Mass Spectrometer Interface

Desktop Application for Reading Instrument Data

Cousins Photosynthesis Lab in the School of Biological Sciences at WSU



**Team Linnaea Borealis**

****

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# Introduction

Plants play a crucial role in regulating the Earth's atmosphere by absorbing carbon dioxide (CO₂) and releasing oxygen (O₂). Understanding the factors influencing plant respiration rates is essential for addressing both past evolutionary patterns and future agricultural advancements. At Washington State University’s Cousins Photosynthesis Lab, researchers use gas chromatography mass spectrometry (GC-MS) to measure plant respiration rates through precise monitoring of gas concentrations. However, the proprietary software currently used generates excessive data and offers limited data processing or exporting, making analysis inefficient.

## Project Overview

The Mass Spectrometer Interface consists of five primary modules, each designed to address specific aspects of data analysis. Modules 3, 4, and 5 are the focus of this report and our attention, since modules 1 and 2 were complete products when we began work. We are still responsible for support for modules 1 and 2, patching small bugs.

### Module 3

Module 3 expands the functionality of the application by enabling isotope ratio analysis and plotting. It calculates the proportion of specific isotopes, such as ¹³C¹⁸O₂, and visualizes their trends over time. Additionally, it introduces a real-time derivative calculation of these ratios, providing researchers with insights into gas exchange dynamics during experiments. The graphical tools in this module allow users to dynamically manipulate scales and isolate key data ranges for precise analysis.

### Module 4

Module 4 addresses a critical need for compatibility with additional instruments. By converting raw data from a second mass spectrometer into a format that Modules 1–3 can process, this module ensures that data streams from multiple devices can seamlessly integrate into the lab's workflow. This enhancement not only improves interoperability but also future-proofs the software for the addition of new instruments.

## Development and Stakeholder Context

## Document Scope

This document provides a comprehensive overview of the **Mass Spectrometer Interface** project, summarizing its progress and technical details. It serves to detail our engineering efforts, including the design, implementation, and testing of key system components. By outlining our current progress, challenges, and solutions, the report captures the essence of our work on the alpha prototype, offering insights into the architecture, functionality, and stakeholder-focused goals of the project. This document also sets the foundation for future development by presenting our findings, demonstrating the prototype, and identifying areas for refinement based on feedback and testing outcomes.

# Team Members & Bios

Our team brings together a diverse set of skills and experiences, ranging from software engineering to data visualization and algorithm development. Each member contributes unique expertise and a shared commitment to delivering a robust and efficient data collection and visualization system.

Erik Holtrop is a dedicated computer science and mathematics student at Washington State University, where he is set to graduate in 2025. His academic journey has honed his skills in software engineering, algorithms, and mathematical computing. Erik’s technical expertise includes Python, C/C++, C#, SQL, and Haskell, along with experience in Python libraries such as MatPlotLib, PyEDA, and PyQT. His responsibilities include managing data structures, debugging, project management, and integrating mathematical algorithms into the system.

Kyler Kupp is a driven computer science student at Washington State University, aiming to complete his degree in 2025. He combines academic excellence with hands-on industry experience, having worked as a Software Engineer Intern at Monson Fruit Company. In this role, Kyler developed monitoring programs, automated reporting systems, and contributed to software managing critical production processes. His technical toolkit includes proficiency in Python, C#, SQL, and JavaScript, with familiarity in libraries like PyEDA and SFML. Kyler is responsible for UI/UX, stakeholder relations, and documentation oversight.

# Project Requirements Specification

When plants breathe, they take carbon dioxide (CO2) out of the air and replace it with oxygen (O2). Determining what affects plants’ respiration rate, or their breathing rate, is incredibly valuable data. These factors point backwards in time, reflecting causes for evolutionary trends, and forwards in time, providing opportunities to improve agriculture. We can use a mass spectrometer to measure this breathing rate. The mass spectrometer measures volumes of gasses, enabling us to see the flow of carbon dioxide and oxygen, and even different isotopes.

The Cousins Photosynthesis Lab in the School of Biological Sciences at Washington State University uses one of these mass spectrometers. These instruments are complicated devices, requiring complex calculations for calibration. The lab uses proprietary software from the mass spectrometer’s manufacturer, but that software outputs massive amounts of data over the course of a multi-hour lab, most of which isn’t needed. This problem has been partially solved with the creation of a Python desktop application, but this application is not perfect. Our task is to improve this application. This application currently faces small bugs, and only works for one instrument. The application is also in process of a UI upgrade. There’s also a few non-spectrometer instruments in the lab that are provide similar data, that would be easier to use if their data-streams were combined.

## Project Stakeholders

Our development process incorporates feedback from key stakeholders, including Dr. Asaph Cousins and the researchers in his lab. As academic researchers, they primarily value accuracy and usability. Our modules need to represent data accurately so that it can be used in academic studies, and it needs to be use-able by researchers from widely varying backgrounds, including a complete inexperience with coding. Focusing on this ease of use for non-technical users, the application uses Python, particularly the PyQt5 library for a robust graphical user interface. The ultimate goal is to create a tool that not only supports current research needs but also lays the foundation for future projects in plant biology and environmental science.

This project builds on prior capstone efforts, enhancing unfinished modules and introducing new functionalities such as multi-instrument data integration. By combining cutting-edge data analysis with practical usability, the Mass Spectrometer Interface will empower researchers to make meaningful contributions to the fields of photosynthesis and respiration research.

## Use Cases

The use cases below describe common scenarios of user interactions with the Mass Spectrometer Interface system, illustrating how various functional requirements are applied in specific situations. These use cases provide a clear understanding of how users will engage with the system's features to achieve their goals. The proposed use cases are visually represented in the use case diagram shown in Figure 1.

A screenshot of a diagram

AI-generated content may be incorrect.  
Figure 1: Use Case Diagram

**Use Case 1: Calculate Bicarbonate/CO2 Ratio**

|  |  |
| --- | --- |
| Use Case | Calculate Bicarbonate/CO2 Ratio |
| Actors: | Lab researcher |
| Pre-condition: | File path to data folder has been selected, and bicarbonate and CO2 have both been calibrated. |
| Post-condition | Bicarbonate/CO2 Ratio is displayed in decimal format. |
| Main Flow | * User selects data acquisition folder. * Starts plotting data. * Selects data segment. * Calibrates bicarbonate and CO2. * Selects calculate Bicarbonate/CO2 button. * Bicarbonate/CO2 ratio is displayed. |
| Alternative Flow | * If bicarbonate or CO2 have not been calibrated, display an error message and retry. |
| Related Requirements | FR-1: Calculate Atom Ratio  FR-2: Center Mean Bars |

**Use Case 2: Plot Derivatives**

|  |  |
| --- | --- |
| Use Case | Plot Derivatives |
| Actors: | Lab researcher |
| Pre-condition: | File path to data folder has been selected. |
| Post-condition | The Atom Percent and its derivative are fully plotted on their respective graphs. Alert user data has run out. |
| Main Flow | * User selects data acquisition folder. * Starts plotting data. * Data is plotted to each graph in real-time. |
| Alternative Flow | * Invalid data in acquisition folder. * User is prompted to select new file path. |
| Related Requirements | FR-3: Plot Atom Percentage  FR-4: Plot Derivative |

**Use Case 3: Convert Data**

|  |  |
| --- | --- |
| Use Case | Convert Data |
| Actors: | Lab researcher |
| Pre-condition: | File path to data folder has been selected. File path to output folder has also been selected. |
| Post-condition | The output folder has been populated with formatted data and the user has been notified by popup that conversion has finished. |
| Main Flow | * User selects data acquisition folder. * Selects output folder. * Starts conversion. * Output file is populated with formatted data. * User is notified that conversion has finished. |
| Alternative Flow | * Invalid data is encountered. * Error message is displayed. * User may select a new input file. |
| Related Requirements | FR-8: Format Data |

**Use Case 4: Select Input Files**

|  |  |
| --- | --- |
| Use Case | Select Input Files |
| Actors: | Lab researcher |
| Pre-condition: | User has opened program. |
| Post-condition | File path has been set. Confirmation message is displayed. |
| Main Flow | * User selects data acquisition folder. * Confirmation message is displayed. |
| Alternative Flow | * Invalid input file is encountered. * Error message is displayed. * User may select a new input file. |
| Related Requirements | FR-9: Select Data Streams |

**Use Case 5: View Graph**

|  |  |
| --- | --- |
| Use Case | View Graph |
| Actors: | Lab researcher |
| Pre-condition: | Input file has been selected. Plotting has been started. |
| Post-condition | Graphs are filled by plotted data. User is notified that end of data source has been reached. |
| Main Flow | * User selects data acquisition folder. * Starts plotting * Graphs are populated * User is notified that end of data source has been reached. |
| Alternative Flow | * Invalid input file is encountered. * Error message is displayed. * User may try plotting again. |
| Related Requirements | FR-10: Plot Data Streams |

**Use Case 6: Manipulate Graph Scale**

|  |  |
| --- | --- |
| Use Case | Manipulate Graph Scale |
| Actors: | Lab researcher |
| Pre-condition: | Program is open |
| Post-condition | Graphs are resized to desired scale. |
| Main Flow | * User hovers over graph * Scrolls up or down to zoom in or out * Graph scales appropriately |
| Alternative Flow | * Maximum or minimum scale is reached * Zooming is limited by maximum size. |
| Related Requirements | FR-11: Manipulate Scale |

**Use Case 7: Change Plotting Speed**

|  |  |
| --- | --- |
| Use Case | Change Plotting Speed |
| Actors: | Lab researcher |
| Pre-condition: | Input file has been selected and data stream has not run out |
| Post-condition | Speed at which data is plotted is changed. |
| Main Flow | * User selects input folder. * Begins plotting. * Sets plotting speed. * Speed at which data is plotted to graph changes appropriately. |
| Alternative Flow | * Data stream runs out. * User is notified and must start over plotting. |
| Related Requirements | FR-12: Change Plotting Speed |

**Use Case 8: Select Data Points**

|  |  |
| --- | --- |
| Use Case | Select Data Points |
| Actors: | Lab researcher |
| Pre-condition: | Input file has been selected and data has been plotted to graph. |
| Post-condition | Vertical bars display the bounds of selected data. |
| Main Flow | * User selects input folder. * Begins plotting. * Selects Mean Bar option * Adjusts Mean Bars’ location |
| Alternative Flow | * If data has not been plotted, the Mean Bars will still appear but contain no data yet. |
| Related Requirements | FR-13: Mean Bars |

**Use Case 9: Calculate Mean**

|  |  |
| --- | --- |
| Use Case | Calculate Mean |
| Actors: | Lab researcher |
| Pre-condition: | Input file has been selected and data has been plotted to graph. Mean bars have been selected and adjusted to the desired location. |
| Post-condition | Mean value within the selected data segment is displayed. |
| Main Flow | * User selects input folder. * Begins plotting. * Selects Mean Bar option. * Adjusts Mean Bars’ location. * Selects calculate mean. * Mean value is displayed. |
| Alternative Flow | * If empty data segment is selected, user is prompted to select a new segment. |
| Related Requirements | FR-14: Calculate Mean |

**Use Case 10: Convert Data**

|  |  |
| --- | --- |
| Use Case | **Convert Data** |
| Actors: | Lab researcher |
| Pre-condition: | EZView data spool file has been selected. |
| Post-condition | A folder is created containing the data from the spool file in the format of modules 1-3 |
| Main Flow | * User selects input folder. |
| Related Requirements | FR-15: Format Data |

## Functional Requirements

#### Calculating Concentrations (Module 1)

|  |  |
| --- | --- |
| **Functional**  **Requirement** | **[FR-1] Calculate Atom Ratio** |
| Description | The system must allow the user to calculate the ratio of bicarbonate to carbon dioxide. The result of the calculation must display the ratio in decimal format. |
| Source | Client |
| Priority | Level 0 (Essential) |
| **Functional**  **Requirement** | **[FR-2] Center Mean Bars** |
| Description | The system must visually present mean bars in the center of the graph window. These vertical bars must be movable by the user so that a segment of data can be selected to calculate the mean for. |
| Source | Client |
| Priority | Level 1 (Desirable) |

#### Analyzing Enzyme Activity (Module 3)

|  |  |
| --- | --- |
| **Functional**  **Requirement** | **[FR-3] Plot Atom Percentage** |
| Description | The system must be able to plot the percentage of carbon dioxide with a mass of 49 out of all present molecules. The graph must be normalized using natural log. |
| Source | Client |
| Priority | Level 0 (Essential) |
| **Functional**  **Requirement** | **[FR-4] Plot Derivative** |
| Description | The system must be able to plot the derivative of the natural log of the percentage of carbon dioxide with mass 49. |
| Source | Client |
| Priority | Level 0 (Essential) |
| **Functional**  **Requirement** | **[FR-5] Copy Table** |
| Description | The system must allow the user to copy the contents of the mean value table. |
| Source | Client |
| Priority | Level 1 (Desirable) |
| **Functional**  **Requirement** | **[FR-6] Plot Datasets Consecutively** |
| Description | The system must be able to plot data from one acquisition folder, stop plotting, and then allow the user to select a new acquisition folder to begin plotting from. |
| Source | Client |
| Priority | Level 0 (Essential) |
| **Functional**  **Requirement** | **[FR-7] Record Sample Name** |
| Description | The system must take user input and record the name of the sample to the mean table in the same row as its corresponding mean value. |
| Source | Client |
| Priority | Level 0 (Essential) |
| **Functional**  **Requirement** | **[FR-17] Mean Bars** |
| Description | Two vertical bars must be included in the derivative graph of the application. The user should be able to move the bars to encapsulate a desired segment of data from which the mean can be calculated. The bar rescale button should center the bars on the derivative graph |
| Source | Client |
| Priority | Level 1 (Desirable) |

#### Data Conversion (Module 4)

|  |  |
| --- | --- |
| **Functional**  **Requirement** | **[FR-8] Accept Data** |
| Description | The system must accept data from the EZ-Tap listener device attached to the secondary mass spectrometer through the USB port. |
| Source | Client |
| Priority | Level 0 (Essential) |
| **Functional**  **Requirement** | **[FR-8] Identify Port** |
| Description | The system must identify which port the EZ-Tap is plugged into and intelligently select it for listening. |
| Source | Client |
| Priority | Level 1 (Desirable) |
| **Functional**  **Requirement** | **[FR-15] Format Data** |
| Description | The system must convert data from the secondary mass spectrometer into a specific format so that it can be analyzed using existing applications. The data must be converted from hexadecimal to decimal format and be resorted into the appropriate column order. |
| Source | Client |
| Priority | Level 0 (Essential) |
| **Functional**  **Requirement** | **[FR-16] Split Data** |
| Description | The system must split the data into many different csv files to match the data file structure used by the primary mass spectrometer. |
| Source | Client |
| Priority | Level 0 (Essential) |

## Non-Functional Requirements

Our project exists in the context of academic plant biology research, and thus has several ideals and values it strives to represent and uphold. These ideals don’t necessarily describe what the program *does*, they rather describe how it *is*. This section clarifies the non-functional requirements which we’ll use to guide our design and development to uphold these ideals and values.

**Modern Visuals:**

The system shall look like a modern 2020’s program. PyQt5’s baseline UI elements meets this standard

**Python For Extendibility:**

The system shall use Python since it is one of the most common languages among Biology students, including those that use the Cousins Photosynthesis Lab. This will enable extension and maintenance.

**Documentation For Extendibility:**

The system shall have documentation for code that’s thorough enough to allow college 4th-year skill level software engineers to extend and maintain it.

**Documentation For Non-Technical Users:**

The system shall have documentation to enable non-technical users to make full use of it. For example, an explanation of how to create executables of each module.

**Accuracy:**

The system shall accurately calculate and portray data. The instruments have their own levels of accuracy, so maintenance of significant figures is our basic metric for accuracy.

**Compatibility:**

Each module shall use compatible formats, where applicable. Particularly, this means using the format of the primary Mass Spectrometer.

**Non-Destructive:**

The system shall not overwrite or otherwise destroy any pre-existing data.

### User Stories

The following user stories outline key tasks that users can perform within the system, highlighting their goals and the reasons behind them. Each story provides a clear and concise description of what the user aims to achieve, along with the expected system behavior, ensuring that user needs are directly addressed and aligned with the system's functionality.

**User Story US1: Calculate Bicarbonate/CO2 Ratio**

As a Lab Researcher, I need to calculate the ratio of bicarbonate to carbon dioxide so that I can log the given output.

Feature: Calculate Bicarbonate/CO2 Ratio

Scenario: Lab researcher calculates bicarbonate/CO2 ratio

Given the mass spectrometer data file has data for HCO-3 and CO2  
AND CO2 and HCO-3 have been calibrated using the plotted data  
When I click the button "BiCarb/CO2"  
Then the correct ratio of BiCarb/CO2 will be computed and displayed.

**User Story US2: Plot Derivatives**

As a Lab Researcher, I need the first and second derivatives of percent CO2 49 So that I can analyze and log it.

Feature: Plot Derivatives

Scenario: Lab researcher plots Atom Percent and its derivative for CO2 data

Given the mass spectrometer data file has data on the CO2 49, 47 & 45 masses.  
When I run module 3 (using the "start" or "unpause" button)  
Then two graphs will show the first and second derivatives of percent CO2 49 respectively.

**User Story US3: Convert Data**

As a Lab Researcher, I need modules 1-3 to work for the second mass spectrometer so that I can analyze its data the same way.

Feature: Convert Data

Scenario: Lab researcher converts data to be compatible with modules 1-3

Given Instrument B (the second mass spectrometer) is outputting data, or has outputted data  
WhenI select the Instrument B option on module 1/2/3  
And I select the Instrument B datastream (likely a directory)  
Then module 1/2/3 functions as normal, including all use cases for module 1/2/3.

**User Story US4: Datastream Combining**

As a Data Researcher, I need data from the LI-COR Leaf-gas Exchange System, Tunable Diode Laser, and Picarro consolidated into one or more spreadsheets so that I can analyze the data more efficiently.

Feature: Datastream Combining

Scenario: Lab researcher combines three streams of data

Given I have data from all three instruments  
When I run module 5  
Then one or more spreadsheets collectively containing all the data, collated by time, is created.

**User Story US5: Data Isolation**

As a Data Researcher, I need to isolate portions of data so that I can view and analyze the most important parts of a multi-hour lab experimentation session.

Feature: Data Isolation

Scenario: Lab researcher isolates data

Given the System has collected a non-trivial amount of data from the mass spectrometer  
When I drag the left and right edges of my selection to a portion of the data graph  
Then only data from that portion of the graph will be analyzed in the calculation dashboard.

**User Story US6: Data Isolation**

As a lab researcher, I need modules 1-3 to work for instrument B (the second mass spectrometer) so that I can analyze its data the same way.

Feature: Data Conversion

Scenario: Lab researcher Converts Data

Given Instrument B (the second mass spectrometer) is outputting data, or has outputted data through EZView

When I select the data spool file

Then module 4 creates a folder containing that data in the format used by modules 1-3.

### Traceability Matrix

The table below links functional requirements to their corresponding use cases and user stories. This mapping ensures that every requirement is fully addressed and connected to relevant user interactions, providing a clear line of traceability throughout the system.

|  |  |  |  |
| --- | --- | --- | --- |
| Functional Requirement | Use Case | User Story | Priority |
| [FR-1] Calculate Atom Ratio | UC-1: Calculate Bicarbonate/CO2 Ratio | US5: Data Isolation | Level 0 |
| [FR-2] Center Mean Bars | UC-1: Calculate Bicarbonate/CO2 Ratio | US1: Calculate Bicarbonate/CO2 Ratio | Level 1 |
| [FR-3] Plot Atom Percentage | UC-2: Plot Derivatives | US2: Plot Derivatives | Level 0 |
| [FR-4] Plot Derivative | UC-2: Plot Derivatives | US2: Plot Derivatives | Level 0 |
| [FR-8] Format Data | UC-3: Convert Data | US3: Convert Data | Level 0 |
| [FR-9] Select Data Streams | UC-4: Select Input Files | US4: Datastream Combining | Level 0 |
| [FR-10] Plot Data Streams | UC-5: View Graph | US4: Datastream Combining | Level 0 |
| [FR-11] Manipulate Scale | UC-6: Manipulate Graph Scale | US4: Datastream Combining | Level 1 |
| [FR-12] Change Plotting Speed | UC-7: Change Plotting Speed | US4: Datastream Combining | Level 0 |
| [FR-13] Mean Bars | UC-8: Select Data Points | US5: Data Isolation | Level 0 |
| [FR-14] Calculate Mean | UC-9: Calculate Mean | US4: Datastream Combining | Level 0 |

# Solution Approach

This section aims to outline our project’s approach. This includes the different parts of the project modules (Architecture Design), data storage and manipulation methods (Data Design), and how the project modules will outwardly look (User Interface Design). These details are intended to elucidate objectives and methods for current and future developers, but to do so using language that can mostly still be understood by stakeholders for overview.

The project is designed to provide a comprehensive platform for managing and interpreting Mass Spectrometer data through various modules. It aims to present data insights through graphical and numerical perspectives while offering flexible data formatting and integration capabilities. The system consists of five primary modules: the first three focus on different ways to visualize and log Mass Spectrometer data, and the fourth module reformats data from a secondary Mass Spectrometer. The general design for each of the modules is to accept input from a file or folder, which is selected by the user, process it in some way (reformat, normalize, derive calculations from, etc.), and then output that processed information, either to graphs on the screen, or to new files.

## Architecture Design

### Overview

Team Linnaea Borealis' architecture design focuses on Module 5. Each module in the system operates as a standalone program, but Module 5 is the primary module requiring architectural design innovation, as most other modules remain stable and do not necessitate changes.

The team has adopted a Pipe and Filter architecture for this design, which is well-suited for this system's data processing requirements. The system requires data to be read from a file, normalized, plotted, and then transformed. This process fits Pipe and Filter architecture well. This approach allows for clear separation of concerns, where data flows through a series of independent filters (or stages), each performing specific tasks such as reading, processing, and visualizing data. This modular design enhances flexibility, scalability, and maintainability, making it easier to integrate new features or modify existing ones without affecting the entire system. By leveraging this architecture, Team Linnaeus ensures a clean and efficient flow of data from input to output, supporting both current and future needs.

The system begins with the User Interface (UI) component, which allows users to specify a file path and view plotted data and calculation results. The UI interacts with the File Reader, which reads raw data from the CSV file provided by the user and passes it to the Data Processor. The Data Processor then normalizes the raw data by applying a natural logarithmic transformation, preparing it for further steps. Once processed, the data is sent to the Graphing Engine, which updates the current graph by integrating the new data. The updated graph is then displayed in the UI for the user and sent to the Calculation Engine. The Calculation Engine performs further computations on the processed data, producing analytical results that are also displayed in the UI such as the mean of a selection of data. This flow of data, facilitated by the modular design, ensures efficiency, flexibility, and ease of maintenance.

A diagram of a system

Description automatically generatedFigure 1: System Block Diagram

### Subsystem Decomposition

This section outlines how the system has been decomposed into its major subsystems, each corresponding to the core components identified earlier: the User Interface (UI), File Reader, Data Processor, Graphing Engine, and Calculation Engine. The decomposition was designed to ensure that each subsystem represents a manageable unit of work for a single developer, with clearly defined responsibilities and minimal overlap. Each subsystem has been assigned a specific functionality: the UI handles user interactions, the File Reader manages data input, the Data Processor handles transformations, the Graphing Engine updates the collection of data, and the Calculation Engine performs analytical operations. The rationale behind this decomposition emphasizes cohesion and coupling. High cohesion is maintained within each subsystem by ensuring that each is focused on a single task or closely related set of tasks. Meanwhile, coupling between subsystems is minimized by defining clear and straightforward interfaces for data exchange, allowing for seamless interaction without unnecessary dependencies. This modular design not only improves the maintainability and scalability of the system but also supports flexible integration of future enhancements.

#### User Interface

##### Description

The User Interface (UI) subsystem is responsible for managing the interaction between the user and the system. Its primary function is to display graph data generated by the Graphing Engine and the results of calculations performed by the Calculation Engine. Additionally, the UI allows the user to input the file path containing the CSV data, which is then passed to the File Reader subsystem for processing. The UI acts as a central hub, presenting outputs from different subsystems in a coherent and user-friendly manner.

##### Concepts and Algorithms Generated

The User Interface subsystem was designed with simplicity and ease of use in mind, utilizing a basic file input mechanism and graphical display capabilities. Concepts such as event-driven programming were considered, allowing the UI to react to user inputs (e.g., file path selection) and update dynamically when data from other subsystems (such as the graph or calculations) is received. The selected solution leverages standard UI frameworks to achieve these goals with minimal latency and high responsiveness. The decision to keep the UI simple was influenced by the need to maintain a clear separation of concerns, ensuring that complex data processing is handled by other subsystems. Trade-offs included balancing performance with usability, ensuring the UI remains responsive even when handling large datasets.

##### Interface Description

Services Provided:

|  |  |  |
| --- | --- | --- |
| **Service Name** | **Service Provided To** | **Description** |
| GetFilePath | File Reader | The GetFilePath service will pass over the user-selected file paths for data acquisition. Three file paths should be returned, one for each instrument utilized by the system. |
| GetDataSelection | Calculation Engine | This service will return the bounds of the data selected by the user using two movable vertical bars. |

Services Required:

|  |  |
| --- | --- |
| **Service Name** | **Service Provided From** |
| CalculateMean | Calculation Engine |
| GetLatestGraph | Graphing Engine |

#### File Reader

##### Description

The File Reader subsystem is responsible for reading data from three different files, each representing data from a distinct instrument used by the system. After reading the raw data from these files, the File Reader passes the data along to the Data Processor for further processing. This subsystem acts as the initial stage in the data pipeline, ensuring that the raw information is properly retrieved and made available for downstream components.

##### Concepts and Algorithms Generated

The File Reader subsystem was designed with the need to efficiently handle multiple file inputs. The concept of parallel file reading was considered to improve performance when handling large datasets, but ultimately, a sequential approach was selected due to the relatively manageable file sizes. The File Reader ensures that each file is opened, its contents are read, and the data is collected into a format that can be easily passed to the Data Processor. Special considerations were made to handle potential file reading errors, such as missing or corrupted files. In such cases, error handling mechanisms trigger notifications to the user. The trade-off involved in this design was balancing robustness with simplicity, ensuring that file reading remains a lightweight process while effectively managing edge cases.

##### Interface Description

Services Provided:

|  |  |  |
| --- | --- | --- |
| **Service Name** | **Service Provided To** | **Description** |
| ReadFileData | Data Processor | This service reads the contents of the three files, each corresponding to an instrument's data. The service accepts the file paths as input (provided by the User Interface) and returns the raw data from all three files as output. The data is passed on to the Data Processor for formatting and normalization. |

Services Required:

|  |  |
| --- | --- |
| **Service Name** | **Service Provided From** |
| GetFilePath | User Interface |

#### Data Processor

##### Description

The Data Processor subsystem is responsible for transforming raw data received from the File Reader into a format that is more suitable for further analysis. Its primary task is to normalize the data using the natural logarithmic transformation, making the data easier to process and visualize. Once the data is formatted and normalized, the Data Processor sends the processed data segment to the Graphing Engine, where the new data is added to the current graph. This subsystem ensures the integrity and usability of the data as it flows through the system.

##### Concepts and Algorithms Generated

The main algorithm used by the Data Processor is the natural logarithmic transformation, which helps normalize the data. This technique was selected because it reduces variance in the data and handles large discrepancies in value magnitudes, making it more suitable for visual representation and computation. Alternative normalization methods, such as z-score normalization, were considered but ultimately not chosen, as the natural log method better aligned with the requirements of the data's structure and scale. Special considerations included handling cases where the raw data contains zero or negative values, as these would cause issues during the logarithmic transformation. Error handling mechanisms and data validation were incorporated to account for such anomalies, ensuring robust processing. The trade-off in this approach involved balancing data transformation speed and the complexity of handling edge cases.

##### Interface Description

Services Provided:

|  |  |  |
| --- | --- | --- |
| **Service Name** | **Service Provided To** | **Description** |
| ProcessData | Graphing Engine | This service receives the raw data from the File Reader, processes it by formatting and applying a natural logarithmic normalization, and then sends the processed data to the Graphing Engine for visualization. The input consists of the raw data from three different files, and the output is the normalized and formatted data ready for graphing. |

Services Required:

|  |  |
| --- | --- |
| **Service Name** | **Service Provided From** |
| ReadFileData | File Reader |

#### Graphing Engine

##### Description

The Graphing Engine subsystem is responsible for visualizing the processed data received from the Data Processor. Its main role is to update the current graph by incorporating the newly processed data segment and rendering it in the user interface. This allows the user to observe real-time visual changes in the data as it is processed. The Graphing Engine ensures that the graphical representation is clear, accurate, and continuously updated as new data is received.

##### Concepts and Algorithms Generated

The Graphing Engine employs algorithms to dynamically update the graph with new data segments. Various graphing techniques were considered, including line charts and bar charts, but a continuous line chart was selected as the best fit for real-time data visualization. The primary concept is to ensure that the graph scales efficiently as more data is added, while also maintaining clarity and responsiveness.

##### Interface Description

Services Provided:

|  |  |  |
| --- | --- | --- |
| **Service Name** | **Service Provided To** | **Description** |
| UpdateGraph | User Interface | This service receives the processed data from the Data Processor and updates the current graph displayed in the User Interface. The input is the normalized data, and the output is an updated visual graph reflecting the latest data. The service ensures that the graph is refreshed in real-time as new data is processed. |

Services Required:

|  |  |
| --- | --- |
| **Service Name** | **Service Provided From** |
| GetProcessedData | Data Processor |

#### Calculation Engine

##### Description

The Calculation Engine subsystem is responsible for performing various calculations on the data, including allowing the user to select a segment of data and calculating the mean of that segment. This subsystem plays a crucial role in providing numerical insights into the processed data, complementing the visual representation provided by the Graphing Engine.

##### Concepts and Algorithms Generated

The primary algorithm used by the Calculation Engine is the calculation of statistical measures such as the mean. The mean is calculated by summing the selected data points and dividing by the number of points. Several approaches were considered, including pre-calculating statistics for all data and storing them for quick access. However, the selected solution was to compute the required statistics on-demand based on the user’s selection. This minimizes resource consumption and ensures that calculations are based on the latest data segment selected by the user.

##### Interface Description

Services Provided:

|  |  |  |
| --- | --- | --- |
| **Service Name** | **Service Provided To** | **Description** |
| CalculateMean | User Interface | This service calculates the mean of the selected data segment. The input is the processed data for the user-selected segment, and the output is the mean value. The mean is displayed in the User Interface as part of the calculation results. |

Services Required:

|  |  |
| --- | --- |
| **Service Name** | **Service Provided From** |
| GetDataSelection | User Interface |
| GetLatestGraph | Graphing Engine |

## Data design

This section covers the different ways our project stores and manages data, both while it’s running, and when the data is stored for later. This overview will be a fairly technical overview, meant mostly for developers. Each subsection covers a different data structure used in the project. The data used in this project is not stored in a database, so the data design revolves around temporarily stored data in memory as well as data exported to files.

### Shared Singleton

A shared singleton is a design pattern that forces only one instance of an object to exist throughout the whole program. Although this design pattern does not usually describe a data structure, in modules 1-3, most important data structures are members of a shared singleton, named sharedData. These members include fileList (subsection IV.2) and dataPoints (subsection IV.3)

### Basic List

In modules 1-3, we use a basic list to store the names of files that are read from. This list is named fileList and is stored in the sharedData shared singleton (subsection IV.1).

### Dictionary

In modules 1-3, we use a Python dictionary to store the mass spectrometer data, named dataPoints. The keys are time points, and the values are tuples of isotope masses. This dictionary is stored in the sharedData shared singleton (subsection IV.1).

### Log Table

In modules 1-3, there are certain data points that can be pulled out from the graph, or otherwise calculated from the data. These can be saved into a table built into the UI. These logs are then stored directly in the PyQT UI component QTableWidget.

### CSV Export

Modules 1-3 can export logged data from the log table (subsection IV.4) into a CSV file, which matches the format of the table.

### Pandas DataFrame

Module 4 uses a DataFrame from the Pandas Python library to store data from Mass Spectrometer 2. This is very similar to a dictionary approach (subsection IV.3), but effectively replaces the need for unique keys with ordering and more importantly allows for the use of Pandas methods like to\_csv at a small performance cost.

### CSV Series

Module 4 exports the DataFrames (subsection IV.6) as CSV’s with ~8 rows each, for use in modules 1-3. Each row contains a time signature and isotope masses. These CSV’s are named with numbers in order of their time signatures.

## User Interface Design

The user interface first allows the user to select data acquisition folders sourced from a mass spectromer instrument. This portion of the interface corresponds with use case UC-4: Select Input Files.

A screenshot of a computer

Description automatically generated

Figure 2: File Selection

The largest section of the user interface will display a black graph such as the one shown in Figure 3. To the left of the graph, color coded labels for each data stream are present to provide an intuitive viewing experience. These labels can also be used to toggle the visibility of different data streams. The graph is populated by line-graphs, color coded for each data stream. This corresponds to the use case UC-5: View Graph. The graph can be scaled easily using the scroll wheel to zoom in or out. Below the graph and to the right of Figure 3, a slider is shown. This slider allows the user to adjust the speed at which data is plotted from 0.5x to 32x. This corresponds to use case UC-7: Change Plotting Speed. On the left of the slider is also a pause/resume button as well as a start button that allows the user to toggle the plotting of data. In addition to the primary graph, modules 1-3 have additional graphs for calculations derived from the primary data.

A screen shot of a graph

Description automatically generatedFigure 3: Graphing and Calculations

Using the leftmost button in Figure 3 that features two vertical lines, the user can toggle the visibility of “mean bars”. These vertical bars pictured in Figure 4 can be shifted left to right using the cursor to select a specific portion of data. This corresponds to the use case UC-8: Select Data Points.

A blue grid with white lines

Description automatically generatedFigure 4: Data Segment Selection

Available calculations are featured below the graph and its controls. Here, the user will be able to use the “Get Mean” button to calculate the mean inside of the selected region. This corresponds to use case UC-9: Calculate Mean.



Figure 5: Mean Calculation

In addition to allowing users to scale the graph using their scroll wheel, users are able to achieve more precise scaling by left clicking the graph to open further adjustment options. As illustrated in Figure 6, users will be able to input the exact bounds of each axis, and the graph will adjust according to their selection.

A screenshot of a computer program

Description automatically generated

Figure 6: Detailed Graph Scaling

Overall, the user interface is designed for an intuitive data acquisition and visualization experience. Users can select acquisition folders for three instruments, with options tailored for each data type, as shown in Figure 2 (UC-4: Select Input Files). The main area features a black graph displaying color-coded line graphs, accompanied by labeled indicators for clarity (UC-5: View Graph). Users can zoom using the scroll wheel and adjust the plotting speed with a slider (UC-7: Change Plotting Speed). Controls for toggling mean bars and selecting data points further enhance functionality (UC-8: Select Data Points), while a “Get Mean” button allows for quick calculations of averages within selected regions (UC-9: Calculate Mean). Additionally, precise graph scaling options enable users to customize their view, ensuring a comprehensive and user-friendly interface.

# Test Plan

This section provides an overview of the steps we take to test different elements of our project. This overview includes the overall flow, the unit tests for individual parts, and integration/system testing for combinations of different parts. The processes outlined are very particular to the context of our project; we’re very aware of our stakeholders and the integration plan that they prefer. Ultimately this section is intended to outline what we consider the ideal methods of testing, in order to keep development in line with those practices.

## Testing Strategy

The following is our loose approach to testing a particular module or feature:

1. Identify the requirement(s) involved in this module/feature. This should either come from the Requirements and Specifications Document or be added to the Requirements and Specifications Document before continuing.
2. Establish the test(s) that will be used. In other words, identify the process of using the module or feature. Document these tests in the Testing Plan Document.
3. Identify any necessary dependencies. This includes other components and input data. Include assumptions about these dependencies in the Testing Plan Document.
4. Build a representation of what acceptable results look like. This must consider our assumptions made in the previous step. For example, an Excel graph of a data acquisition: the particular data acquisition should be clarified in the previous step, with the Excel graph built off it in this step. This mockup(s) should either be included in the Testing Plan Document, or in the relevant module’s “Testing” folder with reference to it in the document.
5. Perform the test(s).
6. If the test(s) is unsuccessful, fix it if possible. If the test(s) is not successful by next standup meeting, prepare a short explanation or document explaining the issue.
7. If the test is successful, move the relevant GitHub issue to Review/QA, or from Review/QA to Done.

Ultimately, our strong connection to our primary stakeholder, Dr. Cousins, allows us to adapt our development process to a more flexible approach that handles opportunities and issues as they come up. Sometimes the requirements are vague, and the following approach may be more effective than generating more specific requirements and a mockup:

1. Implement the most obvious executions of a requirement.
2. Present those executions to the client/stakeholder(s). Receive feedback.
3. If one of the implementations is acceptable, move the relevant GitHub issue to Review/QA, or from Review/QA to Done.
4. If none of the implementations are acceptable, either return with novel implementations or revert to the primary approach, depending on team consensus.

Our delivery process is basically Continuous Delivery. Our client prefers executable files over python scripts, so a new deployment must be manually created by a team member each time. The modular nature of the project lends itself to creating a new iteration of each improved module every sprint. In this regard, our development is continuously integrated with monthly releases.

## Test Plans

This section outlines the comprehensive plan for testing the mass spectrometer interface system, detailing the strategies for unit, integration, system, and user acceptance testing. Each testing phase is designed to identify and address potential faults at different stages of development, from individual software units to the entire integrated system. The testing plan follows a systematic approach, beginning with isolated unit testing to validate the smallest components of the application, followed by integration testing to ensure smooth communication between modules. System testing will then evaluate the application’s compliance with overall requirements, focusing on functional, performance, and stress tests to confirm reliability under varying conditions. Finally, user acceptance testing will involve end-users to validate that the system meets their needs and is ready for operational deployment.

### Unit Testing

The primary objective of unit testing for this system is to validate the functionality and reliability of individual components, or “units,” by isolating them from the rest of the code and checking for bugs or unexpected behavior. Specifically, the unit tests will cover core functionalities, including data parsing from CSV files, data transformations, calculations, and graphical display setup. Unit tests will be designed for each function and method within the modules, verifying both expected outputs and error-handling mechanisms when presented with invalid data inputs. Using Python’s pytest framework, tests will be semi-automated to streamline the process and improve reliability. Mocking will be employed to simulate data inputs and dependencies where necessary, especially for modules that rely on external data sources or interactions. This approach ensures that each unit functions independently and accurately, laying a stable foundation for subsequent integration and system testing phases.

### Integration Testing

The purpose of integration testing in this system is to identify faults that may arise when individual components interact, focusing on groups of components rather than isolated units. This phase will ensure that data flows smoothly between components. For instance, components responsible for parsing CSV files and transforming data will be integrated and tested as a cohesive unit to confirm that each stage performs as expected in the broader workflow. To manage dependencies, a test data set simulating real-world CSV inputs will be used to validate functionality and data consistency across components. Python’s pytest framework will be used for semi-automated integration tests, while pytest-mock will aid in simulating dependencies, ensuring that testing conditions are controlled and predictable.

### System Testing

System testing will be conducted to ensure that the mass spectrometer interface system operates as a cohesive unit, meeting all specified requirements. This phase will involve executing a series of planned tests to validate both functional and non-functional aspects of the system as a whole.

#### Functional testing:

In functional testing, we will develop a comprehensive set of test cases based on the functional requirements outlined in the project documentation. Each functional requirement will correspond to at least one test case. Each standalone system will be tested in realistic scenarios to ensure that they meet user expectations. Test cases will be prioritized to focus on critical user paths and high-risk areas, ensuring that the most relevant features are validated first. Any failures or discrepancies found during testing will be documented and addressed promptly to enhance system reliability.

#### Performance testing:

To assess the system's performance, we will conduct performance testing that focuses on response times, resource utilization, and overall system stability. This will include stress testing the systems by simulating high-load conditions using large datasets to determine how the system performs under pressure. For example, we will measure the speed at which the system can plot all data points from a large sample at once. Key metrics such as processing speed, memory usage, and data handling capacity will be monitored. If any performance issues arise, they will be investigated and resolved to ensure the system meets the expected performance benchmarks.

#### User Acceptance Testing:

User Acceptance Testing will involve lab researchers in evaluating the system based on their operational needs. We will organize testing sessions where lab researchers will perform key tasks, such as loading CSV files, converting data, plotting data, and processing calculations in the same way they would during their academic research. Feedback will be gathered during these sessions to identify any areas requiring adjustment or enhancement. This testing phase is crucial for ensuring that the system is user-friendly and meets the designated requirements. Any issues identified will be prioritized for resolution to ensure the system is fully prepared for operational use.

## Environment Requirements

To ensure comprehensive testing of the mass spectrometer interface system, this section outlines the necessary and desired properties of the testing environment. The setup will enable thorough verification of each module’s functionality, accuracy, and performance in processing and visualizing mass spectrometry data.

The testing environment should be equipped with a Windows 10 or Windows 11 operating system. The environment will rely on Python, version 3.8 or higher, to match the development specifications of the system. Key Python libraries, such as PyQt5 for graphical user interface elements and pandas for handling data and CSV file operations, should be pre-installed. Each module has a requirements.txt file that can be used with pip to install the necessary libraries. Additionally, a sample CSV file will be prepared, including real mass spectrometer data, to evaluate the system’s handling of data directly from a file.

Special tools will aid in testing, such as the pytest framework for semi-automated unit and integration testing. Mocking tools, like unittest.mock or pytest-mock, will be used to simulate various data inputs and scenarios, particularly in modules focused on data handling and conversion.

Module 4 has extra special requirements for its extra specific use case. The module takes in data from a Mass Spectrometer through an EZ-Tap serial-to-usb listener device. Both the Mass Spectrometer and the EZ-Tap are assumed for the testing and usage of module 4. In order to ensure these conditions, we use remote-access to test on the computer that has the EZ-Tap plugged into it. Additionally, the program requires EZView to spool the data from the EZ-Tap before it can be reformatted. EZView is proprietary software from Stratus Engineering, the same company that manufactures EZ-Tap.

These environment specifications aim to provide a controlled, reliable setting that ensures system stability, accuracy, and performance across diverse data scenarios.

# Projects and Tools Used

The table below lists the libraries, frameworks, and tools used to implement our project.

|  |  |
| --- | --- |
| Tool/Library/Framework | What It Was Used For |
| PyQt | GUI library/framework used in Modules 1-3 |
| Pandas | Maintaining data in Modules 1-3 |
| PyQtGraph | Adding graphs to PyQt GUI |
| NumPy | Establishing compatibility between our data and PyQtGraph |
| PyInstaller | Creating .exe executables |
| Excel | Generating example output for tests |
| LabView | Orienting visual design |

The table below lists the languages used in our project.

|  |  |  |
| --- | --- | --- |
| Languages Used In Project | | |
| Python | Markdown | C |

# Description of Final Prototype

With this prototype, Module 3 delivers 100% of its proposed functionality. Users are now able to plot log-normalized atom percentages. This graph shows the percentage of carbon dioxide molecules with a mass of 49. Normalization simplifies data interpretation by eliminating large spikes that would otherwise exceed the viewport. The UI component for this feature is shown in Figure VI.1 where real-world data has been plotted.

Figure VI.1

The system also allows users to compute and plot the derivative of the Atom percentage for trend analysis. This graph is accompanied by vertical bars used for data selection. These bars have been modified to always appear centered in the viewport and scale appropriately with the graph. Both of these implementations are featured in Figure VI.2.

Figure VI.2

In this prototype, data from the mean value table can be easily copied for external use. Additionally, users can input sample names, linking them directly to their corresponding mean values for better organization and reference. The mean value table is displayed in Figure VI.3.



Figure VI.3

Finally, in module 3, users can now plot multiple datasets without restarting the program. This was not possible in the previous solution because users were not allowed to select a second dataset. Now, the system can plot one dataset, stop, and then plot a new dataset as selected by the user.

The team is currently working on Module 4. Much of Module 4’s architecture has already been implemented. This includes data conversion to decimal format and output file creation. However, data importing must still be addressed. A method for selecting the correct port to import data from must be developed and integrated.

The system is now able to accurately plot the normalized percentage of carbon dioxide molecules with a mass of 49. Additionally, the system supports plotting the derivative of this percentage. Mean bars for data selection have been updated to scale appropriately with the graph, as shown in the figure below. The ability to copy data from the mean value table has also been implemented, enabling seamless transfer of information for external use. Furthermore, the prototype allows for consecutive dataset plotting, where users can plot data from one acquisition folder, stop, and then select a new folder to begin a fresh plot without restarting the program. Lastly, the system supports recording sample names, enabling users to input and store identifiers alongside their corresponding mean values, as illustrated in Figure VI.1.1.1. If no further bugs are identified, no work remains to be done on module 3.



Figure VI.1.1.1

Since new versions of the prototype were delivered to the client with each update, several preliminary tests were conducted on module 3. These tests were primarily conducted during weekly meetings with the team and client. Real-world mass spectrometer datasets were utilized to observe the plotted results and compare them to past software solutions as well as ideal outcomes visualized in Excel. The first set of prototypes yielded derivative graphs that did not match expectations. This testing process helped form the ideal calculations for future versions. Lab researchers also helped verify the accuracy of plotting by comparing the plotted values with a previously used graphing software. With later prototypes, all functions mentioned in the previous section were successfully tested with the exception of modifications to the mean table and consecutive dataset plotting which are currently undergoing testing by the client.

As for Module 4, the script for converting data has been written and appears functional. Similarly, the module creates directories for the output streams properly. File creation so far is consistent with what we’d expect. The program successfully connects to some ports but has so far not been able to get useful data from them.

The data format conversion code has been tested on example data and works as expected. When running the program on live data, some ports are inaccessible and one port that may be the correct one only returns “5000” over and over. This port may be the EZ-Tap’s write port instead of the desired read port.

Our next steps are to establish connection through the port, and to develop a method of port selection. Port selection will either be done by the program, if possible, or by the user through a basic UI interface, if necessary.

# Conclusions and Future Work

## Limitations and Recommendations

The primary limitations of this project are in the domain of performance. The most significant place where this stands out is when Modules 1 and 2 are used to take in data from Mass Spectrometer 2. When this is done, it makes use of an integrated version of Module 4. The combined performance delays of Modules 1/2 and Module 4 make for significant delays in information display at times.

Another limitation is the data intake speed when using Mass Spectrometer 2. In this regard, we are limited by the USB connection’s relatively low bitrate. We recommend further development look into the possibility of a direct serial connection.

## Future Work

The clear next step in this project is to create a module for combining the data streams of 3 other instruments in the lab. Our client has expressed interest in this additional module for a while now. This module would involve collating these data streams and displaying them, much like modules 1-3. It would need to synchronize the data as well.