Hochschule für Angewandte Wissenschaften Hamburg
Hamburg University of Applied Sciences

Bachelorarbeit

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Logistic integration of a paternoster rack into sample logistics for MX beamlines

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Faculty of Engineering and Computer Science
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Bachelorarbeit eingereicht im Rahmen der Bachelorprüfung

im Studiengang Produktionstechnik und -management
am Department Maschinenbau und Produktion
der Fakultät Technik und Informatik
der Hochschule für Angewandte Wissenschaften Hamburg

in Zusammenarbeit mit:

Deutsches Elektronen-Synchrotron (DESY)

PETRA III, P11

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22607 Hamburg

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Abgabedatum: 14.02.2024

Hochschule für Angewandte Wissenschaften Hamburg
Hamburg University of Applied Sciences

Zusammenfassung

Thorben Melson

Thema der Bachelorthesis

Logistische Einbindung eines Paternosterregals in die Probenlogistik für MX-Beamlines

Stichworte

Logistik, Warehouse Management, logistischer Prozessfluss, MX Beamlines, ISPyB, Paternoster, Softwarelösung, Datenbank, DESY, EMBL, PETRA III

Kurzzusammenfassung

Diese Arbeit umfasst die Implementierung eines neu entwickelten Logistiksystems für die Probenlogistik der MX-Beamlines an PETRA III ausgeführt. Der Schwerpunkt liegt auf der Entwicklung einer neuen Software zur Verfolgung der Lagerung der dewars, die an die Anlagen geschickt werden. Die allgemeine Handhabung der dewars und ihre Interaktion mit der Umgebung wird beschrieben und der Stand vor dem Projekt aufgezeigt. Anschließend wird die Entwicklung der Software und ihre Funktionsweise beschrieben. Zudem wird die Implementierung in das bestehende System empfohlen und der Bericht endet mit einer Schlussfolgerung und Vorschlägen für die künftige Nutzung und Entwicklung.

Thorben Melson

Title of the paper

Logistic integration of a paternoster rack into sample logistics for MX beamlines

Keywords

Logistic, Warehouse management, logistical process flow, MX Beamlines, ISPyB, paternoster rack, software solution, database, DESY, EMBL, PETRA III

Abstract

This report discusses the implementation of a newly developed logistics system for the sample logistics of the MX beamlines at PETRA III. The focus is the development of new software for tracking the storage of the dewars sent to the facilities. The general handling of the dewars and their interaction with the environment is described and the current state is shown. The development of the software and its functions are described. Implementation into the existing system is then advised and the report ends with a conclusion and suggestions for future use and development.

Acknowledgment

Firstly I want to thank Prof. Dr. Gärtner who gave me the opportunity to be part of this project and giving me the contact to the whole DESY and EMBL team.

Special thanks to Dr. Johanna Hakanpää for monitoring the whole project and the work for DESY. Additionally I want to thank her for the answers to many of my technical questions and the introduction to the whole research done at DESY, especially crystallography.

I want to thank the whole P11 team of Dr. Hakanpää who created a great work environment and helped me wherever help was needed. Especially Dr. Andrey Gruzinov and Olga Merkulova for the support on the programming of the software and Alexander Grebentsov for the help on the hardware side as well as Dr. Michael Agthe of EMBL.

Furthermore I would like to thank family and freinds for their support during the development of this diploma thesis.

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List of abbreviations

2D	two dimensional
API	Application Programming Interfaces
DB	Database
DESY	Deutsches Elektronen-Synchrotron
Door	DESY Online Office for Research with Protons
EMBL	European Molecular Biology Laboratory
EXI	Efficient XML Interchange
GUI	Graphical user interface
HAW	University of applied sciences
HDMI	High Definition Multimedia Interface
HTML	Hypertext Markup Language
IK system	German: Informations- und Kontrollsystem, Internal information and controlling system
IP-address	Internet Protocol address
IP65	International protection class 65
ISPyB	Information System for Protein crystallography Beamtime
IT	Information technology
JSON	JavaScript Object Notation
KB	kilobyte
KPI	Key Performance Indicators
MAC	Media-Access-Control
MXCuBE	Macromolecular Xtallography Customized Beamline Environment
PETRA	Positron-Elektron-Tandem-Ring-Anlage
P11	eleventh beamline for PETRA

QR-Code	Quick Response Code
RFID	radio-frequency identification
RS232	Recommended Standard 232
SQL	Structured Query Language
URL	Uniform Resource Locator
USB	Universal Serial Bus
USB-C	Universal Serial Bus Type C
Vue	pronounced “view”
WLAN	Wireless Local Area Network
XML	Extensible Markup Language

1 Introduction

DESY is a research centre that uses particle accelerators to study the structure, function and dynamics of matter. It is located in the west of Hamburg, in Bahrenfeld, and employs about 3000 people. One of the accelerators is PETRA III. It delivers hard X-ray beams to various research stations. The largest building for PETRA III is the "Max von Laue Halle". It has a single 300-metre-long concrete floor to minimise vibrations. In the research stations P11, P13 and P14 the X-ray will be used for macromolecular crystallography. This is the experimental science of determining the arrangement of atoms in crystals. Beamline P11, operated by DESY staff, operates in UniPuck format at cryogenic temperature (usual energy range of 6-20 keV) with maximum through-put of 30 samples per hour. Remote data collection is enabled and unattended workflows are under development. P13 and P14 are operated by EMBL. EMBL is a different institute using the infrastructure of the DESY synchrotron for similar experiments as the P11 team.

These beamlines require a new way of storing and managing the sample storage containers known as “dry shippers”. These are used to transport samples from different countries to Hamburg for experiments. A closer description can be found in chapter 4.1. Most of the samples have to be cooled with liquid nitrogen. This has to do with the fact that the dry shippers are needed to keep the samples cold during transport. Otherwise the samples might be destroyed. All three beamlines together have about 370 dewars per year with an average storage time of 5.5 days. On average five to six dewars are in storage at any time. Since the synchrotron is out of operation several times a year, there can be peaks of 36 to 45 dewars on site.

A new system with computerised management needs to be developed for storage and logistics. Samples must not be interchanged, as each requires a different treatment and procedure. In addition, the samples must be cooled with liquid nitrogen. Software is required to monitor the dewars within the facility. This software requires different stations to access the software and manipulate the status of the dewars in the databases. The aim is to create a logistics chain that minimises the possibility of human error.

2 Methodology

For the development of a new logistics system for the MX beamlines for DESY and EMBL, a project was initiated in cooperation between DESY and HAW Hamburg.

To get an insight into the general purpose of logistic systems, literature review is conducted. The general concept of logistics is provided in order to compare the concept behind the principles of the research facility with the concepts used in industry. After the brief introduction, a requirements analysis is carried out. It starts with a description of the current state of the logistics system. The analysis also explains some of the terms and concepts used in this thesis and by the people working at DESY and EMBL. This is followed by the identification of the requirements ordered by the different groups that may interact with the system. Special attention is given to the software environment.

The software is the main focus of the project. The development in the given environment is shown and the requirements for the software are shown. The hardware to implement the new software in the facility is selected and the implementation is described. A comparison is then made with logistic systems in the industry and the benefits are assessed. To conclude the project and its findings are summarized and an outlook is given.

3 Basics and definitions

To provide some background information on the basics of the different topics some terms are defined and explained. These are logistic concepts, warehouse management and some terms for the software environment.

3.1 Logistics as a concept

Logistics describes a systematic approach to optimizing the flow of materials and other goods. There are many approaches to the definition of logistics. The main part is the study of planning, organization and control of material flow systems. The focus on warehouse management is the "6Rs" of logistics. They describe the objectives of logistics. The "6Rs" are

- The right product
- At the right time
- In the right configuration
- In the right quality
- In the right location
- At the right price.

"Right" in the sense of these objectives is measured by the customer's assessment [ten Hompel & Schmidt, 2010].

Information is also an important part of logistics. Logistics systems need an information and communication system. Objects controlled by a logistics system are most of the time located far away and are often in motion. To manage every aspect of the parts in the system, a control system is needed. Another characteristic of logistics is to regard it as a whole system. Looking at many processes as one flow in a network. Depending on the objectives of the system within a network, functions should be narrowly defined. Thirdly, logistics deals with physical systems and processes. This involves the design and control of both technical and economic tasks. Logistics is therefore interdisciplinary by nature [Arnold, 2008].

Logistics systems can be divided into macro and micro logistics systems. Macro logistics systems describe the transport systems in a region or economy. This area is mostly covered by transport sciences. Micro logistics systems are the logistics system of a company made up of its subsystems. Transport, storage and handling processes [Arnold, 2008].

Within storage processes, technical aspects must be coordinated. Transport times are determined by storage space. In most storage concepts, parts are defined as different articles to optimize the transport routes. How long an item is stored is determined by the transport and production processes before and after storage. [Arnold, 2008].

The supply of machines and workstations and the handling of incoming and outgoing goods is a primary task of internal logistics systems. This includes of transporting goods within a logistics system for a plant or part of a plant. The way in which goods are handled leads to the creation and reduction of internal stocks. To record, manage and ensure access to these stocks at the required time, storage, buffer and warehouse concepts solve this task. [Arnold, 2008].

In today's ware flow several factors are leading to a supply chain. In some variants every element inside the supply chain is just dependent on the customer and the supplier. Minimal fluctuation in the beginning of a supply chain can lead to major fluctuation at the end of the chain. This is called bullwhip effect. To prevent this effect an information processing system is needed for an efficient supply chain management [ten Hompel & Schmidt, 2010].

3.2 Warehouse management concept

One of the most basic functions of warehouse management is the specification of the storage locations and the units stored in the system. In addition, the continuous optimisation of the system and some control mechanisms should be integrated [ten Hompel & Schmidt, 2010].

This includes the regulation and management of the available storage space. This is defined by the technical infrastructure, such as different shelves and racks, as well as the dimensions and carrying capacity of the storage locations. Warehouse management also includes the technical control of storage and retrieval as well as stock removal. This requires different status updates to organise the available space and capacity. The different storage locations and options therefore receive different options and statuses such as 'occupied' or 'available for ...'. This can be done as a manual system with different cards and papers or as a digital version of a warehouse management system [ten Hompel & Schmidt, 2010].

3.3 IK system

Internal information and controlling systems (short: IK system) process information needed for planning and controlling processes in a logistic chain. Different institutions can get information out of the system to plan their different operations like delivery dates or information of the execution. Information of the status of the items and their status in the logistic chain are also implemented in the IK system [Arnold, 2008].

For the implementation of a warehouse management system (or IK system) different options differ in the scope of

- their functionality,
- in their interfaces,
- in the required hardware,
- in the required operating systems,
- in their operating concepts,
- and the investment.

The decision on the right warehouse management system, or IK system, is largely tied to these parameters. Some of these parameters are difficult to specify for this project, as DESY and EMBL are primarily research institutes and not classic industrial companies [ten Hompel & Schmidt, 2010].

The classical structures of an IK system differ in two ways. One is the mainframe-based architecture, where the IK system runs on a server with a database or a client-server system. The mainframe-based architecture is visualized in **Figure 1**. In the second, a server is connected to different clients with specific functions running on different workstations. This is shown in **Figure 2** [ten Hompel & Schmidt, 2010].

In the mainframe architecture, all processes run on the central computer and are operated by terminals that do not have their own IK system functionality. In client-server systems, these processes are distributed in whole or in part to the intelligent workstations and the server is thus relieved. is thus relieved.

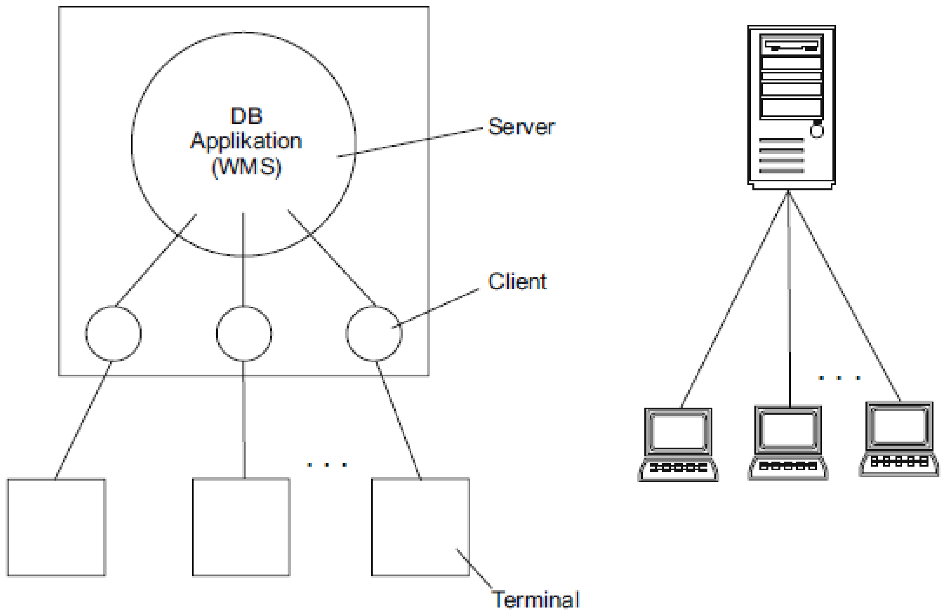

Figure 1: Mainframe based architecture [ten Hompel & Schmidt, 2010]

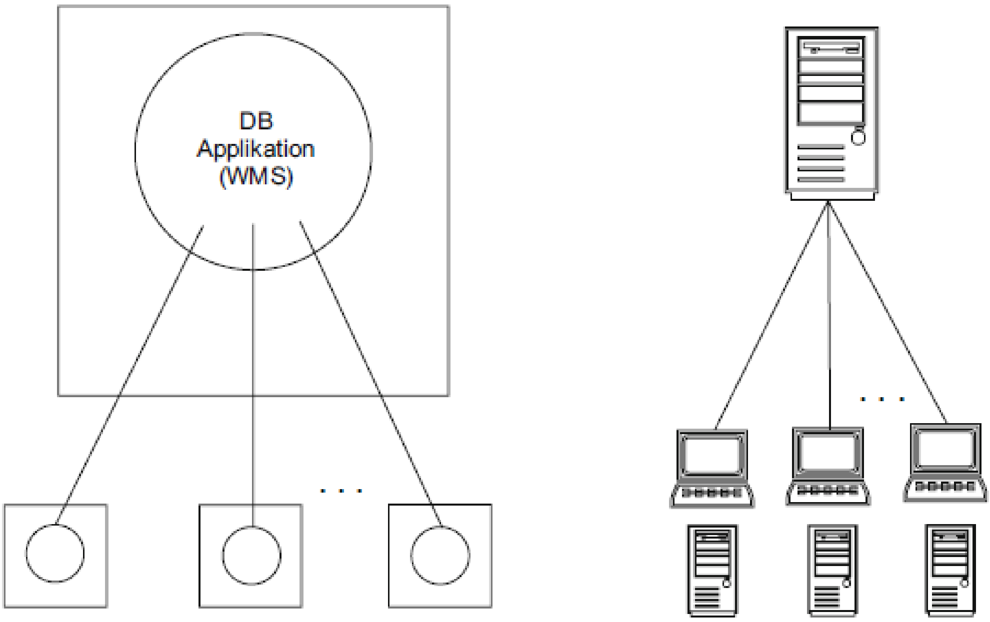

Figure 2: Client based architecture [ten Hompel & Schmidt, 2010]

3.4 Software technologies

To cover basics of software solutions of a logistic system in the following python as a programming language, Flask as a web framework, Vue as a client and MariaDB as a database are introduced.

3.4.1 Python

As a general-purpose programming language, Python can be used for web applications, scripting and other applications. It allows you to write clear and logical applications because of its consistent use of objects and object-oriented programming and its structuring. As well as important features such as the usual control structures and different levels of organisational structure, Python provides an interactive prompt, which makes learning Python and prototyping in python easier than for most other programming languages [Kuhlman, 2013].

3.4.2 Flask

Flask is a web framework for developing web applications. It is a Python module, it is a web application framework. As a web framework, it provides a collection of libraries and modules that help to develop web applications. Flask is therefore written in Python and is based on several toolkits. As a web framework choice, it's easy to get started with because it doesn't have a huge learning curve and it's very explicit for easy readability [Anemaet, 2024].

3.4.3 Vue

A Vue client is a client-side JavaScript web framework. It can be used without any build steps and can be used to create standard web components. These components can be embedded in any HTML page that the client can run itself. This makes it ideal for use with a browser. Vue is designed for building web applications but is not limited to a browser - it can also be used to build mobile or desktop applications [You, 2024].

3.4.4 MariaDB

MariaDB is a relational database created by the original developers of MySQL and guaranteed to remain open source. It provides the same APIs and commands as MySQL, but with additional features and storage engines. Prominent users of MariaDB include Google, Mozilla and the Wikimedia Foundation [Clark, 2013]. A relational database organises data into one or more data tables where data can be related to each other, these relationships help to structure the data. SQL is then used as the language for creating and modifying the database [Gilfillan, 2022] .

4 Requirements analysis

In the following part, the requirements for a new system are defined. First, an overview of the current status of the two institutions, DESY and EMBL, is given. This is followed by the requirements for a new system from a logistical point of view and user's feedback. Finally, all requirements will be prioritised and managed in different phases and categories for a new logistic system.

4.1 Current status

The two institutes handle incoming goods, called dewars, in slightly different ways. dewars are transport boxes that carry a dry shipper. As shown in **Figure 3**, they are about halfway filled with foam to protect the dry shipper and the samples inside. The dewars come with a delivery note for the transport company [Molecular Dimensions, 2023].

Figure 3: Dewar

As mentioned above, inside the dewars are the dry shippers. A picture is shown in **Figure 4**. Dry shippers can safely hold different materials at cryogenic temperatures. The dry shippers has absorbent material that allows the samples to cool down inside the dry shipper. The storage temperature in the shipping room remains at around -150°C until the liquid nitrogen has evaporated from the absorbent material. If the unit tips over, the absorbent material prevents the liquid from spilling out. The cold temperature is necessary to avoid destroying the proteins of the samples inside [Molecular Dimensions, 2023].

Figure 4: Dry shipper

A dry shipper can hold up to seven pucks, depending on the type of puck used. For the beamlines on the DESY campus, mainly UniPucks and SPINE pucks are used. UniPucks, seen in **Figure 5** being used mainly for the P11 beamline. The SPINE Pucks being used more for EMBL which are are shown in **Figure 6**. A dry shipper can hold up to seven UniPucks and four SPINE pucks. The pucks provide additional protection for the samples during transport until they are needed for an experiment [MiTeGen, 2023].

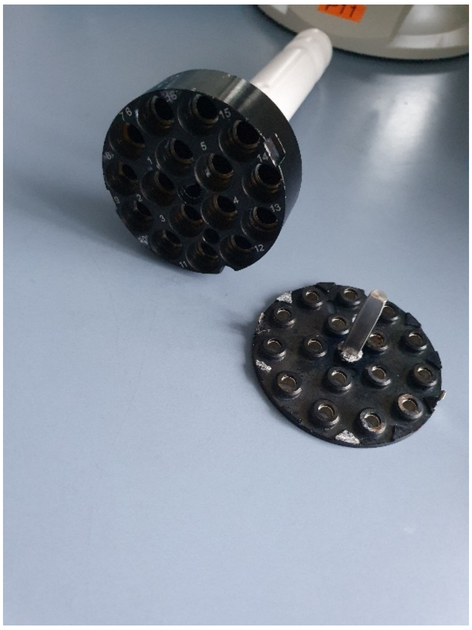

Figure 5: UniPuck

Figure 6: SPINE Puck [EMBL, 2023]

The different pucks can hold different numbers of samples. This might be an important note for future developments of the system. They are attached to a small sample holder that can be stuck into the pucks for transport. A sample holder is shown in **Figure 7.** The samples are atoms, molecules or proteins in some form of crystalline solid.

Figure 7: Sample holder

As previously stated, the two institutions handle the dewars in slightly different ways. Both institutions have a delivery point where the delivery companies can place the incoming dewars. The user’s office of the institution is then notified. The P11 staff at DESY has a digital delivery bell that can be pressed. This sends an automated e-mail to the team and the person in charge can pick up the dewar and process it further. In most cases, this is done by the employee in the user's office. As this person may be absent from the facility for various reasons, a local contact can take care of the dewars instead. A local contact is a scientific staff member who is the point of contact for the research team to which the samples are sent. They prepare the experiments and deal with any problems that may arise. There is no notification system like a delivery bell at EMBL. The user's office takes care of the dewars when they are notified by other means. This can be archived by the universities or by the delivery company in various ways. The EMBL user office has more staff, so they don't need the help of the scientists.

Once the dewar has been registered, it is stored in different areas. At P11 this is a rack in the experimental hall and at EMBL an area close to the beamlines. Dewar registration is tracked in different ways. EMBL has an Excel sheet where all incoming and outgoing dewars are registered and tracked. Communication with customers around the world who send their dewars is done by E-mail. The customers are called users because they use the beamlines or the service provides at the PETRA III beamlines. They just use the synchrotron for their experiments. An important part of tracking is the refill status of the dry shippers. As the liquid nitrogen can evaporate, it needs to be refilled every few days. Normally a dry shipper is filled when it arrives at the facility. If it stays longer than five days, it needs to be refilled to keep the samples cold. The P11 team has another solution for tracking**. Figure 8** shows a small, reusable card attached to one of the dewars. It contains all the necessary information, such as the date of the last refill or the name of the user. The name of the user is blocked due to privacy.

Figure 8: Tracking card

The time when the experiments with a particular sample take place is organised in another interface. When beamtime start, the local contact takes the dry shipper to the beamlines and prepares the experiments. The beamtime is the time the user has booked on the beamline for their experiment. When the experiments are finished, they take the dry shipper back to the facility's storage area. There they then are prepared for shipment. It is labelled with a new delivery note and taken back to the delivery point. Both deliveries are booked by the users.

It should also be mentioned that some users come to the site for their experiments. Some of them bring their dewars with them so that they don't have to be stored.

The shipments of EMBL are tracked via excel sheets. The user’s office tracks the incoming and outgoing dewar in this sheet to identify when which dewars will arrive and when they leave the facility.

4.2 Identification of requirements for the new system

As mentioned in **4.1 Current status** the most important information for the new system that need to be processed are:

- Name of user
- Arrival date
- Beamtime
- Refill status
- Location of the dewar

During the time between the arrival of the dewar and the actual beam time, the dewar must be stored in the facility and constantly checked for refill status. Due to the evaporation of liquid nitrogen, the liquid needs to be refilled every five days. In addition, the arrival of the dewar needs to be tracked so that all relevant people, the local contacts, the user and the user's office know that the dewar is at the facility and further tracking can be initiated. Prior to arrival at the facility, the delivery companies are responsible for tracking the shipment.

The storage space for all versions of dewars and dry shippers is the same because of their limited variety. The current storage facility needs to be replaced. The P11 storage rack is accessible to everyone in the facility. The EMBL storage rack blocks the building's escape routes. Therefore, a paternoster rack system, called “Dewar Hotel “, will be installed for both facilities. This needs to be integrated into the overall material flow.

To track the movement of the dewars, dry shippers and samples an IK system is required.

4.3 Requirement analysis

Information is gathered to process the needs and expectations of the people who impact the material flow and storage. This is then prioritised and organised by importance and workflow. The relevant persons are primarily classified as:

- The local contacts who handle the dewars within the facility between storage cycles and in preparation for beamtime.
- The user's office, which handles the dewars from the point of delivery to the storage location, as well as replenishing the dry shippers. They also manage the return shipment.
- The software engineers, because the IK system will be part of the software structure and will have to be maintained by the engineers themselves. The community of crystallography synchrotrons in the world is not large enough to hire external software companies.

Secondary, are industrial users. They differ from normal users in that their data needs to be processed differently. Normal users have no contact with the material flow within the plant.

4.3.1 Local contacts

The local contacts are responsible for preparing the samples for the experiments. They move the dewars around the facility and remove the samples from the dry shippers to prepare them for the experiments. After the experiments, they return the samples to the dry shippers for storage. The dewars are then ready to be returned to the users. For DESY there is a small additional task. The DESY user’s office is manned by only one employee. If this person isn't available, the local contacts stand in for them.

For the local contacts, the most important part of the supply chain is that the right dewar is available at the right time for the experiments. The user books the beam time and is responsible for the transfer to DESY. For the local contacts, all they need is that the dewar is in the storage area at the time they need to prepare the experiment and that they have the necessary information on the parameters for that experiment. After the experiment they return the dewars to the storage area. The important thing is that there is available space for the dewar. For the information flow, the generated data must be transferred to the users and the information about the successful experiment must reach each relevant person.

In conclusion the local contacts need the dewars to be in the right place at the right time in the right condition. They also need to know the parameters required for the experiment and which dewar is needed for which experiment.

4.3.2 User's office

The role of the user's office in the supply chain is to ensure that the samples are available to the local contacts at the specified time. They do this by liaising with the users to obtain information about the shipment of the dewars and their estimated time of arrival. Once the dewars arrive at the facility the user's office takes them to the storage location. After the experiments have been completed the user's office organises the shipment back to the user's facility. They prepare the dewars for transport and return them to the delivery company.

Once the dewars have been delivered by the selected shipping company, the local contacts take care of them. The first step is to refill the dewars with liquid nitrogen. As the samples need to be cooled with liquid nitrogen and the level of the liquid nitrogen in the dry shipper is unkown, the dewar is refilled on arrival. In addition, the dry shippers are emptied of liquid nitrogen prior to shipment. This is because the absorbent material in the dry shippers absorbs some of the liquid nitrogen to keep the samples cool. This is done because liquid nitrogen is a dangerous liquid that can cause cold burns if spilled during transport. However, some of the absorbed liquid nitrogen will evaporate after delivery, so replenishment is necessary. Users will be notified as soon as this process is complete. Another responsibility of the users office is keeping the liquid nitrogen in the dry shippers at a high level so that the samples don't unfreeze.

The main information required by the user's office is the estimated time of arrival of the dewars, the replenishment status while in storage and the shipment information. This information only needs to be provided as the users book the return to their facility themselves.

4.3.3 Software engineers

The part that the software engineers take in this project is a working IT infrastructure that fits into the existing and planned one. The software engineers are responsible for maintaining the existing IT infrastructure, so the interesting part for them is the IK system. Not only detailed documentation is required also integration with existing software is preferred. For example, a new software tool for the beamlines in MXCuBe. This software controls the parameters at the beamlines for the experiment and is able to start the experiments with these parameters. Since the IK system can and will also hold this information as a communication tool for the users, an interface between the IK system and MXCuBE is a good addition to the software environment.

Most synchrotrons in the world write and use their own software, because there aren't many synchrotrons in the world. It wouldn't be profitable for a software company to write software for just a few customers. Most synchrotrons develop software in collaboration with each other, so the software provided as an IK system needs to be easy to maintain and not expensive at all.

For the software engineers, it is important that the software is easy to maintain and that the data is accessible by other software.

4.3.4 External institutes and industrial users

As already mentioned, it is important to keep the samples cool, otherwise they would be destroyed. Most of the time the samples are unique and an important part of the users' research projects. If they are destroyed during the logistics chain, a lot of work is lost for the users. They also want their experiments done when they have booked their time and they want them done with their parameters and, more importantly, with their samples, not someone else's. As a small bonus, they want their dewars and dry shippers with their samples back.

Some industrial users demand privacy of their data. privacy is for industrial users a valuable asset. Therefore, the collected data and the user’s identity needs to be kept secure.

The most important interest for the external institutes, the users, is that the dewars are in the facility in time and ready for the experiment at the booked beam time. Delivery isn't the responsibility of DESY or EMBL, so the transfer and tracking within the facility is important for the logistical flow. The samples have to be in the right place at the right time for the external institutes.

4.3.5 Requirements management and prioritization

In conclusion the most important requirements of the mentioned persons are determined:

- Information which dewar is inside the facility
- Storage location of the dewar inside the facility
- Refill status of the dry shippers
- Time when the dewar is needed for the experiment
- Information which dewar belongs to which user
- Information on free storage space
- IK system for the process
  - Easy to maintain
  - Interface to other systems
  - Option to hide names of industrial users

All these requirements can be managed with the introduction of an IK system. The priority of these requirements is made by the requirements of Kano’s model of customer satisfaction. The model “(…) distinguishes between three types of product requirements which influence customer satisfaction in different ways when met.” [Sauerwein, Bailom, Matzler, & Hinterhuber, 1996]. The model is designed for customer satisfaction. In this case, the different groups of people interacting with the system are treated as customers for the purpose of prioritising requirements.

Must-be requirements need to be satisfied for the groups of people. Failure to meet these requirements will lead to dissatisfaction in the work environment and lead to a disinterest in this project.

One-dimensional requirements are most of the time demanded by the interacting people. Fulfilment of these will lead to satisfaction.

Attractive requirements have the greatest influence on the satisfaction. These requirements are not expected by the interacting people or expressed by them.

The requirements and the satisfaction can be visualised in **Figure 9**. The most important points of the different types of requirements are displayed in the figure.

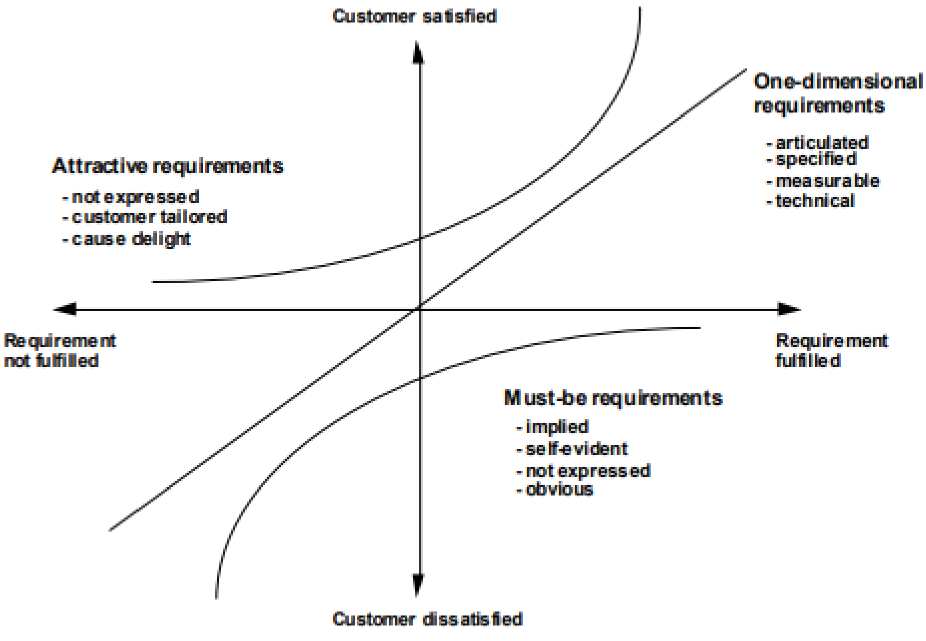

Figure 9: Kano's model of customer satisfaction [Sauerwein, Bailom, Matzler, & Hinterhuber, 1996]

The requirements of the different involved people are categorised by the three categories in Kano's model:

- Must-be requirements
    - Possibility to receive dewars

  - Possibility to send the dewars back
  - Possibility to run the experiments
- One-dimensional requirements
  - Location of the dewars
  - Refill status
  - Information which dewar belongs to which user
  - IK system
- Attractive requirements
  - Storage space inside facility
  - Connection of the IK system to other information systems

Most of the requirements for a new system are therefore met by an IK system. One important point is the refilling status of the dewars. This is because the samples are destroyed without the necessary cooling. As the samples are usually unique, destruction must be prevented, which means that tracking the refill status is essential. These requirements will be the necessities for the development of a new IK system.

5 System design

The design of the new IK system is handled along the workflow how the user's office and the local contacts will use the system in their everyday work. The system should be as insusceptible as possible to human error. The other part of the new system is the new workflow for the two institutes at DESY. To determine parameters for the new system a close look on the workflow is taken and decisions are made based on the necessity of new principles.

5.1 Material flow and design decisions

The Logistics Handbook: A Practical Guide for the Supply Chain Management of Health Commodities [John Snow, Inc., 2011, S. 144] suggests for designing a new logistics system "if it's not broken, don't fix it". The system established at DESY and EMBL has worked well in the past, but parts of this system will change in the future. One important aspect of these changes is the introduction of a paternoster rack, a storage device with movable shelves. The official name for this device by the manufacturer is "LEAN-Lift". The description in the institutes is "„Dewar Hotel“". It is necessary to have a new storage location for all incoming and stored equipment, as space in the experimental hall is limited.

Another reason for changing the logistics system was the susceptibility of the old system to human error. In particular, the tracking of dewars is mainly done manually on small cards attached to the dewars and is hardly digitized as seen in Figure 8. Implementing an IK system at this point is a great opportunity to minimize human error and have a system that manages all relevant information about the goods.

The status as it is in the beginning of the project is described in chapter **4.1 Current status**. In **Figure 10** the flow of the dewars can be seen. As prevously mentioned, EMBL and DESY follow their separate flows, but in the same order. That's because they are handling the same goods and the handling of the goods must be the same. There is a point in the diagram where both institutes follow the same path. On top of this part are the flow stations where the dewars leave the user institutes and are transported by the delivery companies. EMBL and DESY receive the dewars from many different locations in different countries around the world. The shipment can be booked with different delivery companies, which bring the dewars to the site in Hamburg. So EMBL and DESY get their deliveries from different carriers, but not from one in particular. To summarise them in one block, the figure shows them as used by both institutes. Further down in the diagram, the flow of dewars is split between the two institutes. The dewars are received at the institute's user office and then taken to the institute's warehouse. There the dewars are stored and refilled with liquid nitrogen to keep the samples cool. At the time of the experiment, the dewar is picked up and taken to the beamline. That's beamline P11 at DESY and beamline P12, P13 or P14 at EMBL. After the experiment, the material flow is reversed. The dewars are stored again, a return shipment is booked and the user's office hands them over to the delivery companies.

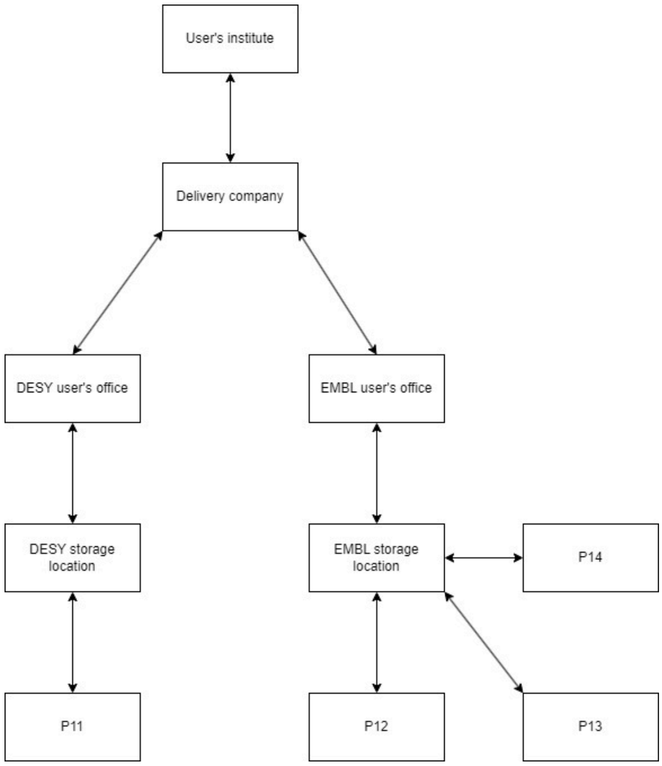

Figure 10: Dewar flow before the implementation of the „Dewar Hotel" [self-created]

For the new logistics system, three variables can be changed besides the implementation of a new IK system. One is the storage location. The current storage locations have shortcomings, characterised by limited capacity and inadequate safety measures due to the blocking of some routes that are designated escape and rescue routes. The new storage facility is ideally designed to address these issues and improve overall efficiency and safety. To this end, a new storage device, the aforementioned „Dewar Hotel", has already been ordered in advance for this project. The „Dewar Hotel" will be used by both institutes. When implemented in the material flow, the flow chart may look as shown in **Figure 11**.

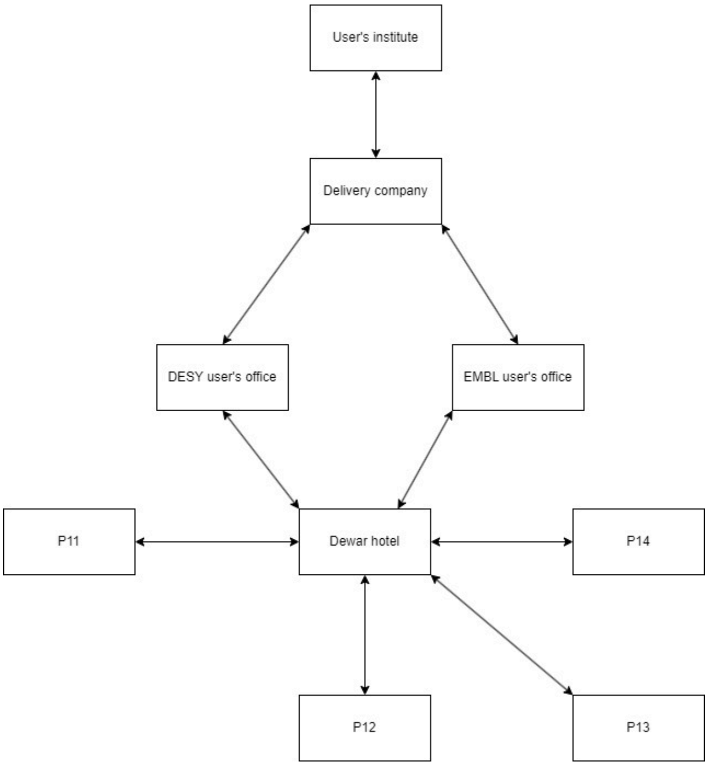

Figure 11: Dewar flow with „Dewar Hotel" [self-created]

The other things that looked at more closely if they are needed to be changed are the delivery companies and the dewar delivery points for the institutes. The dewars are delivered by a number of different carriers and are usually booked by the users who send them to Hamburg. To simplify the process and implement a tracking solution a user interface for the experiments and the delivery, the shipping could be optimised by just one delivery company. Diamond Light Source in Oxfordshire, England, uses DHL exclusively for the EU, Northern Ireland and the UK [Diamond Light Source, 2024]. They pay the delivery company to use them exclusively. The many advantages of this concept include the fact that the payment of the delivery company is difficult to arrange in Hamburg between EMBL and DESY. And the convenience for the users of being able to choose their own preferred delivery company. Therefore, an exclusive contract with a delivery company for Hamburg has been rejected for the time being.

The last point that can be changed is the delivery point. This is the point where the couriers deliver the items and where the institutes user office collects them. Both institutes have their own delivery point and it would be more efficient bring them into one delivery point. Since all the dewars go to the same „Dewar Hotel" the way the dewars are taken from the delivery point to the „Dewar Hotel" could be the same for both institutes. One risk of this concept is the unlikely possibility of dewars being swapped in transit. Each institute's user's office tracks and organises the shipments and dewars differently. The different workflows could lead to shipments being mixed up or some being lost in transit. This could be solved with the new IK system and new ways of communication. The other issue with this concept is the distance between the possible locations of the delivery points. **Figure 12** shows the distance between the current two delivery points for the two institutes, between these entrances to the building is no other option with enough space for another possible delivery point. The user offices are located close to their respective entrances. If one delivery point were to be moved to the other, one of the user offices would have to walk to the other entrance and carry the dewar to the „Dewar Hotel”. EMBEL's entrance (building 48e) is probably closer to where the „Dewar Hotel” will be installed. However, the problem of data management remains. Both institutes cannot and are not allowed to use the same IK system instance on the same servers. The data for the DESY experiments must be on the DESY servers and the same applies for the EMBL data. The data management for the DESY user's office would be unnecessarily complicated if the delivery point for the data would be the one in the EMBL building.

Figure 12: Distance between delivery points [Google Maps, 2024]

In conclusion, and to pick up on the quote at the beginning of this chapter, the only changes to the established system that make sense are the inclusion of the „Dewar Hotel“ in the logistics flow and the implementation of an IK system.

5.2 Selection of technologies and software solutions,

This part is dedicated to the different kinds of hardware and software solutions for the given problems and challenges. The „Dewar Hotel" was ordered by DESY in advance and the other solutions are presented, described and evaluated to justify the selection of these solutions.

5.2.1 „Dewar Hotel"

The „Dewar Hotel" was purchased from "Hänel Büro- und Lagersysteme". This is a German company operating worldwide in the field of automated vertical lift systems and storage carousels. The vertical lift ordered for DESY and EMBL is a "Lean-Lift" that will provide the Hamburg site with 32 dewar racks. The racks are designed to hold up to four dewars side by side on eight shelves. These shelves are moved by an electric motor to different heights inside the vertical lift to store the dewars. The shelves are deep enough to place the dry shippers in front of the dewars themselves for easy access. To illustrate this, the concept is shown in **Figure 13**. The right dewar has its dry shipper placed in front of it and there is space for two more dewars.

Figure 13: Dewars on a rack

The decision to implement the Lean-Lift was based on the space available in the Max von Laue Hall. The facility itself is crammed with all kinds of experimental hatches, experimental stations and other technical equipment needed for the experiments. There was only one space available for the Dewar lift and it was also limited by the ceiling hight and some stairs. One of the smallest models available had to be ordered. The final decisions was between two different sized lean lifts. Both are shown in **Figure 14**.

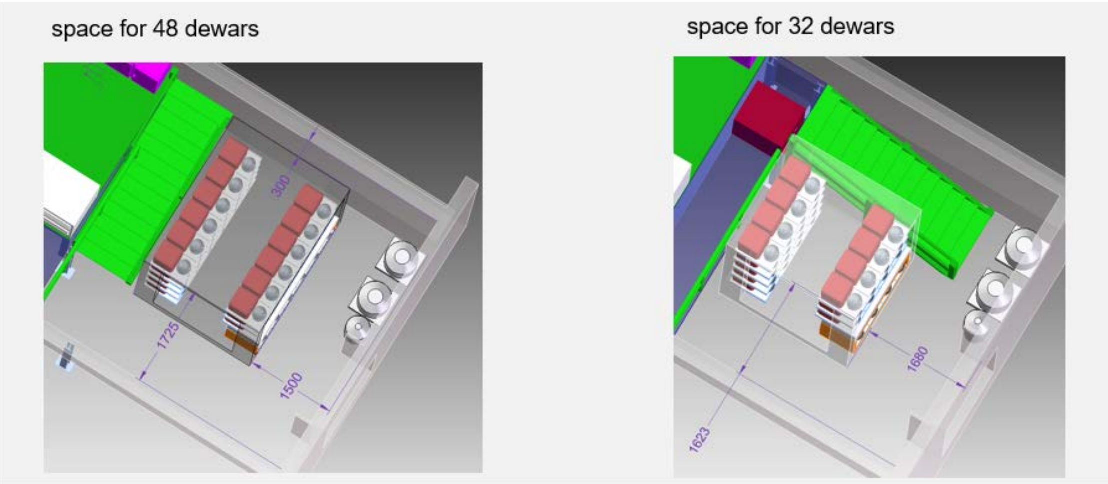

Figure 14: Different "Lean-Lifts" [Storm, 2022]

As seen from the drawings for the larger „Dewar Hotel" with room for 48 dewars, some adjustments had to be made to the interior of the hall. The stairs would have to be moved for the left solution and the upper balcony would have to be shortened. For the illustration on the right, apart from some minor hardware, everything would remain as it is, only the „Dewar Hotel" would be added. The decision was made to go with the smaller version because it was cheaper to order and didn't require any alterations to the building or its interior. [Storm, 2022].

5.2.2 IK system

The best and most convenient solution for an IK system was an extension to the existing ISPyB system, which was already in use or in the process of being implemented by DESY and EMBL. ISPyB is a laboratory information management system. It combines sample tracking and experiment reporting for synchrotron beamlines. It is developed and maintained by a collaboration of synchrotrons around the world. It allows users to easily register and categorise their samples for their experiments and to make the data available to the synchrotron research teams and the people who perform the experiments. One problem with crystallography is that it is a small field compared to the industry and most large companies. Most of the software used is written for the specific needs of crystallographers and their environment. In addition, because the field is so small and most crystallography teams in the world are just small parts of larger research centres, it is not financially viable to buy licences from larger companies that provide such software as a service, such as SAP SE.

The Diamond Synchrotron Light Source has developed an extension to the ISPyB system. ISPyB_logistics is an extension that uses the general structure of ISPyB for dewar management within the facility. The version used by Diamond Light Source is constructed for the environment they have in Oxfordshire and their software and server environment. For EMBL and DESY, some specifications and changes must be made. For example, Diamond Light Source and DESY use different types of user interfaces that communicate with the database and the software. However, both institutes EMBL and DESY, use the same version of ISPyB and the same connected software.

A simple way of using the software is suggested. In industry, most stock management is done via barcodes and scanners connected to a stock management system. The software for DESY and EMBL should be operated in a similar way. Barcodes and scanners minimise the possibility of human error when entering data into the IK system. These entries should be made at several points in the logistic flow. Compared to Figure 11, a revised concept is made. Scanner stations are planned for each relevant material flow between the different stations. This is visualised in **Figure 15**. Scanning stations are located at points where the status of the dewar is changed. The delivery company hands over the dewars to the user's institute. At this point the shipment is delivered and the dewars are in the facility. As soon as the dewars enter the facility, after the user's office has collected them, they scan them into the IK system to register them and store them in the „Dewar Hotel“. This is how the shipment is acknowledged. After that the dewar gets scanned when it is brought to the beamlines for the experiment. The system should then register the movement to the beamlines and the commissioning of that dewar. As soon as the experiment is done, dewar is brought back to the „Dewar Hotel“. There it is scanned in and waiting for the return shipment. All this should be represented in the warehouse management part of the IK system.

The scanning stations are designed to suit this purpose. This is described in the next section.

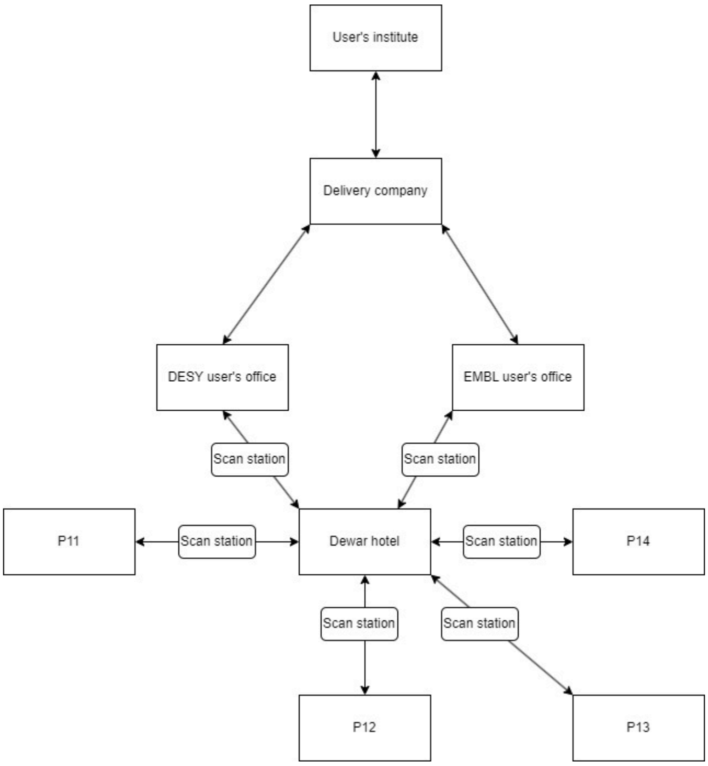

Figure 15: Dewar flow with scan stations [self-created]

5.2.3 Scan stations

As mentioned above, the scanning stations should be designed for the purposes mentioned and yet be as simple as possible. To keep them simple, they consist of just a monitor, a barcode scanner and a computer connected to the Internet.

5.2.3.1 Scanner

The environment in the Max von Laue Hall is quite dusty and the operators spend most of their time working with liquid nitrogen, which is used to cool the samples. The last point in particular suggests a durable solution for the scanners. They should not break from the possible contact with liquid nitrogen. The scanners should also be operated manually. Scanning labels for the logistics system need to be versatile, as there is no standardised way for users to attach the barcodes to the dewars. A static scanning station would require the heavy dewars to be placed in the correct position, while a hand scanner would only need to be moved. The scanner should be able to scan both regular barcodes and 2D barcodes (QR codes) as the software may use both and the regular barcodes may be changed to 2D in the future. To keep the connection to the chosen computers simple, a USB device is an easy option. Most of these connect to the computers like an ordinary keyboard, so the configuration is as simple as possible.

On all these points, the Datalogic PowerScan PD9630 is chosen. It is IP65 and IP67 rated and is able to withstand possible contact with liquid nitrogen. It is also able to scan both types of barcodes and can be reprogrammed if the requirements change [Datalogic S.p.A., 2024]. One of these scanners is shown in **Figure 16**. As seen the scanner is easily used by the operator since it only has one button to operate. It starts the scanning process by activating the optical sensors inside the device and transmits the information via a cable to a processing unit. For processing, the data transfer works like a keyboard input, so it translates the barcodes into a sequence of numbers and letters.

Figure 16: Datalogic PowerScan PD9630

5.2.3.2 Electronic data processing system

According to **chapter 6.2** the software can be controlled via a web interface. All the computer needs to do is run an internet browser and process the information from the scanner. . In addition, a wireless connection is recommended to reduce the cable management. DESY and EMBL have made their networks accessible via wireless communication. The ability to visualise a graphical interface is important for the processing unit. This is essential in order to display all relevant information to the operators and to be able to scan multiple codes.

A Raspberry Pis provide the needed functions. An example of a Raspberry Pi is shown in **Figure 17**. It provides a graphical interface with its own Linux-based operating system, they are also easy to set up and offer a wide range of features. Depending on the model either a HDMI or a mini-HDMI interface for connecting a monitor. It also has several USB-Ports as well as an USB-C Port to connect a power source to the devise. In addition, all third-generation Raspberry Pi models come with built-in Wi-Fi. [Tan, 2021]

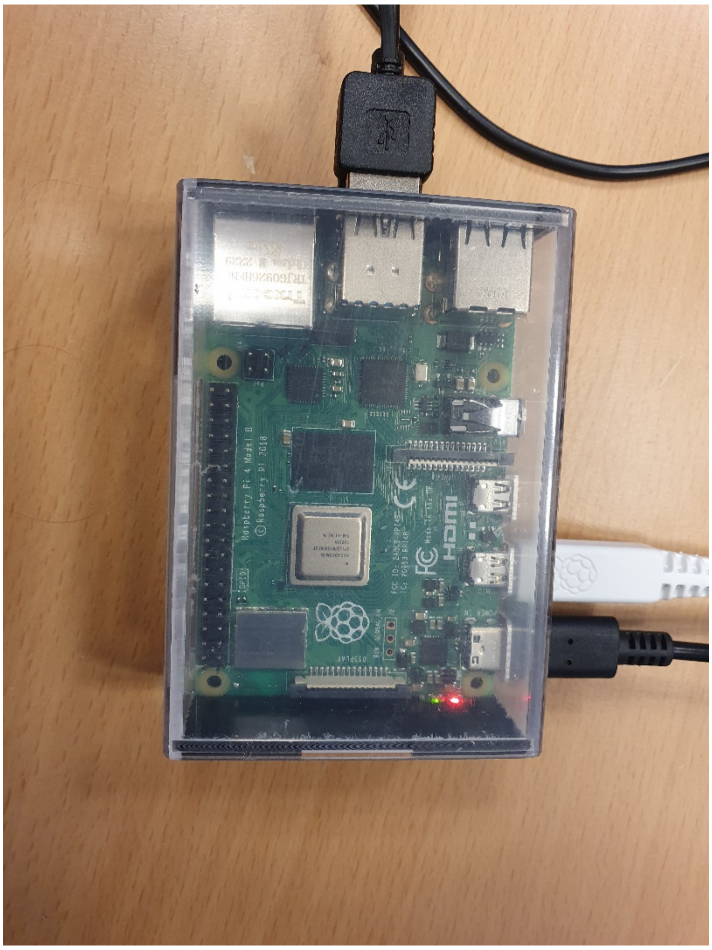

Figure 17: Raspberry Pi

6 Software development

This chapter describes the development of the software needed as the IK system. It starts with the decisions made and follows up with the architecture of the software and the interfaces used. After that the hardware requirements are displayed, and the safety considerations are discussed. In the end communication with other software is displayed.

The main component to be developed for this project is the newly implemented IK system. As discussed in **section 5.2.2**, the most suitable option is the ISPyB logistics developed by Diamond Light Source. The downside with this software is the environment in which it was developed. Specifically the user interface SynchWeb is a specification made for the synchrotron environment at Diamond Light Source. Many data processes work with this specific software. DESY and EMBL do not use this interface because it didn’t exist when ISPyB was implemented. They use EXI or EXI2 as a user interface which doesn't support many of the functions used by ISPyB logistics. Therefore it was decided to use the core part of ISPyB logistics, mainly the front-end part and to write a new back-end solution that fits the software structure of DESY and EMBL. Switching the user software from EXI to SynchWeb isn't an option for either institution because they had problems maintaining ISPyB themselves. DESY and EMBL had difficulties in finding software developers for this software, so that the implementation of some features was already problematic.

Figure 18 shows the software environment and parts of the material flow as well as some of the measurement hardware for the experiments for DESY. It shows the state of the system before the start of the project. Relevant for the project is only the software side that handles the transports and the materials involved. These are ISPyB, Door, the users and the shipments. The figure is used to explain some connections in the DESY environment. It shows the connection between Door and ISPyB as well as the connection between the samples and dewars with the software environment and the scientific measurement devices such as the Goniometer or MXCuBE.

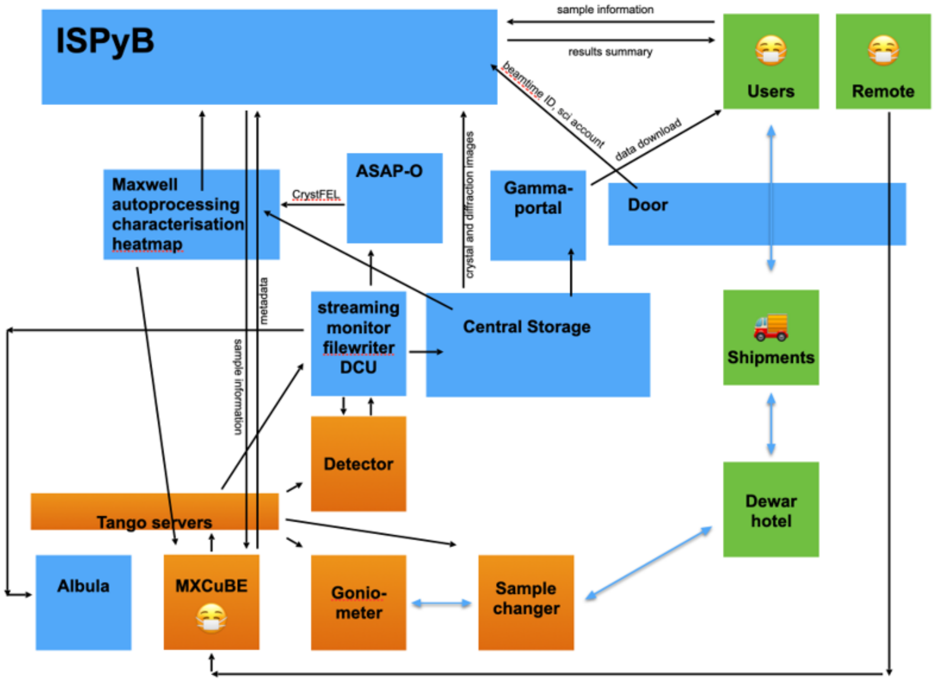

Figure 18: Software environment and material flow [Hakanpää, 2023]

6.1 Software architecture

ISPyB logistics is an extension for dewar management for the software ISPyB. It communicates with the main part of ISPyB by using the same database. It reads and writes information from the database and visualises them for the users. This works with several interfaces between the different structures and components of the program. For the modified version of ISPyB for DESY and EMBL a structure of that is shown in **Figure 19**.

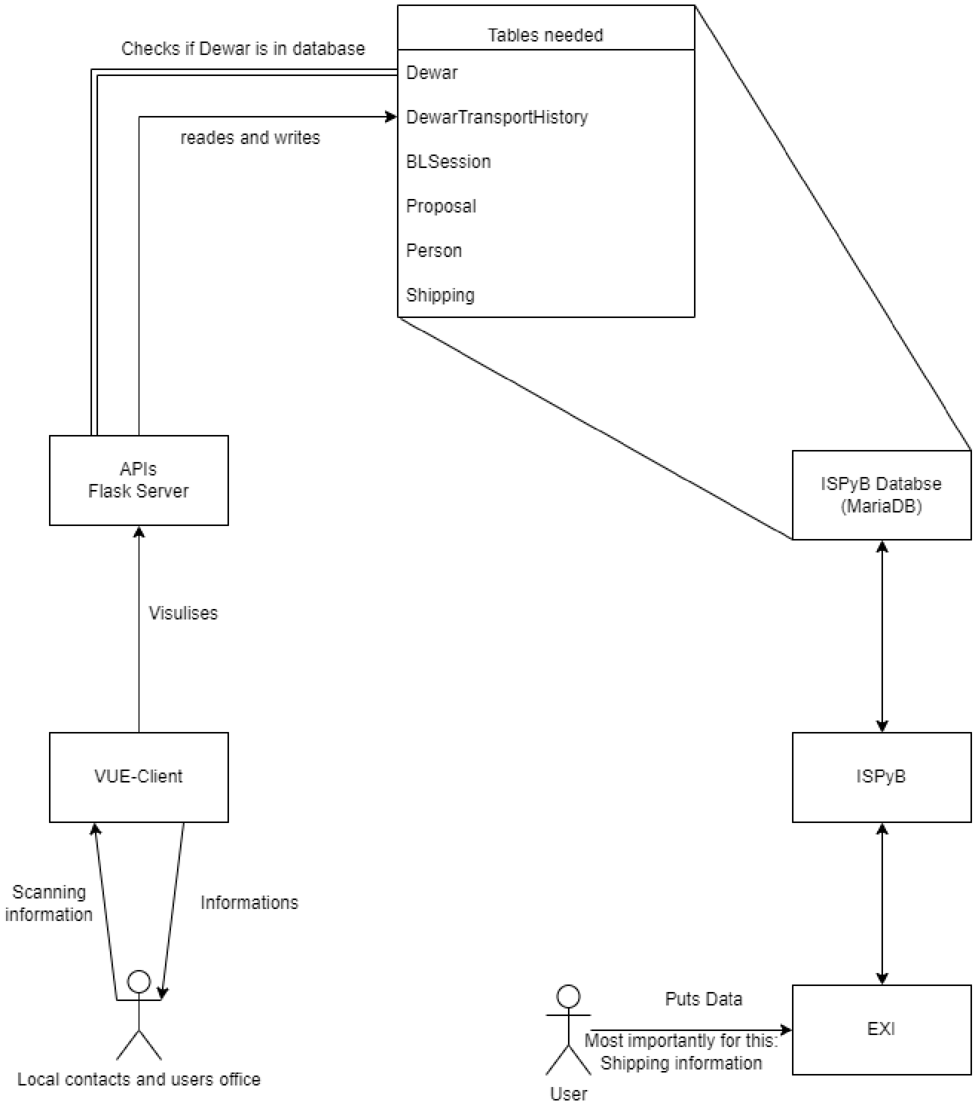

Figure 19: Structure of ISPyB logistics [self-created]

The information flow that was already established is seen in the bottom right area. The users use the EXI interface to provide the data for the experiment. The EXI interface is visualised as a web interface that can be accessed via the internet. The users first need to register themselves and their experiments in a registration tool to get access to EXI and book the beamtime. The tool is called Door where the users also register potential safety concern like toxicity or other safety concerns for their samples and evaluate the safety training for working on site. For EXI the users need their beamline ID given by door and they need their scientific account as shown in Figure 18.

EXI connects to the ISPyB system and its database. ISPyB uses MariaDB as its database system. It is a modified version of MySQL and uses similar tools to MySQL. Both are open-source technologies used by many algorithms and websites [Amazon Web Services, Inc., 2023]. They are used to store data in a tabular format with rows and columns. One difference is the support for storing JSON reports in different ways. MariaDB supports more JSON formats while MySQL doesn't. This is beneficial for the way ISPyB works, since it is written in JavaScript and how it interacts with its database. [Amazon Web Services, Inc., 2023].

As mentioned above the database is structured in tables. Each table can be filled with different information by ISPyB and other related software and websites. For the ISPyB logistics extension only a few tables of the whole structure are required. The required tables are shown in the box at the top of Figure 19. ISPyB logistics needs these tables for different information to work with the shipments. Most of them are used to validate the information progressed.

- Dewar
  This table holds the main part of the information on the dewars. It holds everything from the shipping identification numbers to a reference to the user of that dewar.
- DewarTransportHistory
  The entire movement of each dewar within the facility is recorded in this table. The moment the dewar is scanned into the ISPyB logistics system via a web interface the movement is recorded in this table. Each movement to another storage location and to a beamline is written to this table by the APIs. Therefore, a lot of information about the logistics system is stored in this table with the relevant time stamps.
- BLSession
  This table is mainly used to validate the user's existing beamtime and to validate the time of the experiment. If this information is not found, the dewar can't enter the experiment.
- Proposal
  The proposal table was needed to provide a link between different tables within the database. Some information could later be used in some functions to exchange information about the samples with other software directly at the beamline.
- Person
  To make the connection between the different tables such as Dewar and BLSession, the username is always required. This table holds information about the user who has sent a dewar to the facility. For some automation in the process, such as sending mails about the arrival of a shipment or giving users information about the status of the dewar via EXI.

- Shipping
  This table holds information about the shipment of the dewar via a delivery company and links this to the dewar. It is implemented in the code of the program for possible automated tracking in the future.

In order to use these tables from the database, APIs are required to provide various information between a user interface and the database. The database can be accessed by its own IP-address and port via the network. These APIs need to be able to periodically check the database for changes in the relevant tables. This has been solved at Diamond Light Source with the already mentioned SynchWeb software. Since this is not an option for DESY and EMBL, these APIs were the main part to be changed for the ISPyB logistics system for the two institutes.

To tackle this task, a Flask server was set up. A Flask server is a web framework written in Python. It can support dynamic websites and web services. The idea is that the user interface would run in a browser, making it accessible from anywhere in the network. The Flask server, like the database, is accessible via an IP-address. It connects to the database interacts with it as required. At the same time, the server frequently checks the database for changes that need to be displayed to local contacts and the user's office. Most of the APIs used by Diamond Light Source were not usable in the DESY environment due to the missing SynchWeb instance. The majority of the APIs are rewritten or adapted to the different software structure. However, some parts were necessary to adapt the software for the ordered „Dewar Hotel" and the different use of the ISPyB logistics. In addition, this whole structure and work enabled the possibility of future customisation and further interfaces for other software or control and processing units.

A Vue client was provided by Diamond Light Source to build the user interface for operating the programs. It is an open-source front-end system for building user interfaces. It is a command line interface that creates and manages Vue.js projects. These projects use the JavaScript library to visualise certain features written in their code. The client visualises specific information provided by the Flask server. It connects to the server via its IP-address and triggers the APIs when input is made to the interface. The main visual structure of various objects was taken from the Diamond Light Source version and adapted for DESY purposes. An example of the final version is shown in **Figure 20**.

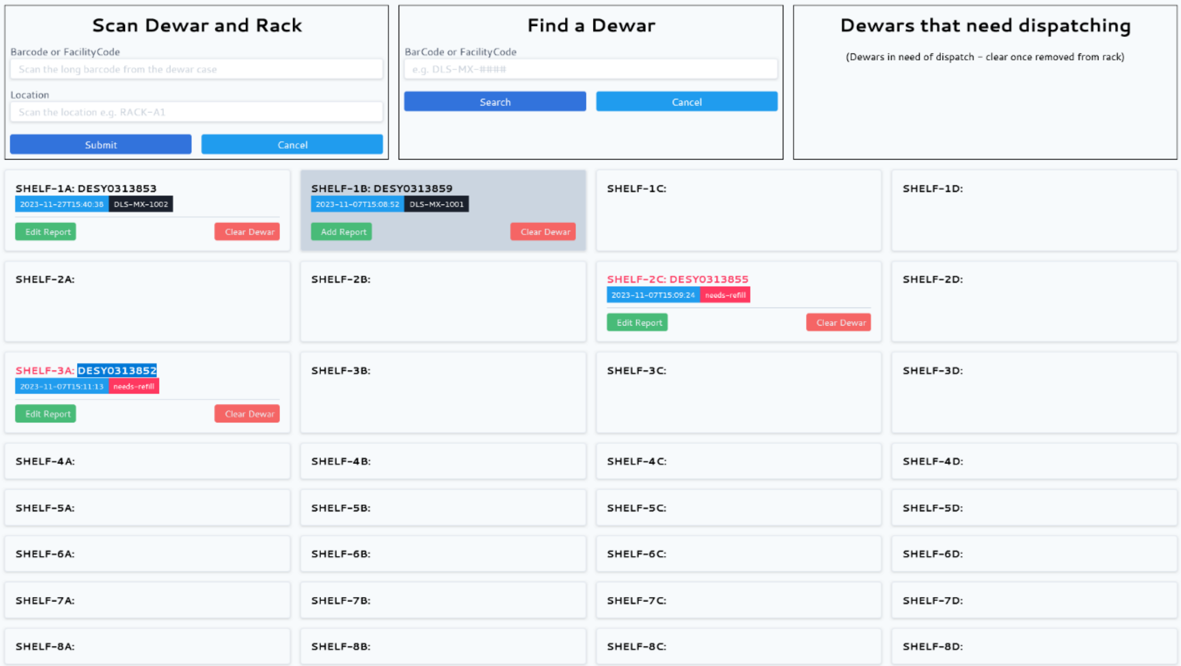

Figure 20: Screenshot of the ISPyB logistics dewar management interface

An additional feature running on the Vue client is the checking of the respective refill status of the dewars. As shown in Figure 20, some dewars are marked in red. The client periodically checks the status of the last refill via the flask server. This information is written to the database tables. If the time of the last refill is more than five days in the past, the dewar is displayed in red and the local contacts and people in the user's office can easily see the dewars that need to be refilled with liquid nitrogen.

All these different clients, servers and databases all run on a server. The architecture ist chosen to be centralized in contrast to be distributed. This reduces the risk of potential firewall errors while providing access to all in the network via the IP-address.

6.2 Interfaces

Different interfaces are needed to connect the hardware and the different software parts. To ensure good communication between the systems, most of this is standardised. This makes it easier to implement the environment and the system for the two different institutes. An overview of the different interfaces and ports used can be seen in **Figure 21**.

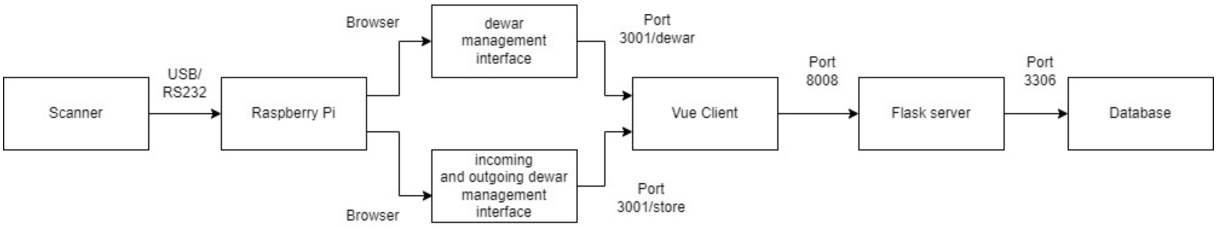

Figure 21: Interfaces and ports [self-created]

Most of the software interacts through ports and IP-addresses. As the regular ISPyB system is already running for the institutes, the IP-addresses have been set for the software and for the database. In order to keep the connections and configuration parameters simple, it is advisable to run the ISPyB logistics on the same machine as the ISPyB system. That insures the IP-addresses of both systems are the same and can be connected more easily without having to bypass EMBL or DESY security rules. However, all IP-addresses used by ISPyB logistics to connect to the different running servers and the IP-address of the database can be configured for different environments.

As shown in Figure 21, the connections are graphically visualised from the point where people interact with the system to the ISPyB database where all the information is stored. The interacting people use the scanners to interact with the IK system. The scanner is connected by a cable to a Raspberry Pi. This has either a USB port or a RS232 port but the USB port would be easier to use since it is the more common interface for cables today. The barcodes and QR codes needed for interaction are provided by the graphical interfaces, the information on the dewars or at different points in the facility, such as the „Dewar Hotel" for the different racks and locations. The Raspberry Pi is connected to the network and is able to access the various graphical user interfaces via a standard internet browser. These are either the Dewar Management Interface for the storage in the „Dewar Hotel", shown in Figure 20, or the Store Management Interface, shown in **Figure 22**. This interface handles incoming and outgoing dewars. It also provides the relevant QR codes for use with the scanners.

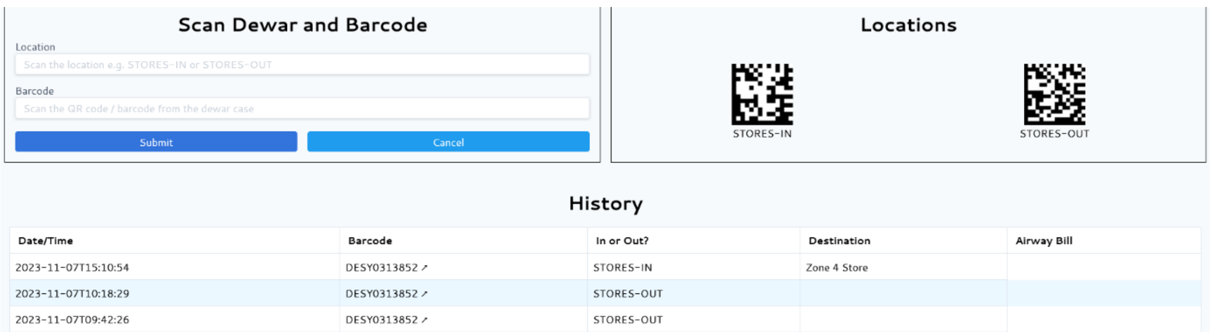

Figure 22: Screenshot of the ISPyB logistics store management interface

The different graphical interfaces run on the Vue client. The client runs on port 3001 with different paths for the different interfaces. The Vue client connects to the Flask server running on port 8008. The Vue client sends user input to the server as it is made and automatically checks for updates from the server every five seconds. The Flask server, on the other hand, checks the database for updates to the relevant tables every five seconds. When input is received from the Vue client, the Flask server makes an update to the database and immediately checks the tables for the new updates to serve to the GUI. The database runs on port 3306 and can be accessed by the Flask server on that port.

6.3 Hardware requirements

The hardware requirements for the various components and the server are minimal for this environment. The scanners have some requirements as they are used in an environment that is not as common. This is discussed in section 5.2.3.1. The requirements for the Raspberry defined in chapter 5.2.3.2.

The software itself is about 864KB in size and requires minimal effort to run. The only important thing for the software is the open ports in the firewall to connect the different running instances.

6.4 Safety Considerations

To access the network where the software is running, devices must be registered to access the instances running on the network. Therefore, the ISPyB logistics user interface can only be accessed by devices inside the network. The Raspberry Pis have to be registered with their MAC address via the network services and the IT staff of the different institutes. For DESY, for example, some forms have to be filled for the devices and the purpose of the device. Otherwise, the user interfaces can't be accessed. Access to other parts of the software environment is not possible via the GUI. The Raspberry Pis on which the user interface can be accessed are not password protected which should not be a security issue for the software environment itself, as the graphical user interfaces could simply tamper with the information stored in the database regarding the location of the dewars. In addition, the software always checks that the dewars have been registered in ISPyB via EXI and doesn't allow the use of different strings to those already registered in the system.

The software itself runs on a password-protected server instance that is only accessible within the DESY network. In order to configure and change the code, people need to have access to the network and the corresponding password for the instances on the servers where the software is running. At DESY, the software engineers and some higher-ranking employees have the password. With the firewalls provided by the institute's IT infrastructure, no external person should have access to the software.

6.5 Communication with other systems

Communication with other systems used by DESY and EMBL is an optional addition to the possibilities offered by the ISPyB logistics. Besides the already implemented in different software other communication might come into mind. The first is the MXCuBE software mentioned above which can be used to monitor and control experiments at the beamlines. MXCuBE uses ISPyB information that users have fed into the system via EXI. Therefore, some of the data generated by the ISByB logistics, such as the position of the samples in the different pucks, could be used. This part of the software used by Diamond Light Source can visualise this information directly at the beamline. MXCuBE can then use this data to bring the correct samples directly to the beamline via a robot to perform the experiments.

Another possible addition to communicate with other parts of the logistics system is the ability to control the „Dewar Hotel" via a web host interface. Depending on the accessibility of this web host, ISPyB logistics could interact with the „Dewar Hotel" and directly control the different racks to be present when the „Dewar Hotel" users use the scanners to interact with the software. This integration was out of scope for this thesis because software training by the company providing the software for the dewar hotel, Hänel, was not available until the end of the project.

7 Implementation

In order to implement the new logistics environment with all the new software and hardware, a rough schedule was drawn up at the beginning of the project. One of the difficulties is that the project was planned for a hardware engineering student with little experience of programming and coding and not as a full-time job. Students in Germany are allowed to work 20 hours per week besides their studies and additional tasks to be done for the student. Much of the planned time was spent learning the new programming languages and writing the code for the new IK system. The implementation was primarily made for DESY but could be adapted for EMBL later.

7.1 Planning and timeline for implementation

The mentioned schedule is shown in **Table 1** and then visualised in a Gantt chart in **Figure 23**. The important fixed date for this was the installation of the ordered „Dewar Hotel" between 16 October 2023 and 20 October 2023. The choice of this week was based on the time needed for the construction company to build the „Dewar Hotel" and it had to be in a shutdown week when the synchrotron beam was offline. Otherwise the construction work would have interrupted the ongoing work on the beamlines while the beam was up. The schedule of experiments on the beamline is made months in advance and could be changed. The demand for beam time is also too high to take the beamlines offline for an extra week. The schedule was adapted while the project was in progress.

Table 1: Dates for Gantt diagram [self-created]

Nr.	Start	End	Process
1	01.02.2023	02.04.2023	Learning programming
2	05.04.2023	28.04.2023	Getting into the environment
3	01.05.2023	13.10.2023	Software development
4	01.10.2023	01.12.2023	Orders for hardware
5	16.10.2023	20.10.2023	Installation dewar hotel
6	23.10.2023	30.10.2023	Training on operation
7	01.11.2023	31.12.2023	Installation of hardware

As can be seen, the major part of the project time was spent creating the software. After the kick-off most of the time was taken for learning programming, getting into the environment and understanding how the software is working and then developing the software itself. The tasks, after the program was finished, were mainly planned for the hardware. Ordering the hardware through the university was planned with several months, as the process of ordering hardware through a state institution takes some time. The detailed implementation of all the different components is described in the next chapter.

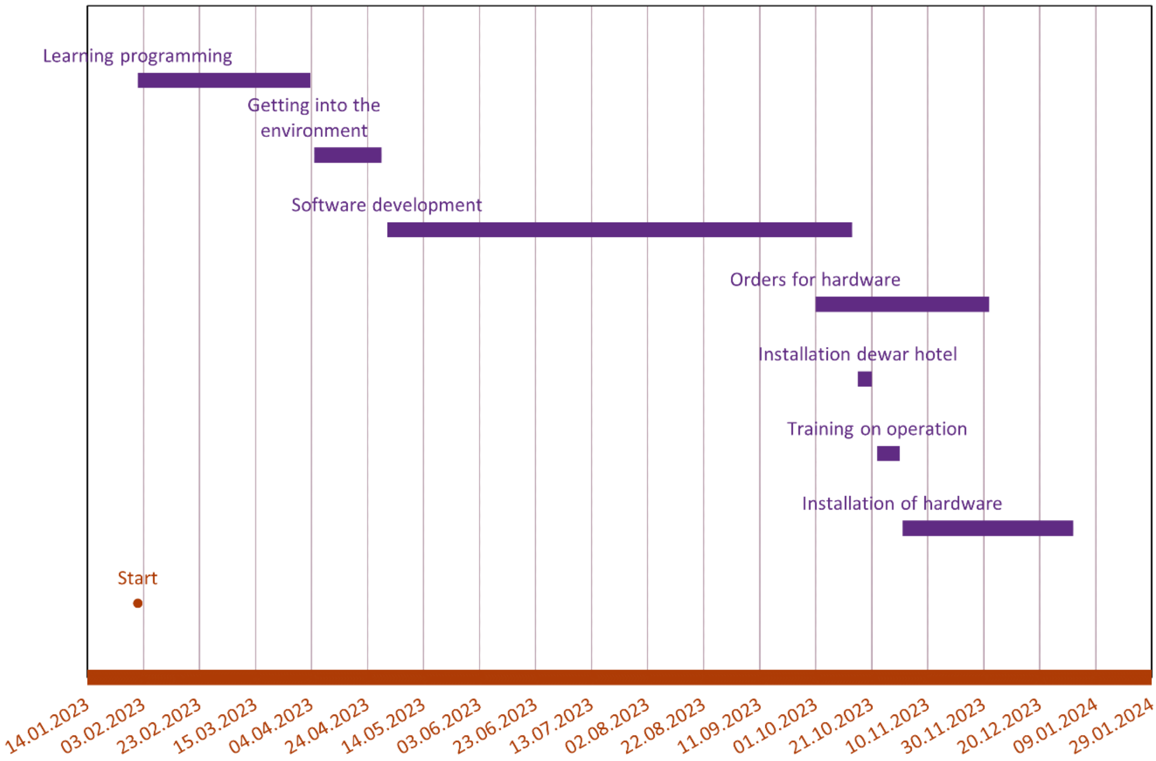

Figure 23: Gantt chart [self-created]

7.2 Step-by-step implementation

The project started on the 01 February 2023. The „Dewar Hotel" had already been ordered and the installation was planned for the week starting 16 October 2023. After a quick introduction week, the project began with learning a new programming language. The backend of the original software was written in Python, so it made the most sense to learn that language. This was done through several online workshops and tutorials. This took almost two months.

Once the basics of the language had been learned, the software environment of existing software such as ISPyB had to be taken into account. During this time, the original version of ISPyB logistics from Diamond Light Source was installed on DESY's virtual machines and prepared for adaptation. This meant that all necessary ports were opened and access to the other software was provided via different users and passwords. At this point, the software itself was able to run, but since the connection to the database was made through a software that was not used by DESY. The software simply responded with errors on every input and wasn't able to visualise the information from the database. Only the general interface was visual.

Programming of the new software then began. The process was not as strict as the Gantt chart shows, as the first coding attempts were made on the original software. The idea was to change a few small lines of code to bypass Diamond Light Source's SynchWeb software. After a few failed attempts, it was decided to rewrite the API server, leaving only the basic structure. This took up most of the project and wasn't finished until almost the end.

While the software was being developed, the first hardware orders had to be placed. First, a full sample of a scanning station was ordered to test if the hardware could meet the requirements. A monitor, a Raspberry Pi, a scanner and the necessary cables for the connections were ordered. The initial tests were promising, so the rest was ordered for the other scanning stations.

The week of the „Dewar Hotel" installation required some preparation. The area where it was to be installed had to be cleared and access secured. The best place to deliver the parts for the „Dewar Hotel" was to the north of the Max von Laue Hall. There wouldn't be any stairs in the way. However, there were still about 300 meters to go to the „Dewar Hotel" construction site. During the first few days of construction, some adjustments had to be made to the building. Some threaded rods were drilled and glued into the floor and ceiling. The ones in the ceiling were to help with the construction. With the limited space to work in, it wasn't an option to use a lift or crane. Eyebolts were screwed onto the screws in the ceiling. The rods in the floor were required by the DESY building department. In order to limit the vibrations of the „Dewar Hotel" and to avoid disturbing the experiments, the „Dewar Hotel" had to be mounted on the cement floor. With these adjustments, construction was completed by the end of the week.

After the construction was completed, a week was spent training DESY staff in the use of the „Dewar Hotel". The construction workers from Hänel showed some of the staff how to use the „Dewar Hotel". The rest of the staff still needs to be trained in the use of the „Dewar Hotel". The new unit took up space that had previously been used to store some of the dewars that were now missing. Even though the whole new logistics system hadn't been implemented yet, the „Dewar Hotel" had to be used immediately. Several training sessions were held on the new equipment and a basic manual to operating the „Dewar Hotel" was created until the rest of the system was implemented. This can be seen in **Figure 24**. Only trained staff were allowed to operate the „Dewar Hotel".

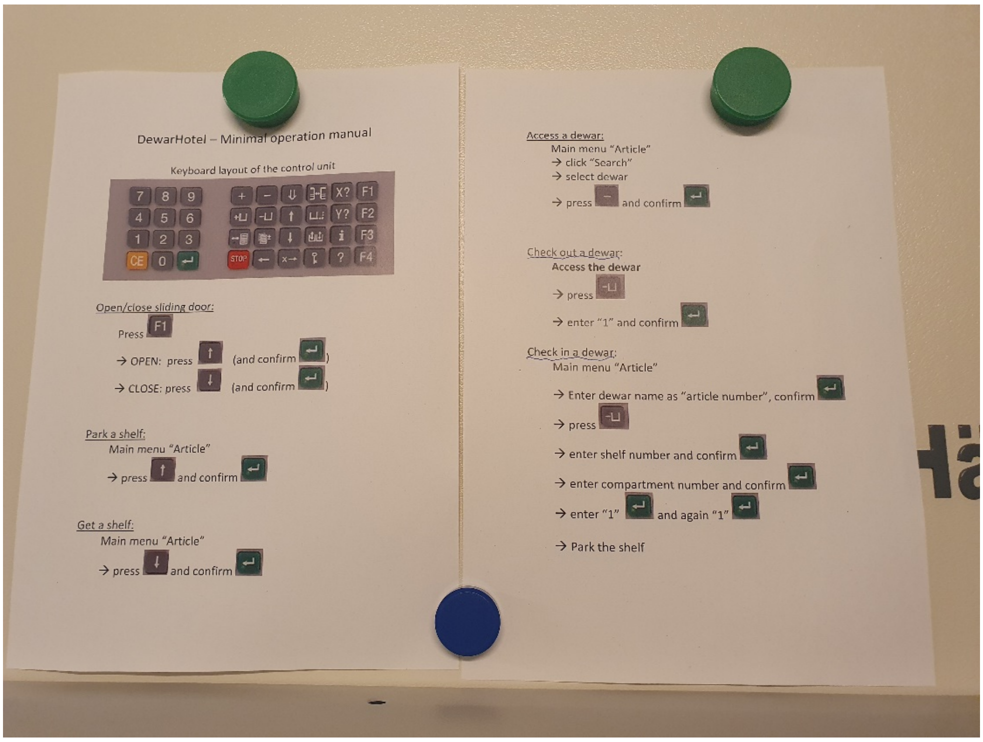

Figure 24: „Dewar Hotel" manual

Once the „Dewar Hotel" was implemented into the day-to-day operations of the staff, the scanning stations were configured and ready for use. The Raspberry Pis were registered on the network and configured to show one of two different user interfaces on startup. This made it easy to access the ISPyB logistics if the Raspberry Pis somehow lost power. Two of the computers were configured to display the ISPyB logistics store interface, as shown in Figure 22. The remainder were configured to display the Dewar Management interface as shown in Figure 20. The store interface was only needed to register the dewars in the system, so two were needed for the two dewar collection points. One at the locations where the delivery companies would drop off and pick up the dewars coming in and going out of the facility and one for DESY and one for EMBL. The others were configured for dewar management. Unfortunately, due to problems with the two networks and servers, the scanning stations weren't up and running at the end of the project, but they were configured and ready to go. A configuration manual was produced and a user's manual for the operating staff of ISPyB logistics.

8 Comparison to logistic principles

This chapter compares the discussed and developed system with the principles presented in **Chapter 3**. Starting with the basic concepts of logistics principles and the concept of warehouse management concepts and ending with the developed IK system. The system for DESY and EMBL can be defined as a micro logistics system. It only covers the transportation, storage and handling processes inside one facility.

Starting with the basic concepts of the '6Rs' of logistics. Some of these objects are difficult to evaluate for a research institution, as the research institution differs from industrial companies, e.g. the profit-oriented motivation. In Germany, the funding of research institutions is mainly from the government and foundations. Nevertheless, the principles of the '6Rs' will be compared with the logistics concept before and after this project.

The points that haven't changed much in this project are that the product has to be available at the right time and in the right quality. The samples are sent by the external users to the research facilities in Hamburg, and they are still responsible for sending the right samples to the right place with a delivery company of their choice. The delivery must take place before the users beamtime starts, and DESY and EMBL don't have much influence on this. Arguably, the quality of the product can be determined by the correct parameters of the experiment performed on the samples, but this hasn't been changed in this project. Only the motivation to use EXI and ISPyB more bindingly, although the implementation of ISPyB logistics can make it easier to give the right parameters to the research staff.

The right quality falls into the same grid as this discussion. The quality of the samples doesn't really depend on the project. The new IK system helps to track the refilling status of the dewars, minimising the risk of samples being unfrozen and destroyed.

For the right product, better tracking of dewar storage minimises the error of taking the wrong dewars to experiments. Getting the right dewar to and from the correct place has also changed. With the new system, a new storage system has been implemented that merges the two storage locations of EMBL and DESY into one. However, the implementation of the new IK system helps, and the linking of a dewar and its samples to a barcode and the associated information in the database makes it easier to find the right dewar and bring it to the right location.

For the right price, the cost of the experiment and transport to the facility hasn't changed. Only the amount of storage space required has been reduced. The „Dewar Hotel" is able to store the dewars several metres high, so some of the space previously used for storage is now available for other uses. This may not affect the price of the product itself, but the overall use of space within the Max von Laue Hall. The fire regulations are fulfilled as the corridors are not full of stored dewars.

Transport times and routes have only changed slightly. For EMBL, the transport time hasn't changed because the „Dewar Hotel" was built in the previous storage area. For DESY, the total distance from the delivery point to the storage area has become slightly longer, but the distance to the beamline is almost the same. This negative point is outweighed by the positive aspects of the newly implemented system. The storage time hasn't changed. It is linked to the time of delivery and the time of the experiment, but the principle is the same as before the project.

The handling of incoming and outgoing products in the central storage area has changed for both institutes. The operators are the same as before. Only the information system and the control of the dewars have optimised in a more convenient way. The use of scanners and scanner stations directly at the various points makes handling easier for the user's office and the local contacts. ISPyB logistics is accessible from any browser on the network, so the handlers can make their inputs into the IK system via the scanner stations and get the relevant information and status of the dewars by accessing the system from any computer on the network. This helps with the handling of the dewars. This negates the bullwhip effect as much as possible. The logistic chain is monitored from the point of the dewar entering the facility until it leaves it.

Storage locations are defined specifically for the warehouse management concept. dewars are standardised in size and weight. The „Dewar Hotel" and the shelves inside are therefore optimised for this standard. Theoretically, there is space for 32 dewars. This is more storage space than before and should cover the heated months for experiments. Another principle of storage management is to continually optimise the system. The ISPyB logistics system is designed to be expanded and optimised.

The developed IK system has a mainframe-based structure. Users interact directly with the system via an interface provided by the running system.

The decision for the newly developed IK system was based on the environment provided by EMBL and DESY. The easiest way was to use software that interacts with the existing software structure. ISPyB logistics is not affected by the different operating systems used by the users, only by the server on which the main framework runs. The software also works directly with the database used, which makes it easier to link the necessary parts. The financial investment was kept to a minimum. The student's development hours were paid for by the collaboration between DESY and HAW Hamburg, and the software itself is open source, like much of the software used by the research institutes.

9 Conclusion and outlook

The task for this thesis was to implement a new logistics system with a focus on a new IK system for dewar handling for EMBL and DESY. The new system was framed by the installation of the so-called „Dewar Hotel", a paternoster rack for storing the dewars while they are inside the facility. The centrepiece of this new logistics system is the newly implemented IK system. ISPyB logistics is an adapted and partially developed software for warehouse management, especially for dewar management for experiments at the beamlines for DESY and EMBL. It is implemented and communicates with the existing software environment. In addition, it tracks the parameters relevant for the storage and the refill status of the dry shippers inside the dewars.

A limitation of this study was the lack of explicit data to measure success and implementation KPIs. Most KPIs are defined by financial comparison or time spent on certain processes before and after the project. Both factors are difficult to analyse for this explicit case because the financial structure hasn't changed and time is not a critical factor for the defined area. A negative point is the unfinished implementation of the hardware. This limited the ability to conclude that the project was successful. A recommendation would be to reflect on the installed hardware and software after a few months.

A number of developments are possible for the future. The IK system is designed to evolve. It has the ability to communicate with ISPyB and therefore EXI. Automated emails to users on the status of their dewars and samples are a quality-of-life update for the user's office. An extension to track samples within the dry shippers is also possible. The pucks can be bar-coded or even tagged with an RFID chip for tracking [MiTeGen, LLC, 2024].With the right equipment, the information can be displayed in red and used directly at the beamline, even under liquid nitrogen. This helps in positioning the samples for experiments. The need to use two instances of ISPyB logistics for the two institutes could also be changed in the future. This is a discussion that is held on the level of security of the institutions. Direct control of the dewar lift or dewar lift interface is another improvement that could be implemented in the near future for further quality-of-life improvements. Users wouldn't need two interfaces at the „Dewar Hotel". They could then control the hotel via the ISPyB logistics interface or interact with ISPyB logistics via the „Dewar Hotel" interface.

In conclusion, the project has been a success for the development of the new warehouse management system. Instead of dealing with Excel sheets or paperwork for dewar management, the people involved are now able to use an extension of software. The tracking of dewar refill status helps to identify dewars that need refilling, greatly reducing the time spent searching for these dewars and minimising the possibility of samples being destroyed due to thawing. The logistical concept is primarily designed to facilitate the work of the user's offices and local contacts. The clearly defined storage area of the „Dewar Hotel“ and the additional storage capacity help to keep escape routes clear and to organise the handling and storage of the dewars.

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