons and neutrons in an atomic nucleus

Mass Percent: 100 times the ratio of the mass of a component to the total mass of the sample

Monochromator(mono): an optical device that transmits a mechanically selectable narrow band of wavelengths of light from a wider range wavelengths available at the inputs.

N

Nucleus: the small, dense, positively charged region at the centre of the atom

O

Oxidation: a loss of electrons: an increase in oxidation number

P

Parallax: apparent shift of an object against a background due to a shift in the position of an observer

Periodic Table: A table that organizes the elements by atomic number and chemical properties into groups and periods.

Photon: an individual particle of radiant energy

Plot: drawn graphical representation of data

Point defect: A misplaced or missing atom in a real crystal

Polychromatic: a broad spectrum of wavelengths

Polycrystalline: composed of many crystals/grains

Q

R

Resolution (spectral): a measure of the ability of a spectrograph to differentiate features in the electromagnetic spectrum. It is usually defined as $R = \lambda/\Delta\lambda$, where $\Delta\lambda$is the smallest difference in wavelengths that can be distinguished at a wavelength λ.

S

Session: A slice of time allocated to do tasks.

Spectrum: a plot of light intensity as a function of frequency or wavelength

Strain: average linear strain is defined as the ratio of the change in length to the original length of the same dimension.

Stress: defined as the force per unit area

Synchrotron light: is produced at the Synchrotron Radiation Source (SRS) when an electron beam travelling close to the speed of light is accelerated in a magnetic field. The light covers a broad area of the electromagnetic spectrum, from infrared through to hard X-rays. Synchrotron X-rays are much more intense than those from a conventional laboratory source, enabling researchers to carry out experiments in a very short time. The light from the SRS has other important properties making it different to ordinary light; it comes in regular pulses, allowing data to be collected like a movie on samples which vary with time. The light is also very highly polarised, linearly in the centre of the beam and circularly above and below centre.

T

Task: (is an activity) a way of classifying a small number of activities that people do such as experiments into a general category. A task is made up of slices of time.

V

Very Sensitive Elemental and Structural Probe Employing Radiation from a Synchrotron (VESPERS): Determine trace elements and crystal structure in microsamples. Research is applicable to mineral ores and metals.

X

X-ray Absorption Spectroscopy (XAFS): is a technique whereby the effect of the absorption of the X-rays by the central atom of a molecule is studied. This provides element-specific chemical information about matter in virtually any physical state: gases, liquids, amorphous materials, or crystalline solids. XAFS analysis determines chemical bonding, valence and oxidation state, and can give quantitative data on short-range structure. Data studied can provide detailed information about the structure and properties of the molecule in question. A major advantage of XAFS for structural determination is that a crystalline sample is not required. This feature is particularly helpful in the geochemical sciences, catalysis studies, electrochemistry, materials science, and the environmental sciences where pure crystals of a sample usually do not exist. In addition, the penetration power of hard X-rays permits the study of various complex systems in situ (in their natural or original position) without treatment or chemical preparation. The XAFS spectrum can be divided into two different regions; the XANES (X-ray absorption fine structure) and the EXAFS (extended X-ray absorption fine structure) region (see XANES and EXAFS).

XANES (X-ray absorption near edge structure): the threshold, or pre-edge and near-edge regions of the XAFS spectrum from ~5 eV below to 40-50 eV above the absorption edge. XANES yields information about the oxidation state and local geometry around the absorbing atom.

EXAFS (extended X-ray absorption fine structure): the EXAFS region extends beyond 40-50 eV above the absorption edge. The EXAFS region yields information about the number neighboring atoms around the absorbing atom, bond length, and disorder.

X-ray Diffraction (XRD): An instrumental technique used to measure the spatial dimensions of a crystal structure by measuring the diffraction patterns caused by x-rays impinging on the crystal

X-ray Fluoresence (XRF): An instrumental technique that is used to detect the presence of chemical elements (i.e., iron, calcium etc.). Fluorescence is the emission of light from an excited state and x-rays are used to excite the atoms into an excited state- for example, higher energy core electron fills empty electron shell, and ejects an x-ray of fixed energy that allows the element to be identified.

3.0 REQUIREMENTS OVERVIEW

Stakeholder Requests are all requests made for features, fixes, changes, or enhancements to the new or existing system. The requests can be made by users, managers, developers, or other interested stakeholders. If new or changed functionality is accepted, new system requirements will be created. Requirements define the analyzed and approved requested capabilities of the system.

3.1 REQUIREMENTS SUMMARY

The following are the main high level requirements for the system (as elaborated in "RBA Preliminary Requirements, Architecture and Design May, 2006"):

- Remote access to (ability to create and update)
    - User metadata which will be used to
        - provide information to Beamline Scientists
        - automate many beamline processes
        - provide data for analysis techniques (input into analysis tools)
        - organize accessed results (images, scans, analysis, processing)
    - Running Experiments, as required
    - Experimental results (beamline data results)
- Collaboration services
    - Collaboration with other scientists
    - Collaboration with staff
        - Proof of Concept Functional Requirements for Remote User Control and Access on a Simulation Beamline

3.2 PROTOTYPE REQUIREMENTS (PHASE I REQUIREMENTS)

The requirements for the capabilities of the remote access and control of the prototype beamline were set out in the following prototype beamline diagram. The Prototype Beamline provides a model for future system usability guidance and development and hardware configuration techniques:

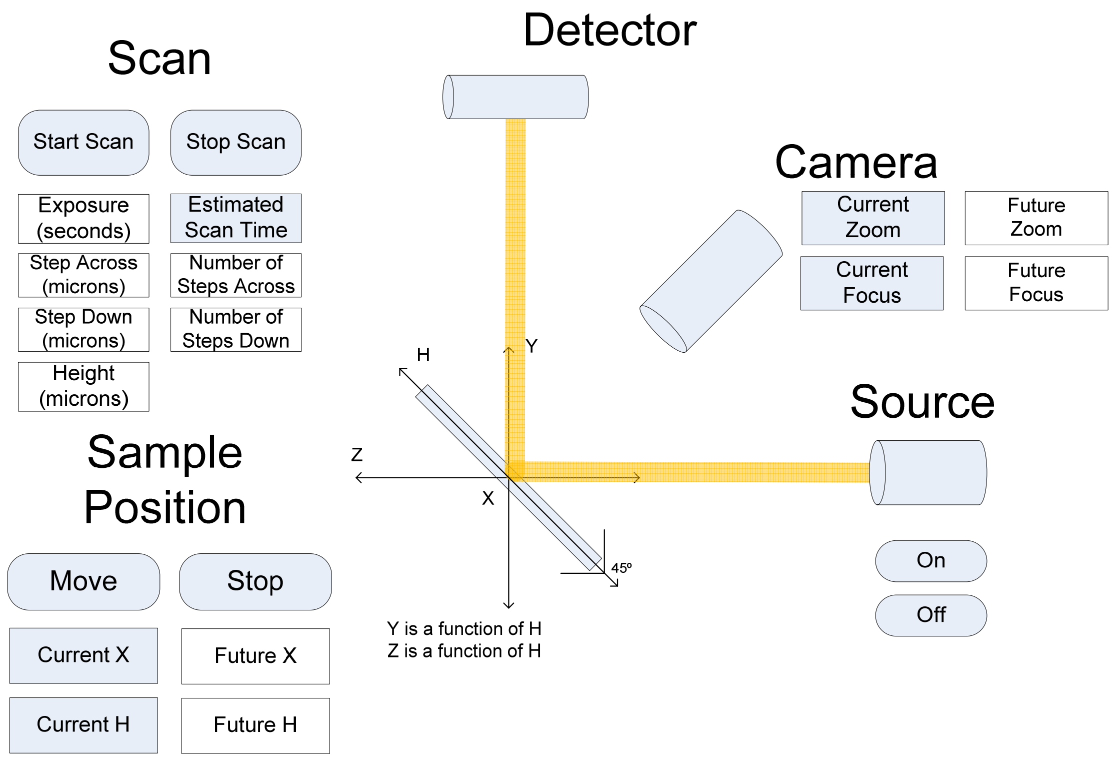

Figure 3: Prototype Beamline

The use case flow that the proof-of-concept will support is as follows:

- User logins in
- User creates project
- System generates a Project Lead Role and associates the User to this role
- User creates project roles associating team members to the role
- User creates sample within project context
- User creates beamline session within project context
- User associates sample to session from available project samples
- Beamline Scientist starts a beamline session making it active
- User joins an active beamline session (either prototyped beamline or one of the simulation Beamlines)
- User loads a sample into the active beamline session
- User moves sample tray to find region to scan
- User zooms and focuses camera to better identity scan region
- User selects scan type: spot, line or area scan and scan exposure in seconds
- If a line scan is selected, the user selects either a number of scan points or step size
    - System calculates either the step size or the number of scan points based on user's choice

- If area scan, the user selects either a number of scan points or step size and a height
    - System calculates either the horizontal step size or the horizontal number of scan points based on user's choice. Vertical step size and vertical number of scan points are determine by the horizontal step size and the user's choice of height
- The user can select where on the sample to scan, depending on scan type a spot, line or rectangle will be drawn on the image to represent the scan area
- The user selects start scan and can monitor the scan's progress by the time remaining and the progress bar
- While the scan is running the user can view the experiment's results as they come in, in the form of a scan plot and as raw unplotted data
- To see the results at a previous scan point, the user hovers over the point and the scan plot is displayed
- The user can copy the scan image and the scan plot into a word processing document
- The user can archive their session (or project), all the data stored as XML is moved to their own hard drive
- The user logs out

3.3 REQUIREMENTS

The Proof of Concept must demonstrate the following capabilities:

- Create a framework that is flexible, that can be used to control a large number of divergent devices
- Remote control of a physical motor
- Show the feed from a physical camera
- Show the feed from a physical detector
- Use the CANARIE Lightpath network
- User can join more than one beamline session at a time
- User can switch between beamline sessions
- A team of users can see the same session view of a running experiment.
- Rich easy to maintain client, preferably browser based
- The developed frameworks can be open sourced
- The architecture be based on open standards
- The architecture not be tied too closely to non open/proprietary development and production solutions
- Development of some useful UI widgets with the capability of easily creating others. The following list was identified as the UI widgets to develop:
    - tab control
    - tree navigation control

  - window pane to window pane communication
  - overlay graphics onto images
  - copy and paste application images and data into other applications
- User friendly, useful and intuitive UI for experienced and novice users both
- Responsive UI
- Change the look or skin of the UI from altering a style sheet
- Common template for displaying and editing business objects
- Provide a framework for supporting multiple beamlines potentially with a unique beamline UI
- Provide a framework for being able to access multiple Beamlines
- Provide a framework that is flexible enough for integrating
  - third party analysis tools
  - other business systems like the Proposal System
  - a common authentication and authorization system

After 5 years the business users would like to be able to accomplish the functions outlined in the diagram below:

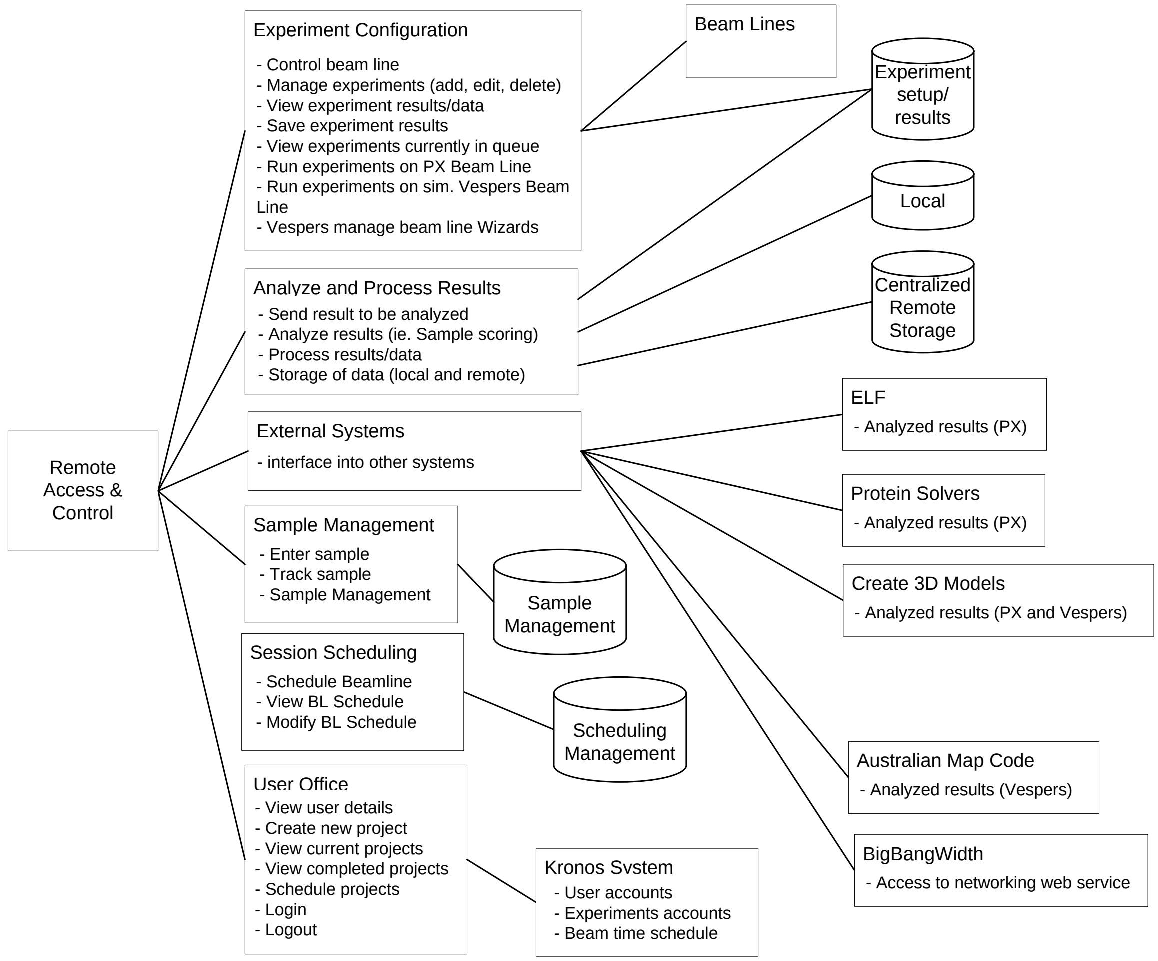

Figure 4: Business User Requests for Remote Access

Stakeholder requests evolve as the stakeholder gets a better idea of the capabilities of a system. They will make additional requests. These requests should be documented and analyzed to see if they will become useful requirements for the evolution of the system.

3.3.1 Additional Non Functional Requirements

General

- Number of participants (people who will or could be involved in conducting experiments)
  - 30-50
- Number of participating institutions conducting experiments
  - 10-15
- Additional growth of institutions per year
  - 2-4
- Additional growth of participants per year
  - 5-15
- Any special characteristics for an institution (institution types)?

  - On the light path or not on the light path (off light path means access via internet)
  - Universities, research institutes, and industries
- How many beam lines do we need to support
  - 2-4 (?) for next a few years

Experiments

- Number of experiments per year
  - ~50-100
- Number of participants per experiment
  - ~3-5
- Min/max/average number of days/hours for an experiment
  - 2-7 days

Sessions

- Number of sessions (with the beam line) for an experiment
  - N/A
- Characteristics that determine when subsequent sessions are conducted (e.g. fixed time, analysis time, etc.)
  - N/A
- Average duration of an experiment session
  - N/A
- Min/max/average time between experiment sessions
  - N/A
- Number of online participants, by role, for a session
  - 2-3

Experiment Conductor

- Avg/max number of control commands issued per experiment
  - ~100 (not included sequence commands created by control system)
- Max number of control commands which might be reasonably required within an experiment (i.e. what is a good objective for responsiveness)
  - ~1000 (?)
- Responsiveness of request/response and publish/push
  - Undermined. As responsive as possible.

4.0 SCENARIO OR USER STORY

A user story is a logical and conceptual description of system functionality for a specific scenario, including the interaction required between the system users and the system. A user story "tells a specific story".

Jane S. arrives at SSW/UWO at 8am Tuesday morning. She greets Barry as she enters the office she shares with Barry and two other colleagues. Jane turns on her computer, removes her coat and puts away her personal belongings. As her computer is firing up, she gets a cup of coffee from the coffee station down the hall. She runs into Ray, her supervisor, on her way back to her office.

Ray: Jane, I left a message from a prospective client on your voicemail. Mel Y. from metal forming company B called late yesterday afternoon. They are looking at changing a part of their process and want to analyse test samples for elastic/plastic strain. They also want elemental mapping analysis to check for contamination. I thought that this would be a good project for you to handle.

Jane: Thanks Ray. I'll listen to his message and give him a call.

Jane sits down at her desk and accesses the UI for the RBA database. A message on her message board shows that search results for a project she has recently been working on are ready. Another system message informs her that a project report for Project Biohaz is due by the end of today. She accesses the project and pulls out the report and reads it. She pulls out the associated X-ray fluorescence (XRF) results and reviews them again. Jane looks at a scan and copies it and pastes it into the report and rewrites a section of the report. Jane then phones the secretary Sarah and tells her that the report for Project Biohaz is ready. Sarah will access the database and pull out the report for final editing. The company information is also in the database and Sarah will get the report out today.

Jane then checks her personal folder and notes a reminder of an appointment with her dentist coming up this week on Thursday.

It is now 10am and Jane gets another cup of coffee and sits down at her desk and listens to the message from Mel Y. from metal forming company B. Jane looks up a resource list on the database and puts in the analysis requirements and searches for resource/device capabilities to match the requirements. The search results indicate that the HXMA beamline at the Canadian Light Source (CLS), the synchrotron facility located in Saskatoon, Saskatchewan, has the capability to do X-ray fluorescence analysis (XRF). The elemental mapping information could be obtained on the samples using this beamline. However, the VESPERS beamline at (CLS)has the capability to do both the XRF and Laue XRD analysis on the same sample volume at the same time. Laue XRD would give the requested elastic/plastic strain information.

Jane pulls out a fee list for the beamlines at CLS. To make effective, efficient use of the beamlines, Jane feels that pre-screening of the samples should be done at SSW and she pulls out a fee list for the services provided at SSW and adds it to the fee list document she has created from the CLS information.

Jane calls Mel at the metal forming company to discuss analysis options. She advises Mel that the VESPERS beamline would give the company the information that they are looking for. She suggests to Mel that pre-screening of the samples should be done at SSW and then the pre-selected samples be sent out to CLS from SSW.

Jane: The samples will likely have to be cut to be accommodated on the VESPERS end-station. We'll take optical images of the samples at SSW and also do some initial screening of the samples by having them analysed by scanning electron microscopy combined with energy dispersive X-ray analysis (SEM/EDX). SEM/EDX gives elemental composition information. Mel, I'm going to send you the beamline capabilities documents and the fee list for the analysis options I've recommended.

Mel: Your recommendation seems very sound.

Jane: If you decide to go ahead with the analyses we've recommended, fill out the online form and submit it. Then ship your samples to us and notify us that the samples are on the way. You can do this through the online service as well.

Mel: Thanks Jane, we'll be in touch.

It is now 10:45am and Jane talks with a team member to check on the progress of a project. Stephen is busy taking optical images of samples he has just finished cutting and is saving the images into the database under the project. He makes notes as he takes images and enters the notes directly into the database along with the images. Bob will then do SEM/EDX analyses of the samples and enter the results into the database under the project and appropriate task category. The client of the project will be contacted tomorrow and the results will be discussed online with the client able to view the results as they are being presented. Samples will be chosen for analysis at CLS and Stephen will mount the samples onto the samples trays and then ship the samples to CLS.

Jane is also working on a project with Joe A. from mining company Alchemy Borealis. They are doing exploratory work in northern Ontario looking for gold. They are also interested in the mineral phases associated with any gold. Samples have already been pre screened at SSW and shipped out to CLS. A beamline session is planned for 1pm today and Jane checks the online database for messages from the beamline scientist, Renfei. Renfei has sent a note that the samples will be loaded at 1pm and Jane's remote session will start at 1:15pm. Jane contacts Joe and reminds him of the beamline session. Joe will be observing the session remotely from Timmins and assisting Jane in setting up the remote experiments by helping her select the sample areas to be analysed.

It is now 11:25am and a graduate student comes in to see Jane for help in assessing Laue XRD data from an experiment the student ran last week with Jane's help. With more experience, the student will soon be running their own experiments remotely. At noon, Jane goes to lunch.

At 1:04pm, Jane logs into the system from the beamline remote access site at SSW. Joe logs into the site from Timmins, as an observer. Jane and Joe chat online about sample strategy. Joe has questions about the SEM/EDX data and Bob at SSW logs in as an experimenter and chats with Joe and explains the data that he collected. At 1:15pm Jane joins the active experiment session. The plan is to select 9 samples for automated analysis. Jane selects and loads (brings into view) a sample from the loaded sample tray. Jane and Joe chat online and decide on a sample area to be analysed. Jane takes an image of the sample area and inputs the parameters for the experiment. This process continues until all the experiments are entered. Jane then selects the analysis tools for processing the data and also requests the system to stream the data for processing.

Jane then starts the experiments from her remote site. The system sends her a message that the experiments are estimated to take approximately 1.5 hours, which is within her session time window. It is now 1:45pm. Jane and Joe plan to rejoin the online system at 3:30pm and assess the processed data together.

Jane then attends a talk given by a visiting scientist. The talk is scheduled from 2-3pm. After the talk, Jane has a chance to check her email and sends out responses and queries. Jane grabs a cup of coffee and walks over to the remote station. She logs into the system and changes her status to available. She checks Joe's status and sees that he is available and pings him to alert him that she is ready to begin chatting and reviewing the data.

At 3:30pm, Jane and Joe login to the system and begin looking at the processed data. They chat online about the data and assess the next stage of sample analysis. After reviewing the data, they decide to go back and re analyse the samples, changing some of the experimental parameters. They request a 10 hour slot and are scheduled an active session starting at 6pm. Gerry from Queens University has a screening session at present and his experiments will finish at 5:30pm.

At 5:25pm Jane logs into the system from SSW, and Joe from Timmins logs in as an observer. They join the active session, load the first sample and begin the process of setting up the experiments. At 6:10pm the experimental setup is complete and Jane starts the experiments. The system lets Jane know that the experiments will be completed at 3:19am. Jane and Joe log out and Jane checks her job list, notes any tasks that were not completed today and reschedules them for tomorrow and heads for home.

5.0 ESSENTIAL OR BUSINESS USE CASES

A use case is a technique for capturing functional requirements of systems and systems-of-systems[6]. Each use case provides one or more scenarios that convey how the system should interact with the users called actors to achieve a specific business goal or function. Use case actors may be end users or other systems.

An essential use case is a refinement of the general use case. In Usage-centric design, essential use cases are used to describe the user's intentions for a system and the system responsibilities in response to the user intention. It is similar to a Business Use Case in RUP.

The use cases presented in this document were the initial use cases used by the development team. Much has changed. The terminology and concepts has become clearer and an understanding of what the system needs to be able to do is also clearer. New use cases should be developed to indicate the functional requirements for the next major phase of development.

5.1 USER ROLE

A user role is a role that users of the system can play when interacting with it.

5.2 PHASE I: USER ROLES

Project Lead (alias User in Use Cases)

Beamline Scientist

Experimenter (alias User in Use Cases)

Observer

[6] This definition of "Use Case" has been taken from Wikipedia. http://en.wikipedia.org/wiki/Use_case

5.3 PHASE II: USER ROLES

Project Lead (alias User in Use Cases)

Beamline Scientist

Experimenter (alias User in Use Cases)

Observer

Controller of Device

Device Operator

User Office

System Administrator

Client

5.4 PHASE I: USER ROLE MAP

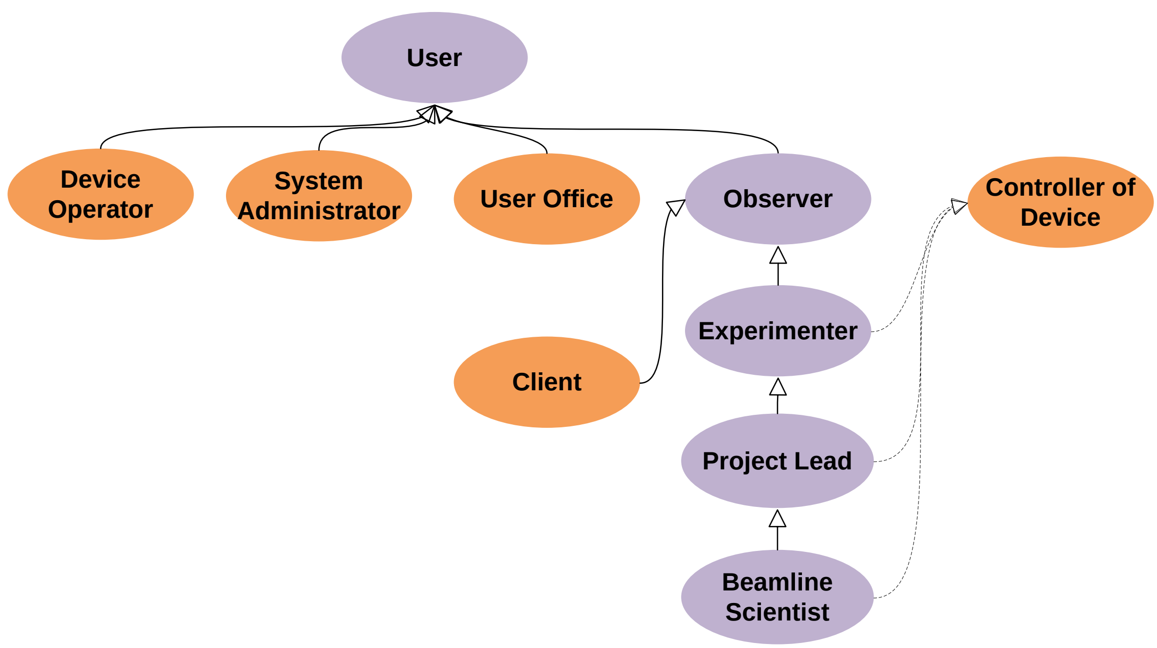

Figure 5: User Role Map

5.5 PHASE I USE CASE SUMMARY

Use Case Summary

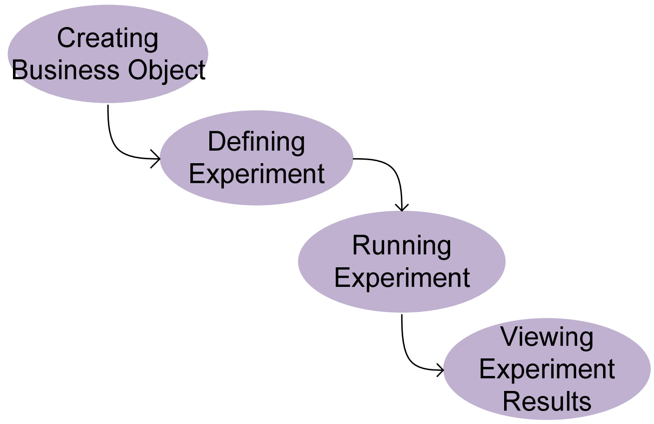

Figure 6: Use Case Summary

Creating business object

- Creating Project
- Creating Sample
- Creating Person (optional)
- Creating Experiment

Defining experiment

- Associating Sample to Project
- Associating Experiment to Project
- Associating Sample to Experiment
- Adding Person with Role to Project
- Creating Note associated with Business Object

Running experiment

- Setting up experiment
- Aligning beam (moving detector and slits)
- Finding x-ray beam position in lab space (using phosphor sample)
- Positioning beam on sample (moving sample)
- Changing beam spot size (changing slit position)
- Setting detector parameters (Exposure and readout times (duration))
- Picking Spot Line or Scan Area
- Choosing Data Analysis
- Opening/Closing Shutter

Executing experiment

- Starting/Activating experiment by command
- Viewing experiment results
- Viewing Raw Data Image
- Viewing Processed Data Image

5.6 PHASE I USE CASE MAPS

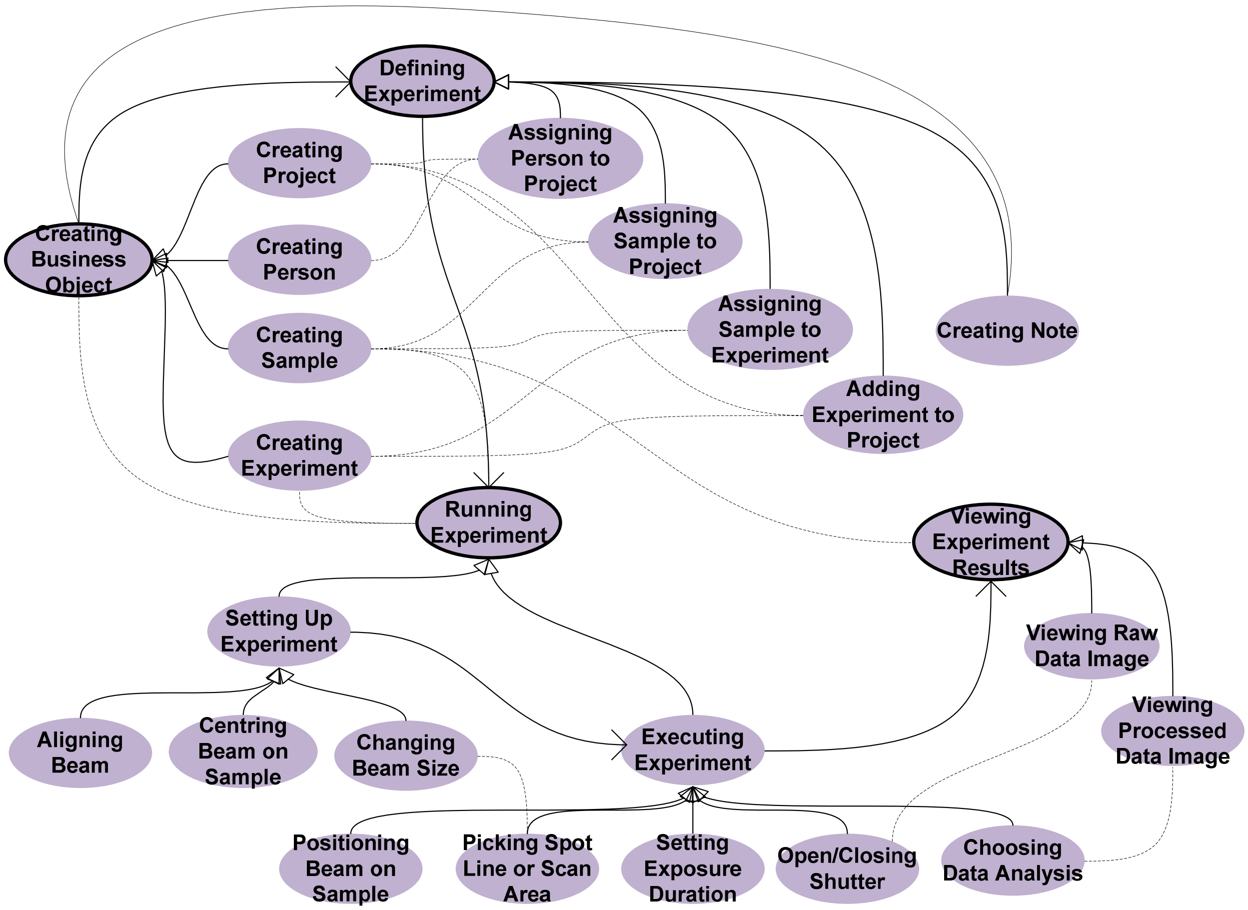

Figure 7: Use Case Map

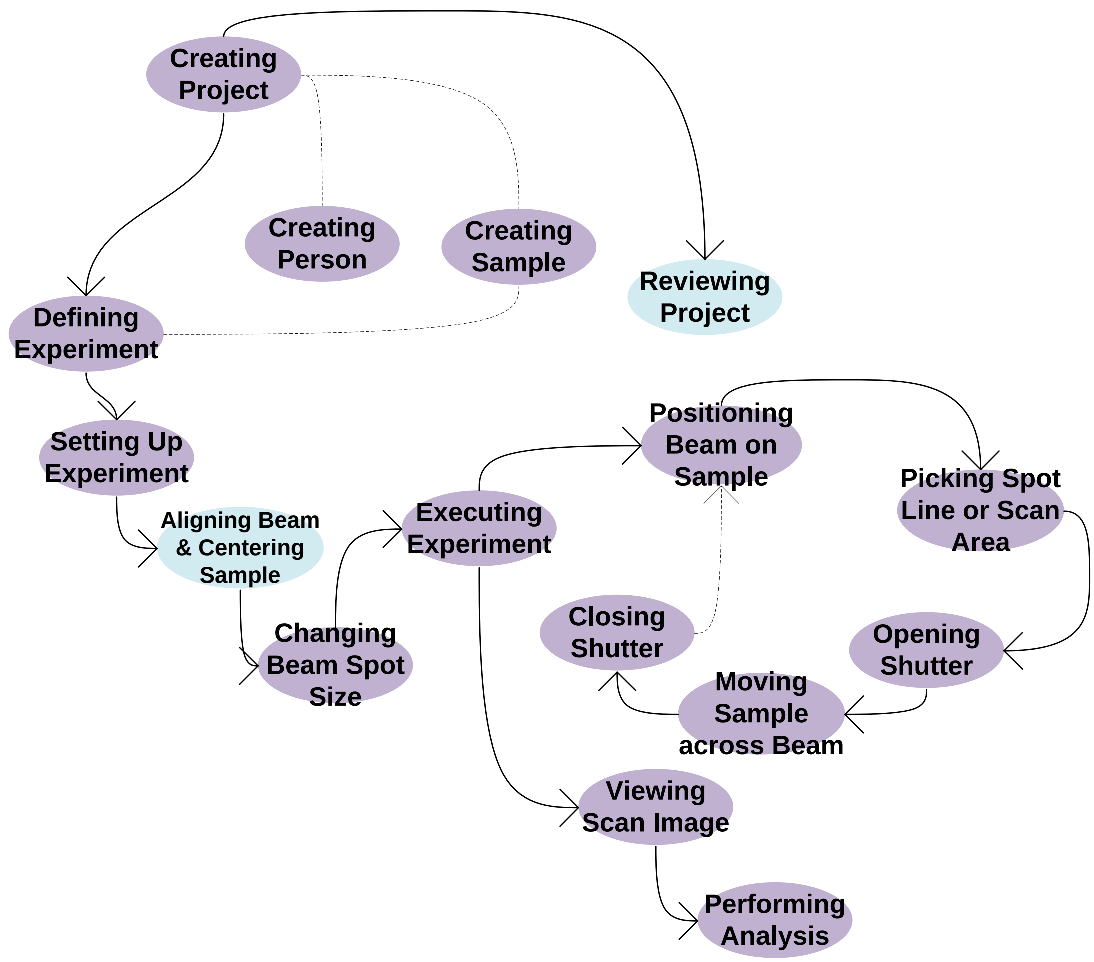

Figure 8: Use Case Flow

5.7 PHASE I DETAILED USE CASES

Creating business object

Contextual Purpose

The user needs the ability to be able to create and modify business objects. Once the user has created a business object, the user needs the ability to find and be able to navigate to the business object. The ability to create or modify business objects depends on the user authority within the system to do so. These business object, or business documents and their relationships is an important part of the system.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating project
- Creating sample
- Creating person
- Creating experiment
- Creating note

Process

Pre-conditions

User has access to the control for producing a list of new objects types.

User is authorized to create the new object

User intentions/System responsibilities

User Intentions	System responsibilities
	1. Depending on business object, the system may provide the user with a list of possible business objects (for example, project, sample, experiment, person)
2. Depending on business object the user picks a business object, and requests the creation of new object or adding a new object (except for creating projects, user chooses objects within the context of a project)	3. system creates a link for the new business object, creates the object in the system, and passes link to this new object, back to user
	4. system provides a form for the user to fill out corresponding to the business object chosen.
5. user fills out form (optionally, user requires a pick list to choose one or more associations) and indicates task is finished	6. system validates form, updates the business object, and sends to user some form of confirmation of success
7. user receives confirmation of successful data correction	

Modifying business object

Contextual Purpose

Once a business object has been created, it is important to be able to make changes to the object.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating project
- Creating sample
- Creating person
- Creating experiment

Process

Pre-conditions

User has access to the control for producing a list of object type to modified

User has authorization to modify the objects.

The business object to modified exists

User intentions/System responsibilities

User Intentions	System responsibilities
1. User selects a business object and chooses to edit it 3. Users updates business object form 5. user receives confirmation of request	2. system validates request, retrieves business object, responds to user with business object form with the current state of its contents 4. system validates form, updates the business object, and sends to user some form of confirmation of success

Finding business object

Not completed yet.

Creating Project

Contextual Purpose

The user helps clients define their problems. The user analyzes the problem to develop possible strategies or solutions for solving them. Because there are multiple clients with multiple problems, the user needs some way of organizing their work. The organization of work aids the user in:

- identify tasks and activities;
- planning, scheduling and prioritization of task and activities;
- improving the user focus required to complete and to track the status of tasks/activities.

All the information associated with carrying out these task and activities should be included in the same organization. This organization and information contained within, could be shared with other team members and could be used as a tool to help improve communication.

It was decided that the root organizational concept would be the project. Here the user and systems can put person information, notes, samples information, beamline configurations, beamline device values, experiment information, raw data images, raw results, processed results, system alerts, etc.

The user submits project to CLS User Office (CLSUO) and asks for beamtime on appropriate beamlines. The project is peer reviewed and accepted/rejected. If accepted, CLSUO creates (schedules) a beamline session to perform experiments related to the project.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Associating sample to project
- Adding person with role to experiment
- Creating business object

Process

Pre-conditions

User has a new problem that needs to be solved or a new solution area.

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses new project 3. User fills out project form	2. System creates new project and responds with project form 4. System validates, saves form and confirms action

Creating sample

Contextual Purpose

The user needs to store information about a sample. The sample is generally provided by the user's client and the client often wants to learn something about it, what it looks like at a micro level, how are its elements arranged, what is it's make up, what are its properties, how will it behave in a certain circumstance. The user needs to enter certain information about the sample, for example, it's dimensions, where to scan on the sample, a possible centre point for calibration, images taken, analysis techniques to try on it, its location, its shipping date and receiving date. The sample will be associated to one or more projects and to one or more experiments. Image scans and analysis data produced from the sample must be within the system associated to the sample.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Associating sample to project
- Associating sample to experiment
- Creating business object

Process

Pre-conditions

The project in which the sample is to be added exists.

User intentions/System responsibilities

User Intentions	System responsibilities
  2. User chooses to create a sample. 4. User fills out sample form 6. Optionally, do assigning sample to project	1. System provides choice of objects to create. 3. System creates new sample and responds with a new sample form 5. System validates, saves form and confirms action 7. System validates, updates association and confirms action

Creating person

Contextual Purpose

A person in this system is a user of the system. A person will have a role in the context of a project. For example, person A may have the Team Lead role on Project A but the Scientist role on Project B. A person object is required for authentication, to logging into the system and verifying the user. The person role is also used for authorization. Different roles (and the users that have these roles) are allowed to do different things on the system. For example, at one point, creating a person on the system may only be done by a person that has the Scientist User Team Lead role on the current project.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating business object
- Adding person with role to project

Process

Pre-conditions

None.

User intentions/System responsibilities

User Intentions	System responsibilities
	1. system provides choice of objects to create
2. User chooses to create a new person	3. System creates a new person object and responds with a new person form
4. User fills out the person form	5. System validates, saves form and confirms action

Creating experiment

Contextual Purpose

A user needs time on a beamline in order to perform experiments using techniques which have been designed to solve a problem/question posed by a client. The experiments are part of a project generated by the user to solve the problem. An experiment is performed on a beamline during a beamline session. A project may have more than one experiment associated with it.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating business object
- Associating sample to experiment
- Running experiment
- Viewing experiment results

Process

Pre-conditions

User is within a project context.

User intentions/System responsibilities

User Intentions	System responsibilities
	1. system provides choice of objects to create
2. user chooses to create a new experiment	3. system creates a new experiment, associates the experiment to the current project context and responds with a new experiment form
4. User fills out the experiment form	
5. User chooses to associates samples to an experiment	6. system provides a list of valid (active) samples
7. User choose one or more samples to associate to an experiment	
8. User saves/submits experiment form	9. System validates, saves form and responds with confirmation

Defining the experiment

Contextual Purpose

The user needs to provide context for an experiment before starting it. This is to allow for automatic organization of the data that this produces. The user will define the experiment in the user proposal to the CLSUO in a request for beamtime. The experiment defines the type of beamline that will be used for the experiment. The defined experiment in the proposal allows for the peer review to determine the feasibility of the experiment. Also, the beamline scientist should see the defined experiment as the beamline scientist also has good knowledge to determine whether the experiment can be successfully carried out on the beamline. The types and numbers of samples associated with the intended experiment as well as the type of information that the user/client wants to obtain are outlined in the proposal. As well, the user should have some idea as to how much beamtime will be needed to carry out the experiment.

As well, defining the experiment will in the future allow the user to better collaborate and share information with team members.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Associating sample to project
- Associating sample to experiment
- Adding person with role to project
- Creating a note associated with a business object
- Changing experiment time (optionally supported)

Process

Pre-conditions

User picks an active project context

User chooses active person

User chooses active sample

User chooses active experiment

User is authorized to set up an experiment

User intentions/System responsibilities

User Intentions	System responsibilities
	1. System a list of projects
2. User picks a project as the context of their work	3. System validates request, set the project context, responds confirmation
4. Do adding person with role to project	5. system validates, executes and confirms with response
6. Optionally, do creating note associated with person added to project	7. system validates, executes and confirms with response
8. Do associating sample to project	9. system validates, executes and confirms with response
10. Optionally, do creating note associated with sample associated to project	11. system validates, executes and confirms with response
12. Do adding experiment to project (can be done when creating experiment)	13. system validates, executes and confirms with response
14. Optionally, do creating note associated with experiment added to project	15. system validates, executes and confirms with response
16. Do associating sample to experiment	17. system validates, executes and confirms with response
18. Optionally, do creating note associated with sample associated to experiment	19. system validates, executes and confirms with response

Associating sample to project

Contextual Purpose

To help organize the large amount of data generated from experiments using samples, it is important to be able to quickly navigate and find that information. For this reason, samples are associated to a project. Samples can be associated to one or more projects. Within a project, a sample can be associated to one or more experiments.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating project
- Creating sample

- Defining experiment

Process

Pre-conditions

None.

User intentions/System responsibilities

User Intentions	System responsibilities
	1. System provides choice of projects.
1. User chooses a project.	3. System indicates user is within the chosen project's context.
4. User adds a sample to this project	5. System responds with a choice of samples
4. User picks one or more samples to associate with this project	7. System updates the association and confirms action

Associating sample to experiment

Contextual Purpose

To help organize the large amount of data generated from experiments using samples, it is important to be able to quickly navigate and find that information. For this reason, samples are associated to an experiment. Within a project context, a sample can be associated to one or more experiments.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating sample
- Creating experiment
- Creating association

Process

Pre-conditions

User has access to a list of active experiments

User has access to a list of active samples

User has access to the control for associating samples to an experiment

User has authorization to modify the association.

The business objects to be associated exists

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses a project	2. System provides project context
3. User chooses a specific experiment from this project context	4. system provides experiment context

5. User selects to associate a sample to this experiment 7. User picks one or more samples	6. system provides a list of active samples associated with this project 8. system validates, updates the associations, and responds with confirmation

Adding person with role to project

Contextual Purpose

Adding a person with a role to a project will be used to determine who has authorization to perform some task on a project. Eventually, the user can use this association as an aid in collaboration and communication. The user will be able to view and access the project team and members will be kept informed of the tasks/activities assigned to them. Task assignments organized around projects allows for specific metrics.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating project
- Creating person
- Modifying business object

Process

Pre-conditions

None.

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses a project 3. User selects to associate a person to this project 5. User picks a person and role to associate to this project 7. Optionally user repeats steps 5 to add additional persons	2. System provides project context 4. system provides a list of active persons 6. system validates, updates the associations, and responds with confirmation

Creating note associated with a business object

Contextual Purpose

Users are currently entering notes in their note books about many things associated with the experiments they are running. For example, why did they choose to use this sample? These explanations are hard to find after the fact but are very important explanations about why something was done.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Creating business object
- Modifying a business object

Process

Pre-conditions

User is authorize to attach note to business object

User has access to business object

User has the business object context

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses to add note to a business object 3. User fills out note form	2. system creates notes object and responds with the note form 4. system validates, updates the note object and responds with confirmation

Running experiment

Contextual Purpose

Once all the organizational information has been created, for example the project, associated experiments and samples, and the experiment's beamline session is ready, the user can now run an experiment. Note that the user defines the intended experiments to be run in the proposal but it is actually during the running of the experiment that the final determination and choosing of the experimental parameters is done. The running of the experiment is defined as setting up the experiment (determining and choosing experimental parameters) and then executing the experiment (starting (using a command) the experiment, viewing the raw data actively, processing the data and reviewing data, etc).

The Beamline Scientist and user will initially set up the experiment. The Beamline Scientist will align the beamline, making sure the beam is coming down the beamline and not blocked by anything so that there is good beam intensity/flux at the end of the beamline. The Beamline Scientist/user will centre the sample within the beamline and/or ensure that the beam is hitting the sample in relation to a reference coordinate system. This can be accomplished by placing a fluorescing sample (a phosphor) at the end of the beamline, along with the user's samples that are to be analysed. The x-ray source needs to be 'on' for this task. The position on the phosphor where the x-ray beam hits the phosphor sample lights up (fluoresces) and the user/beamline scientist can see this by using a camera to view the phosphor in the beamline. The user will then mark the position on the screen where the phosphor fluoresces as this is the x-ray beam position. The user now knows the x-ray beam position in the lab space and moves the sample into camera view. The user then moves the sample so that the sample area/ feature to be analysed coincides with the marked x-ray beam position.

During the setup procedure, the user will also choose the x-ray beam spot size (for the synchrotron case). The user will also set up the detector parameters such as exposure and readout times. Note [strongly] that experimental setup is generally an iterative process and the user may likely test certain settings before actually starting the experiment. The software for experimental setup should be designed to be a cyclic process as the user will test and likely modify certain parameters before starting the experiment. For example, the exposure time for the detector may be tested with the detector and x-ray beam on. If the exposure time is too high, the detector readings will be saturated (too much signal) and the user will have to use a smaller exposure time value.

Part of the setup process is determining the sample area to be analysed. The user may choose to do a single spot analysis or a line scan or an area scan. If a single spot analysis is chosen, then the sample spot is positioned to coincide with the marked x-ray beam position. If a line/area scan is chosen, then the user must determine the scan step size (the distance between analysis positions) in the x- and/or y-directions.

Once the experiment has been set up, the user is ready to execute (start) the experiment. This would involve pressing a key to activate the experiment. During an experiment, the devices all work as set or programmed, for example, the detector counts or collects data during the exposure time, the collected data is read and the channels emptied to get ready for the next analysis point, the stage motors then move the sample to the next analysis point (distance set by scan step size), and the detector is then activated to count, and so on. The user wants to actively view the data as it is being collected. The user may choose to process the raw data in parallel to its collection or have it processed once the experiment has been stopped.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Determining x-ray beam position in lab space (using phosphor)
- Changing beam spot size (changing slit position)
- Choosing detector parameters
- Choosing sample area for analysis
- Executing experiment
- Choosing data analysis (choosing data analysis algorithm) (optional)

Process

Pre-conditions

User is within an active project context

At least one person has been assigned to the project

Experiment date and time matches current date and time

User is authorized to run an experiment

Experiment has been defined with project and sample associations

Beamline is on and operational (detector is functioning properly)

Sample is in position

Test of beamline has been successfully executed

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses to run an experiment 3. do setting up experiment	2. system sends user the running experiment view 4. system validates, executes and confirms

	with response
5. do executing experiment	6. system validates, executes and confirms with response
7. do viewing raw data image	8. system validates, executes and confirms with response
9. do choosing data analysis (can also be done before step 5. so that data collection and processing run in parallel)	10. system validates, executes and confirms with response
11. do Viewing processed data image	12. system validates, executes and confirms with response
13. user reviews returned data analysis image	14. system validates, executes and confirms with response

Setting up the experiment

Contextual Purpose

Note that the user defines the intended experiments to be run in the proposal but it is actually during the running of the experiment that the final determination and choosing of the experimental parameters is done. The running of the experiment is defined as setting up the experiment (determining and choosing experimental parameters) and then executing the experiment (starting (using a command) the experiment, viewing the raw data actively, processing the data and reviewing data, etc).

The Beamline Scientist and user will initially set up the experiment. The Beamline Scientist will align the beamline, making sure the beam is coming down the beamline and not blocked by anything so that there is good beam intensity/flux at the end of the beamline. The Beamline Scientist/user will centre the sample within the beamline and/or ensure that the beam is hitting the sample in relation to a reference coordinate system. This can be accomplished by placing a fluorescing sample (a phosphor) at the end of the beamline, along with the user's samples that are to be analysed. The x-ray source needs to be 'on' for this task. The position on the phosphor where the x-ray beam hits the phosphor sample lights up (fluoresces) and the user/beamline scientist can see this by using a camera to view the phosphor in the beamline. The user will then mark the position on the screen where the phosphor fluoresces as this is the x-ray beam position. The user now knows the x-ray beam position in the lab space and moves the sample into camera view. The user then moves the sample so that the sample area/ feature to be analysed is moved to coincide with the marked x-ray beam position.

During the setup procedure, the user will also choose the x-ray beam spot size (for the synchrotron case). The user will also set up the detector parameters such as exposure and readout times. Note [strongly] that experimental setup is generally an iterative process and the user may likely test certain settings before actually starting the experiment. The software for experimental setup should be designed to be a cyclic process as the user will test and likely modify certain parameters before starting the experiment. For example, the exposure time for the detector may be tested with the detector and x-ray beam on. If the exposure time is too high, the detector readings will be saturated (too much signal) and the user will have to use a smaller exposure time value.

Part of the setup process is determining the sample area to be analysed. The user may choose to do a single spot analysis or a line scan or an area scan. If a single spot analysis is chosen, then the sample spot is positioned to coincide with the marked x-ray beam position. If a line/area scan is chosen, then the user must determine the scan step size (the distance between analysis positions) in the x- and/or y-directions.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment (setting up and starting experiment)

Process

Pre-conditions

User is within a current active project context

User is within an active project context

At least one person has been assigned to the project

At least one sample is associated to the project

At least one experiment is assigned to the project

At least one sample is associated to the project

Experiment date and time matches current date and time

User intentions/System responsibilities

User Intentions	System responsibilities
1. do choosing beam spot size 3. turning on/opening shutter to get x-ray beam 5.do determining x-ray beam position in lab space 7. do setting detector exposure and readout times 9. do positioning sample analysis area with x-ray beam spot position in the beamline 11. optionally, do testing experiment parameters by running analysis on sample spot 13. Reviewing raw data 14. Optionally, processing and reviewing raw data 16. If not acceptable, repeat from or modify	2. system validates, executes and confirms with response system 4. system validates, executes and confirms with response system 6. validates, calibrates the position of the sample and responds to user when ready with the coordinate details added to the experiment view 8. system validates, executes and confirms with response 10. system validates, executes and confirms with response 12. system runs test analysis using chosen experiment settings and sends collecting data view to user 15.system processes raw data using chosen algorithm

one of above setup steps.	17. system validates, executes and confirms with response

Aligning beam at beamline (done by beamline scientist)

Contextual Purpose

The Beamline Scientist will align the synchrotron beam at the beamline, making sure the x-ray beam is coming down the beamline and not blocked by anything so that there is good beam intensity/flux at the end of the beamline. In order to maximize the energy of the beam it must occasionally be aligned with the detector. This is done by moving the detector and slits. It is done by the Beamline Scientist before using the beamline. It is an optional step, done only when required.

This use case is out of scope of what we are prototyping.

Supported Roles

Beamline Scientist

Relationships

- Prior to running experiment

Process

Pre-conditions

Setting up experiment

User intentions/System responsibilities

User Intentions	System responsibilities
1. Aligning synchrotron x-ray beam at beamline.	2. system validates, executes and confirms with response

Determining beam position in lab reference space (using reference phosphor sample)

Contextual Purpose

Users needs to know where the x-ray beam is hitting the sample. This would be visualized by looking at an image from a camera. A fluorescing reference sample (phosphor sample) is placed in the beamline with the user's samples. The user moves the phosphor into position (into view of camera) and then opens the shutter to get x-ray beam (or in the case of the prototype which is an anode source, turns on the x-rays). The x-ray beam hitting the fluorescing sample will be bright (fluoresce) where the beam hits the sample and the user can see this and determine the beam position on the sample in the view of the camera. The user then marks the screen with cross-hair to represent the beam position in the camera screen view. It would be good to have the beam position in the center of the screen but this would necessitate moving the camera?

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment

Process

Pre-conditions

Phosphor sample has been chosen

X-ray beam is on

User intentions/System responsibilities

User Intentions	System responsibilities
1. User activates stage motors to move phosphor (fluorescing) sample into camera view. 3. user sees bright spot on phosphor sample which is the x-ray beam position in lab space 4. User marks this bright spot with forexample, cross-hairs, using the computer command	2.system validates, executes and confirms with response system 5. system validates, executes and confirms with response system

Positioning beam on sample (moving sample)

Contextual Purpose

Analysing the appropriate sample area within the sample may lead to the solution/answer to the problem, hence the user needs to be able to pin point on the sample where the beam will hit. The user may have already marked on the sample useful places to look.

If the sample is larger than the beam size, scanning the entire sample (in micron steps) would produce too many images to review. To be able to mark off an area to scan, either a line or box, will a useful enhancement.

Once the user has determined where the beam is on the sample, with the aid of markings (the user may have predetermined the direction and distance from the markings the sample is to be moved to get to the analysis spot), the user will move the sample so that the beam is on the sample spot/area that the user wishes to analyse.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment

Process

Pre-conditions

Do setting up experiment

Sample has been chosen

User is on the running experiment view

User intentions/System responsibilities

User Intentions	System responsibilities
	1. system provides the valid coordinates that can be entered (as calculated from the sample dimensions entered on the sample form)

Changing beam size (changing slit position)

Contextual Purpose

The size of the features that are to be measured on the sample will influence the beam spot size, i.e., small features require smaller spot size. Depending on the beamline, the flux available would also influence the spot size choice. The user chooses the x-ray beam spot size on sample from a list. The spot size depends on the beamline intermediate focussing slit size. Beam spot sizes are measured in microns.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment

Process

Pre-conditions

Do setting up experiment

Sample is chosen

User is on the running experiment view

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses to change the beam size 3. User chooses a beam size	2. system validates request and responds with beam sizes (slit positions) 4. system validates request, sets beam size and responds to user when the chosen slit position has been reached

Executing experiment

Contextual Purpose

After an experiment has been set up to run, the user is ready to execute the experiment, i.e., to start collecting raw data. When experiment setup is complete, the user would push "start experiment" to activate the experiment sequence. For XRF analysis, the x-ray source should be on and the detector is programmed to collect counts. The time for collecting counts is typically called exposure time. Then the detector needs time to read signal (called readout time). This is programmed using detector software. The stage motor then moves sample to next analysis position and the detector is activated, and so on.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment

- Setting up experiment
- Aligning beam
- Changing beam size
- Setting exposure duration

Process

Pre-conditions

Do setting up experiment

Hutch is closed and no one is inside

User is on the running experiment view

User intentions/System responsibilities

User Intentions Optionally at any time: do aborting scan	System responsibilities
1. Optionally, do positioning sample on beam. 3. Optionally, do picking spot line or scan area and do setting the scan step size 5. Optionally, do setting exposure duration 7. User opens shutters	2. system validates request, sends message to EPICs, handles response and sends back acknowledgment 4. system validates the request and confirms with response 6. system validates the request and confirms with response 8. system validates the request, starts the scan, responds to the user when scan has started. 9. system notifies user when scan complete and responds with either a link to the raw data image or the raw data image

Picking spot, line or area scan

Contextual Purpose

The user is in the process of setting up the experiment. The user moves the sample to the sample area to be analysed. If a single spot is chosen for analysis, then the sample spot is positioned to coincide with the marked x-ray beam position. If a line/area scan is chosen, then the user must determine the scan step size (the distance between analysis positions) in the x- and/or y-directions. The distance between analysis points is called the scan step size (in microns). In determining and setting the scan step size the user takes into account the size of the x-ray beam (spot size) and the size of the feature to be measured on the sample. There is more than one option for setting up line or area scans. One option is to choose the centre point of a line, or the center point of an area and then define the number of analysis points in the negative and positive sense of the center point. The analysis will start from the most negative point towards the positive end.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment
- Executing experiment
- Choosing sample area

Process

Pre-conditions

Do setting up experiment

Sample/sample area is chosen

Sample area line or area scan is chosen

User is on the running experiment view

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses single spot/line/area scan 3. Do choosing of step scan size	2. System validates the request, updates the experiment, and responds with confirmation 4. System validates the request, updates the experiment, and responds with confirmation

Setting scan step size

Contextual Purpose

The user is in the process of setting up the experiment. The user has chosen an area on a sample and has chosen to do a line or area scan. For the line or area scan, the user must determine the distance between analysis points in the x and/or y direction. The distance between analysis points is called the scan step size (in microns). In determining and setting the scan step size the user takes into account the size of the x-ray beam (spot size) and the size of the feature to be measured on the sample.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment
- Executing experiment
- Choosing sample area

Process

Pre-conditions

Do setting up experiment

Sample/sample area is chosen

Sample area line or area scan is chosen

User is on the running experiment view

User intentions/System responsibilities

User Intentions	System responsibilities

1. User sets step scan size.	2. System validates the request, updates the experiment, and responds with confirmation

Opening/Closing Shutter

Contextual Purpose

The user needs to be able to access the x-ray source during the running of the experiment, in other words, the user must be able to turn the x-ray source on and off. In the case of the prototype (anode source), the x-ray source needs to be turned on and off. For the synchrotron source, shutters need to be opened to get x-ray beam from the storage ring, down the beamline to the sample at the endstation, and closed when the x-ray source is not required.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist, Storage ring

Relationships

- Running experiment
- Executing experiment

Process

Pre-conditions

Do setting up experiment

Sample is chosen

User is on the running experiment view

User intentions/System responsibilities

User Intentions	System responsibilities
1. User communicates intention to turn on/turn off x-rays (open shutters/close shutters)	2. System validates the request, updates the experiment, and responds with confirmation

Setting detector parameters (counting time/exposure time and readout time)

Contextual Purpose

The detector settings need to be determined and set by the user. The counting or exposure time is the time during which the detector collects signal/data. This time will depend somewhat on the flux of the x-ray source. Too much signal (too high a counting time) will saturate the detector and too little signal (too small a counting time) will not yield good signal to noise ratio. The user may try some preliminary tests (exposure/counting times) to determine the best setting and the software should allow the user to do this before the actual experiment is run. The readout time is the time that is required to readout out and empty the detector channels. The detector channels need to be emptied before the next reading (data) is taken.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment

- Executing experiment

Process

Pre-conditions

Do setting up experiment

Sample is chosen

User is on the running experiment view

User intentions/System responsibilities

User Intentions	System responsibilities
1. User sets the exposure time and readout time in seconds for a scan	2. System validates the request, updates the experiment, and responds with confirmation

Choosing data analysis

Contextual Purpose

User receives raw data and needs to process the data in order to determine whether the raw data is acceptable and yields an answer/or part of the solution to the problem. If not acceptable, then the user may want to rerun the experiment using a different technique, or changing the parameters with respect to the technique, or by analysing another sample area. User creates process data by choosing a data processing algorithm and then activating the algorithm. The raw data may have been reviewed prior to activating the algorithm or the algorithm will have been pre-selected prior to starting the experiment so that the raw data streams in to the data processing environment.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Running experiment
- Executing experiment duration

Process

Pre-conditions

Raw data image exists

Plot analysis has not been done

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses a raw data image	2. system validates request, retrieves image and responds with image
3. User chooses a point on the image for a plot	4. System validates the request and determines that plot analysis does not exist for point chosen
	5. system does plot analysis, generates and saves plot data

	6. system generates and saves jpg from plot data 6. system responds with confirmation when done (either with jpg of plot image or a link to the plot scan)

Viewing experiment results

Contextual Purpose

Once a scan has been carried out, the user will need to be able to view the results. They will be able to view the raw data image, be able to choose an analysis technique to apply to the scan (in this case a basic plot of a point on the raw data image) and view the results of the scan analysis.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Viewing raw data image
- Viewing processed data image

Process

Pre-conditions

Creating Business Objects

Defining experiment

Running Experiment

User intentions/System responsibilities

User Intentions	System responsibilities
1. do viewing raw data image 3. do choosing data analysis 5. do viewing processed data image 7. user reviews returned processed data image	2. system sends user the running experiment screen 4. system validates, executes and confirms with response 6. system validates, executes and confirms with response

Viewing raw data image

Contextual Purpose

The user receives a scan (raw data) and reviews it. If the scan is not acceptable the user may want to redo the scan and perhaps change some parameters. Or if the scan is acceptable, the user may want to send the raw data off for processing or send the data to another location such as the home institution.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Viewing experiment results
- Executing experiment

Process

Pre-conditions

None.

User intentions/System responsibilities

User Intentions	System responsibilities
1. User chooses a raw data image 3. Optionally: User chooses to see raw scan data	2. system validates the request, retrieves and responds with raw data image 4. system validates the request, retrieves and responds with raw scan data

Viewing processed data image

Contextual Purpose

The user receives the process data and reviews it. If the process data is acceptable, then the user may continue with other experiments related to the project; if not, then the user may want to go back to the sample and reanalyse it, perhaps changing the sample area or changing experimental parameters or by analysing a different sample area. If the process data provides an answer to the problem then the user may stop. If the process data does not provide an answer, then the user may want to redefine the project. The user may want to direct the process data to another location for storage.

Supported Roles

Scientist User, Scientist User Team Lead, Beamline Scientist

Relationships

- Viewing experiment results
- Viewing raw data image

Process

Pre-conditions

Do choosing data analysis

User intentions/System responsibilities

User Intentions	System responsibilities
1. User choose a processed data image or chooses point on the raw data image 3. Optionally: User chooses to see raw processed data	2. system validates the request, retrieves and responds with processed data image 4. system validates the request, retrieves and responds with raw processed data

6.0 BUSINESS MODEL

A business modeling discipline models the business context. It identifies and describes the business processes, business roles, business entities and the business rules. It is used to describe the business context of where the system fits in the overall business.

Business modeling was only touched on in this project. It should be expanded in subsequent phases.

6.1 INITIAL BUSINESS MODELING

The following represents some of the work in initially modeling the business problem space. In order to explore the business process, a Role-Process-Entity (RPE) diagram was developed. The following diagram describes how to read a RPE diagram.

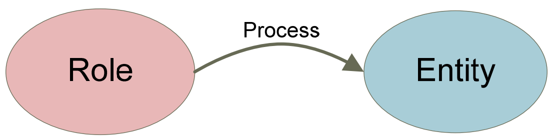

Figure 9: Role-Process-Entity Diagram Legend

Role

A resource, a person, system or device that is responsible for, or has some rights in regards to, some action (process) on entities

Process

An action a resource role carries out on an entity or the input required from another entity

Entity

A business object, for example a document segment within a document, a record in a database, a file in a file system, an instantiation of a class in an object model

The following RPE diagram describes a very high level view of the business user's managing their problem.

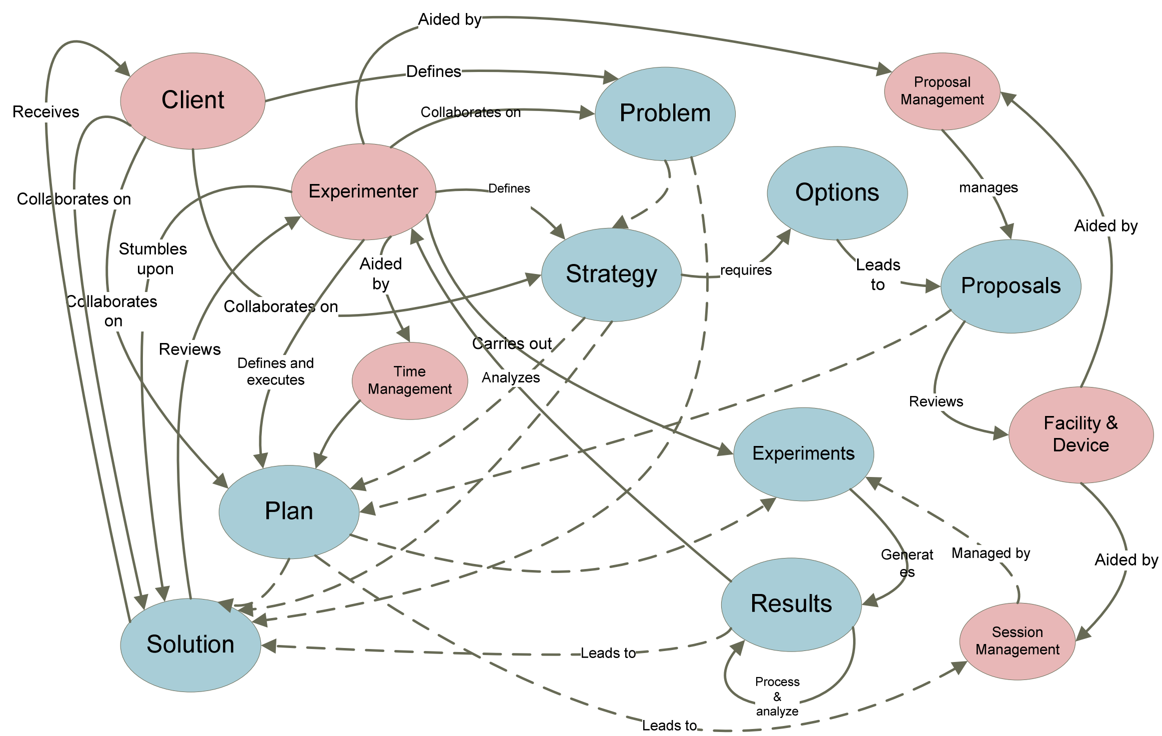

Figure 10: RPE Diagram Experimenter Manage Problem

An experiment (scientist), works on solving client problems. Together the experimenter's client and the experiment define a problem to be solved. The experimenter, often with the help of the client defines a strategy and a plan for solving the problem. This produces potential options which get narrowed down into one or more proposals to use scientific devices, like CLS Beamlines. Experiments are devised and scheduled to be carried to on a device. The experiment results are processed and analysed and may ultimately lead to a solution to the problem that is communicated back to the client. This generally produces a research paper. In order for the experimenter to manage the problem they need to take advantage facilities that contain the devices to run experiments, proposal management and session management for the scheduling of experiments on devices. A next step would be to understand these process areas.

6.2 INITIAL INFORMATION MODELING

Some initial work was done on information modeling. This will be used for the organization of the tree. The following tree structure is one proposed way of organizing the information. Note in the proof of concept, the task concept was not implemented.

Projects

<project name>

Persons

<person name>

Samples

<sample name>

Images

<image name>

Experiments

<experiment name>

<scan point 1>

Tasks

<task name>

Sessions

<session name>

Samples

Images

<image name>

Experiments

<experiment name>

<scan point 1>

6.3 BUSINESS RULES

6.3.1 General Object Rules

The following diagram shows the relationship between some of the main business objects.

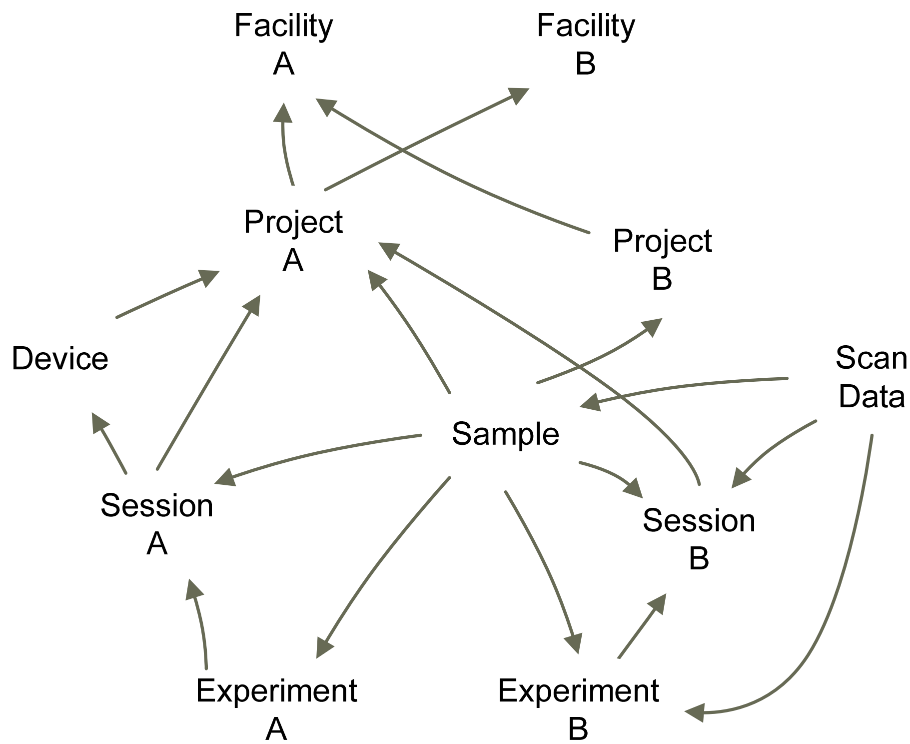

Figure 11: Relationship between the main business objects

The following describes some of the general relationships rules:

- Projects can be associated to multiple facilities. CLS is an example of one facility.
- Sessions can be associated to only one project.
- Experiments can be associated to only one session (current definition. This may change in the future).
- Samples can be associated with multiple projects and experiments.
- A Scan is associated to one sample, one experiment and one session context and one sample area
- A Project can be associated to multiple facilities, multiple Beamlines, multiple instruments
- People/roles are associated with Projects and Experiments
- A session can be associated to only one beamline

There are four roles in the system, system administrator, project lead, experimenter and observer.

System Administrator role

- can do anything to any object
- Proeject Lead of the Master project.

- Can create new users into the system

Project Lead role

- when user creates a project, they are automatically assigned the Project Lead role for that project
- can add any object in a project context
- can modify any object that belongs to a project that they are a member
- can delete any object that belongs to a project that they are the Project Lead for and the object is not linked to another project.
    - If object belongs to another project, deletion of the object will delete the object link to project where the delete was initiated.
- can add project roles to a project.
- can belong and be project leads of multiple projects
- eventually when implemented (not in phase I), when any object is deleted, it is a logical delete not a physical delete.
- eventually when implemented (not in phase I), the project lead can review deleted associations and permanently delete from system.

Experimenter role

- identical to the project team lead role except that the Experimenter cannot view or permanently delete objects that have been logically deleted

Observer role

- can view all objects within a project they are a member of
- cannot modify any objects
- cannot delete any objects
- cannot add any object to an existing project context
- can create projects
- can belong to multiple projects

6.3.2 Person Object Rules

- Project Roles are always created within the context of a project
- People are assigned to roles within the context of a project
- At any time, a person may have one, and only one role within the context of a Project
- Persons can be associated to more than one project
- Within a project context a person can always be associated

- Person's have either an active or inactive status. The status is not used within the system at this time.
- A person has a location, currently online and offline. This location is reflected in the tree control by an icon or colour.

6.3.3 Project Object Rules

- Any user can create a project
- Once a project has been created, the project cannot be deleted
- The project's Project Lead and Experimenters can associate persons within context of the project
- The project's Project Lead and Experimenters can associate roles to team members.
- A project can have only one Project Lead, the person that created the project
- Project's have either an active or inactive status. The status is not used within the system at this time.

6.3.4 Sample Object Rules

- Samples can be associated with more than one project.
- Samples can be associated with more than one experiment.
- Samples are always created in the context of a project.
- A project's Project Lead or Experimenter role can create Samples.
- Sample's have either an active or inactive status. The status is not used within the system at this time.
- A sample has a location. The location can be one of the following: Home, CLS, Loaded, In View, In Transit, Unknown, Destroyed. The location is reflected in the tree control by an icon or tree control.
- A sample has a life indicator. The life indicator is either Ok or Done. The system does not do anything with indicator at this time.
- Samples will have a type. Type field is to be determined. Need placeholder for samples that can be partially placed in a beamline, for example powders.

6.3.5 Experiment Object Rules

- An experiment can be created by a Project Lead or Experimenter associated to the project.
- An experiment can be associated to only one project.
- Numerous experiments can be associated to one project.
- Creating and defining experiment(s) within the context of a project for submission of a proposal is a guideline to the CLSUO, BLS and peer review panel to determine the merit and feasibility of a project.

- Many devices and device parameters are indicated within the created experiment.
- During an active beamtime session, only one team member of the team at a time, may set/use devices remotely. Project Lead and Experimenters can assume command. The person with control must accept giving up control.
- The BLS may at any time interrupt an experiment during a beamtime session and send a message to the team lead that session has been interrupted with some explanation as to why.
- The parameters associated with devices may be changed/edited during setting up/running of an experiment.
- When running an experiment, the experiment must be aborted before changing any parameters.
- The same experiment (see definition) may be performed on more than one sample and more than one area per sample, however it is treated as a different experiment with a different experiment label.
- An experiment has the either an active or inactive status.
- An experiment has the following phases: setup, active running, stopped running, analysis, closed.
- Once a project has been closed, experiments may not be created.