

Module Interface Specification for SpectrumImageAnalysisPy

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1 Revision History

| Date | Version | Notes |
|-------------------|---------|---------------|
| November 29, 2017 | 1.0 | Initial draft |

2 Symbols, Abbreviations and Acronyms

See **SRS** documentation at https://github.com/icbicket/SpectrumImageAnalysisPy/blob/SpectrumImageAnalysisPy_dev/Doc/SRS/SRS.pdf.

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3 Introduction

The following document details the Module Interface Specifications for SpectrumImageAnalysisPy, a library created for the data processing of spectrum image datasets.

Complementary documents include the System Requirement Specifications and Module Guide. The full documentation and implementation can be found at https://github.com/icbicket/SpectrumImageAnalysisPy/tree/SpectrumImageAnalysisPy_dev.

All modules within SpectrumImageAnalysisPy are accessible by the user from terminal commands. Some modules will interface with each other, but the workflow of SpectrumImageAnalysisPy is driven by the user.

4 Notation

The structure of the MIS for modules comes from [1], with the addition that template modules have been adapted from [2]. The mathematical notation comes from Chapter 3 of [1]. For instance, the symbol $:=$ is used for a multiple assignment statement and conditional rules follow the form $(c_1 \Rightarrow r_1 | c_2 \Rightarrow r_2 | \dots | c_n \Rightarrow r_n)$.

The following table summarizes the primitive data types used by SpectrumImageAnalysisPy.

| Data Type | Notation | Description |
|----------------|--------------|----------------------------------------------------------------------------------------------------------------------------------|
| character | char | a single symbol or digit |
| string | str | a sequence of characters |
| integer | \mathbb{Z} | a number without a fractional component in $(-\infty, \infty)$ |
| natural number | \mathbb{N} | a number without a fractional component in $[1, \infty)$ |
| real | \mathbb{R} | any number in $(-\infty, \infty)$ |
| complex | \mathbb{C} | any combination of real and imaginary numbers, in the form $a + bi$, where a and b are real and i is the imaginary number |

The specification of SpectrumImageAnalysisPy uses some derived data types: sequences, strings, and tuples. Sequences are lists filled with elements of the same data type. Strings are sequences of characters. Tuples contain a list of values, potentially of different types. In addition, SpectrumImageAnalysisPy uses functions, which are defined by the data types of their inputs and outputs. Local functions are described by giving their type signature followed by their specification. It should be noted that each state variable is assumed to have a setter and getter accessible through module.variable_name.

5 Module Decomposition

The following table is taken directly from the Module Guide document for this project. The modules in this document are listed in the order in which they appear in this table.

| Level 1 | Level 2 | Level 3 |
|-----------------------------|----------------------|--------------------------------------------------------------------------------------------|
| Hardware-Hiding Module | | |
| | Import | csv dm3 h5 rpl |
| | Export | csv h5 png rpl |
| Behaviour-Hiding Module | Data processing | Richardson-Lucy Deconvolution Normalization Gain correction Background correction |
| | Data extraction | 1D slice 2D mask 3D mask |
| | Display | 1D spectrum plot 2D image plot 3D spectrum image plot |
| Software Decision Module | Data | Spectrum Image Spectrum Image |
| | Array Data Structure | |
| | Plotting Library | |

Table 1: Module Hierarchy

6 MIS of Hardware Hiding Module

[You probably don't need to document this module, unless you need it to make the specification for other modules clear. —SS]

6.1 Module

HardwareHiding

6.2 Uses

N/A

6.3 Syntax

6.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|---------------|----------|-----------|------------|
| InputDevices | Hardware | Read out | - |
| OutputDevices | Hardware | Write out | - |

6.4 Semantics

This module handles the interface between the hardware being used and inputs to the software

6.4.1 State Variables

N/A

6.4.2 Environment Variables

- Keyboard
- Mouse
- Screen
- Long Term Storage
- Temporary storage

[Yes, these are environment variables. There seems to have been some confusion on this topic, but you get it. :-) —SS]

6.4.3 Access Routine Semantics

InputDevices():

- input: Hardware allowing the user to input instructions to the computer software, *e.g.* mouse, keyboard, long term or temporary memory
- transition: N/A
- output: Software instructions corresponding to the desire of the user (*e.g.* registering a mouse click, reading a variable from memory, accessing a file on the harddrive)
- exception: N/A

OutputDevices():

- input: Hardware allowing the user to see output from the computer software, *e.g.* screen, storage
- transition: N/A
- output: Interface to allow software to communicate output to the user (*e.g.*, it provides the capability for the software to output something onto the screen or write to a file on a harddrive, or write to memory)
- exception: N/A

[It is nice if each module starts on a new page. —SS]

7 MIS of Import csv Module

7.1 Module

ImportCSV

7.2 Uses

- Data 1D Spectrum
- Array data structure
- Hardware-hiding

7.3 Syntax

7.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|---------|------------|----------|------------------|
| ReadCSV | fname: str | Spectrum | NO FILE, NOT CSV |

[Having exception names with spaces in them might be a problem for your implementation. —SS]

7.4 Semantics

This module imports data from csv files and initializes a Spectrum object.

7.4.1 State Variables

N/A

7.4.2 Environment Variables

filesystem [What is the type of your environment variable? Usually a file is abstracted as a sequence of strings. —SS]

7.4.3 Access Routine Semantics

ReadCSV():

ReadCSV reads a .csv file and creates a Spectrum object with the appropriate assignments to intensity and energy range.

- input: *fname: str*
- transition: N/A
- output: **Spectrum** [You have inputs for the constructor for Spectrum; you should identify them here. —SS]
- exceptions:

| Exception | Condition |
|-----------|---------------------------------------------------------------------------------------------|
| NO FILE | The filename does not correspond to any file in the filesystem $fname \notin filesystem$ |
| NOT CSV | The indicated file is not a *.csv format $fname \notin \{files files \in .csv\}$ |

8 MIS of Import dm3 Module

8.1 Module

ImportDM3

8.2 Uses

- Array data structure
- Hardware hiding
- Data Spectrum Image
- Data 1D Spectrum
- Data 2D Image

8.3 Syntax

8.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|---------|---------------|-----------------------|------------------|
| ReadDM3 | fname: string | SI Spectrum Image | NO FILE, NOT DM3 |

8.4 Semantics

This module imports data from .dm3 and initializes the appropriate data type.

8.4.1 State Variables

N/A

8.4.2 Environment Variables

- filesystem: the filesystem of the computer on which SpectrumImageAnalysisPy is being run

8.4.3 Access Routine Semantics

ImportDM3():

- input: *fname: str*
- transition: N/A
- output: Spectrum Image or Spectrum or Image

- exception:

| Exception | Condition |
|-----------|---------------------------------------------------------------------------------------------|
| NO FILE | The filename does not correspond to any file in the filesystem $fname \notin filesystem$ |
| NOT DM3 | The indicated file is not a *.dm3 format |

9 MIS of Import h5 Module

9.1 Module

ImportH5

9.2 Uses

- Array data structure
- Hardware hiding
- Data Spectrum Image
- Data 1D Spectrum
- Data 2D Image

9.3 Syntax

9.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|--------|---------------|-----------------------|--------------------|
| ReadH5 | fname: string | SI Spectrum Image | NO FILE, NOT H5 |

9.4 Semantics

This module handles the reading of .h5 files and assignation of the data contained therein to the appropriate data type.

9.4.1 State Variables

N/A

9.4.2 Access Routine Semantics

ImportDM3():

- input: *fname*: *str*
- transition: N/A
- output: **Spectrum Image** or **Spectrum** or **Image**
- exception:

| Exception | Condition |
|-----------|-------------------------------------------------------------------------------------------------------------------------|
| NO FILE | The filename does not correspond to any file in the filesystem $fname \notin filesystem \Rightarrow \text{NO_FILE}$ |
| NOT H5 | The indicated file is not a *.h5 format |

10 MIS of Import rpl Module

10.1 Module

ImportRPL

10.2 Uses

- **Array data structure**
- **Hardware hiding**
- **Data Spectrum Image**
- **Data 1D Spectrum**
- **Data 2D Image**

10.3 Syntax

10.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|---------|---------------|-----------------------|---------------------|
| ReadRPL | fname: string | SI Spectrum Image | NO FILE, NOT RPL |

10.4 Semantics

This module handles the reading of .rpl files and assigns the data contained within to the appropriate data type.

10.4.1 State Variables

N/A

10.4.2 Access Routine Semantics

ImportRPL():

- input: *fname*: *str*
- transition: N/A
- output: **Spectrum Image** or **Spectrum** or **Image**
- exception:

| Exception | Condition |
|-----------|-------------------------------------------------------------------------------------------------------------------------|
| NO FILE | The filename does not correspond to any file in the filesystem $fname \notin filesystem \Rightarrow \text{NO_FILE}$ |
| NOT RPL | The indicated file is not a *.rpl format |

11 MIS of Export csv Module

11.1 Module

ExportCSV

11.2 Uses

- **Data Extraction 1D Slice**
- **Data Extraction 3D Mask**
- **Data 1D Spectrum**
- **Display 1D Spectrum**
- **Hardware Hiding**

11.3 Syntax

11.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|----------|----------|------|-------------|
| WriteCSV | Spectrum | file | FILE EXISTS |

11.4 Semantics

This module writes Spectrum data to a csv file.

11.4.1 State Variables

N/A

11.4.2 Environment Variables

- filesystem

11.4.3 Access Routine Semantics

WriteCSV():

- input: **Spectrum**
- transition: N/A
- output: csv file containing spectrum data, written to filesystem
- exception:

| Exception | Condition |
|-------------|---------------------------------------------------------------------------------------------------------|
| FILE EXISTS | The filename already exists in the filesystem $fname \in filesystem \Rightarrow \text{FILE_EXISTS}$ |

12 MIS of Export h5 Module

12.1 Module

ExportH5

12.2 Uses

- Data 1D Spectrum
- Data 2D Image
- Data 3D Spectrum Image
- Data Extraction 1D Slice
- Data Extraction 2D Mask
- Data Extraction 3D Mask
- Display 1D Spectrum
- Display 2D Image
- Hardware Hiding

12.3 Syntax

12.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|---------|--------------------------------------|------|-------------|
| WriteH5 | Spectrum Image Spectrum Image | file | FILE EXISTS |

12.4 Semantics

This module writes Spectrum data, Image data, or Spectrum Image data to an h5 file.

12.4.1 State Variables

N/A

12.4.2 Environment Variables

- filesystem

12.4.3 Access Routine Semantics

WriteH5():

- input: Spectrum | Image | Spectrum Image
- transition: N/A

- output: h5 file containing spectrum data, image data, or spectrum image data (including any metadata), written to filesystem
- exception:

| Exception | Condition |
|-------------|--------------------------------------------------------------------------------------------------------|
| FILE EXISTS | The filename already exists in the filesystem $fname \in filesystem \Rightarrow \text{FILE EXISTS}$ |

13 MIS of Export png Module

13.1 Module

ExportPNG

13.2 Uses

- Data Extraction 2D Mask
- Data Extraction 3D Mask
- Data 2D Image
- Display 2D Image
- Hardware Hiding

13.3 Syntax

13.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|----------|-------|------|-------------|
| WritePNG | Image | file | FILE EXISTS |

13.4 Semantics

This module writes Image data to a png file.

13.4.1 State Variables

N/A

13.4.2 Environment Variables

- filesystem

13.4.3 Access Routine Semantics

WritePNG():

- input: **Image**
- transition: N/A
- output: png file containing image data, written to filesystem
- exception:

| Exception | Condition |
|-------------|---------------------------------------------------------------------------------------------------------|
| FILE EXISTS | The filename already exists in the filesystem $fname \in filesystem \Rightarrow \text{FILE_EXISTS}$ |

14 MIS of Export rpl Module

14.1 Module

ExportRPL

14.2 Uses

- **Data 1D Spectrum**
- **Data 2D Image**
- **Data 3D Spectrum Image**
- **Hardware Hiding**

14.3 Syntax

14.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|----------|--------------------------------------|------|-------------|
| WriteRPL | Spectrum Image Spectrum Image | file | FILE EXISTS |

14.4 Semantics

This module writes Spectrum data, Image data, or Spectrum Image data to an rpl file.

14.4.1 State Variables

N/A

14.4.2 Environment Variables

- filesystem

14.4.3 Access Routine Semantics

WriteRPL():

- input: **Spectrum** | **Image** | **Spectrum Image**
- transition: N/A
- output: rpl file containing spectrum data, image data, or spectrum image data (including any metadata), written to filesystem
- exception:

| Exception | Condition |
|-------------|---------------------------------------------------------------------------------------------------------|
| FILE EXISTS | The filename already exists in the filesystem $fname \in filesystem \Rightarrow \text{FILE_EXISTS}$ |

15 MIS of Data Processing Richardson-Lucy Deconvolution Module

15.1 Module

RLDeconvolution

15.2 Uses

- **Array Data Structure**
- **Hardware Hiding**
- **Data 3D Spectrum Image**
- **Data 1D Spectrum**

15.3 Syntax

15.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|-----------------|------------------------------------------|----------------------------|----------------|
| RLDeconvolution | Spectrum, PSF, iterations | deconvolved Spectrum | DIVIDE BY ZERO |
| SIDeconvolution | Spectrum Image, PSF, iterations, threads | deconvolved Spectrum Image | - |

15.4 Semantics

This module performs the Richardson-Lucy deconvolution algorithm on either a Spectrum or Spectrum Image, following [IM2](#) in the SRS. [\[Referencing the SRS is a good idea. —SS\]](#)

15.4.1 State Variables

N/A

15.4.2 Environment Variables

- threads: \mathbb{N} , number of processing threads to use during Spectrum Image deconvolution

15.4.3 Access Routine Semantics

RLDeconvolution():

- input:
 - **Spectrum**, the spectrum to be deconvolved
 - Point Spread Function: **Spectrum**, the point spread function to deconvolve from Spectrum
 - iterations: \mathbb{N} , the number of iterations of the algorithm to perform
- transition: N/A
- output: Deconvolved **Spectrum**
- exception:

| Exception | Condition |
|----------------|---------------------------------------------------------------------------------------------------------------------------------|
| DIVIDE BY ZERO | The algorithm encounters a 0 in the denominator $\sum_l I_{PSF}(E) I_{real(l)}^c(E) = 0 \Rightarrow \text{DIVIDE_BY_ZERO}$ |

SIDeconvolution():

- input:
 - **Spectrum Image**, the spectrum image to be deconvolved
 - Point Spread Function: **Spectrum**, the point spread function to deconvolve from Spectrum Image
 - iterations: \mathbb{N} , the number of iterations of the algorithm to perform
 - threads: \mathbb{N} , the number of processing threads to use in deconvolving the Spectrum Image
- transition: N/A
- output: Deconvolved Spectrum Image
- exception: N/A

16 MIS of Data Processing Normalization Module

16.1 Module

Normalization

16.2 Uses

- **Array Data Structure**
- **Data 3D Spectrum Image**
- **Data 1D Spectrum**
- **Data Extraction 1D Slice**

16.3 Syntax

16.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|---------------|----------------------------------|---------------------|-------------------|
| Normalization | Spectrum Spectrum Image, slice | Normalized Spectrum | DIVIDE BY ZERO |

16.4 Semantics

This module normalizes either a Spectrum or Spectrum Image to the sum over the range defined by the user, following **IM1** in the SRS.

16.4.1 State Variables

N/A

16.4.2 Access Routine Semantics

Normalization():

- input:
 - **Spectrum**, the spectrum to be normalized, or **Spectrum Image**, the spectrum image to be normalized
 - **slice**
- transition: N/A
- output: Normalized **Spectrum** or **Spectrum Image**
- exception:

| Exception | Condition |
|----------------|---------------------------------------------------------------------------------------------------------------------------------|
| DIVIDE BY ZERO | The algorithm encounters a 0 in the denominator $\sum_{E(k=k_1)}^{E(k=k_2)} I(E(k)) = 0 \Rightarrow \text{DIVIDE_BY_ZERO}$ |

17 MIS of Data Processing Gain Correction Module

17.1 Module

GainCorr

17.2 Uses

- **Array Data Structure**
- **Data 3D Spectrum Image**
- **Data 1D Spectrum**

17.3 Syntax

17.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|----------------|----------------------|------------------------------|----------------------------------|
| GainCorrection | data, Gain Reference | Gain Corrected Spec- trum | DIVIDE BY ZERO, SIZE MISMATCH |

17.4 Semantics

This module corrects either a Spectrum or Spectrum Image using a gain reference (obtained from the acquisition camera hardware), following IM4 in the SRS.

17.4.1 State Variables

N/A

17.4.2 Access Routine Semantics

GainCorrection():

- input:
 - data: **Spectrum**, the spectrum to be corrected, or **Spectrum Image**, the spectrum image to be corrected
 - Gain Reference: **Spectrum**, a reference Spectrum obtained from the hardware
- transition: N/A
- output: Gain-corrected **Spectrum** or **Spectrum Image**
- exception:

| Exception | Condition |
|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| DIVIDE BY ZERO | The algorithm encounters a 0 in the denominator $g(E) = 0 \Rightarrow \text{DIVIDE_BY_ZERO}$ |
| SIZE MISMATCH | The size of the gain correction is different from the size of the input data spectral range $\text{len}(g(E)) \neq \text{len}(\text{data.Srange}) = 0 \Rightarrow \text{SIZE_MISMATCH}$ |

18 MIS of Data Processing Background Correction Module

18.1 Module

BkgndCorr

18.2 Uses

- Array Data Structure
- Data 3D Spectrum Image
- Data 1D Spectrum

18.3 Syntax

18.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|----------------------|----------------------------|-------------------------------|----------------------|
| BackgroundCorrection | data, Background Reference | Background corrected Spectrum | Cor- SIZE MIS- MATCH |

18.4 Semantics

This module corrects the background noise for either a Spectrum or Spectrum Image, following **IM3** in the SRS.

18.4.1 State Variables

N/A

18.4.2 Access Routine Semantics

BackgroundCorrection():

- input:
 - data: **Spectrum**, the spectrum to be corrected, or **Spectrum Image**, the spectrum image to be corrected
 - Background Reference: **Spectrum**, a reference Spectrum representing the background noise in the camera
- transition: N/A
- output: Background-corrected **Spectrum** or **Spectrum Image**
- exception:

| Exception | Condition |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SIZE MISMATCH | The size of the background correction is different from the size of the input data spectral range $len(b(E)) \neq len(data.Srange) = 0 \Rightarrow \text{SIZE_MISMATCH}$ |

19 MIS of Data Extraction 1D Slice Module

19.1 Module

Slice1D

19.2 Uses

- Data 1D Spectrum
- Display 1D Spectrum

19.3 Syntax

19.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|----------------|--------------------|----------|----------------------------|
| CreateSlice | data, $[k_1, k_2]$ | slice | RANGE OUTSIDE BOUNDS |
| IntegrateSlice | slice | integral | - |

[What is the type of data, or is data a type? It looks like data is of type Spectrum, so the Input types should be Spectrum. If you would like to show the variable name, you could use the notation data: Spectrum. —SS]

19.4 Semantics

This module allows the user to extract slices from a 1D dataset for further analysis with other modules.

19.4.1 State Variables

- slice: interval of Spectrum between $[k_1, k_2]$

19.4.2 Access Routine Semantics

CreateSlice():

- input:
 - $[k_1, k_2] \in \mathbb{R}^2 \mid [\max(\min(k_1, k_2), \min(data.Srange)).. \min(\max(k_1, k_2), \max(data.Srange))]] \in data.Srange$
 - data: Spectrum
- transition: Creation of slice

- output: slice
- exception:

| Exception | Condition |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| RANGE OUTSIDE BOUNDS | The user tried to select a range of values which was wholly outside the data's spectral range $[max(min(k_1, k_2), min(data.Srange)..min(max(k_1, k_2), max(data.Srange)))]$ $data.Srange \Rightarrow$ RANGE_OUTSIDE_BOUNDS |

IntegrateSlice():

- input
 - slice
- transition: N/A
- output: integral over slice, $\sum_{k_1}^{k_2} data.data$
- exception: N/A

20 MIS of Data Extraction 2D Mask Module

20.1 Module

Mask2D

20.2 Uses

- [Data 2D Image](#)
- [Display 2D Image](#)

20.3 Syntax

20.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|------------|-------------------------|-------------|----------------------|
| CreateMask | vertex list, size(data) | mask2D | RANGE OUTSIDE BOUNDS |
| ApplyMask | data | masked data | SIZE MISMATCH |
| ModifyMask | vertex list | mask2D | RANGE OUTSIDE BOUNDS |

20.4 Semantics

This module allows the user to extract portions of a 2D dataset for further analysis with other modules.

20.4.1 State Variables

- mask2D, $\forall value \in mask, value \in \{True, False\}$, mask of boolean values representing the desired mask from the user

20.4.2 Access Routine Semantics

CreateMask():

- input
 - vertex list: $[x_i, y_i], x_i, y_i \in \mathbb{N}$, a list of (x, y) ordered pairs of indices to access an array of size(data)
 - size(data): \mathbb{N}^2 , the size of the data to which the mask and vertex list refers
- transition: Creates mask
- output: mask2D
- exception:

| Exception | Condition |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| RANGE OUTSIDE BOUNDS | The user tried to select a mask with a vertex outside the data boundaries $[x_i, y_i] \notin [0..size(data_x), 0..size(data_y)] \Rightarrow$ RANGE_OUTSIDE_BOUNDS |

ApplyMask():

- input
 - data: **Image**
- transition:
- output: masked data: **Image**
- exception:

| Exception | Condition |
|---------------|--------------------------------------------------------------------------------------------------------------------------------|
| SIZE MISMATCH | The size of the data is not the same as the size of the mask $size(mask) \neq size(data) \Rightarrow \text{SIZE_MISMATCH}$ |

ModifyMask():

- input
 - vertex list: $[x_i, y_i], x_i, y_i \in \mathbb{N}$, a list of (x, y) ordered pairs of indices to access an array of size(data)
- transition: Update mask to the new set of input vertices
- output: mask2D
- exception:

| Exception | Condition |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| RANGE OUTSIDE BOUNDS | The user tried to select a mask with a vertex outside the data boundaries $[x_i, y_i] \notin [0..size(data_x), 0..size(data_y)] \Rightarrow \text{RANGE_OUTSIDE_BOUNDS}$ |

21 MIS of Data Extraction 3D Mask Module

21.1 Module

Mask3D

21.2 Uses

- Data 3D Spectrum Image
- Display 3D Spectrum Image

21.3 Syntax

21.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|---------------|-------------------------|-------------|-------------------------|
| CreateMask3D | vertex list, size(data) | mask3d | RANGE OUTSIDE BOUNDS |
| ExtrudeMask2D | mask2D, size(data) | mask3d | SIZE MISMATCH |
| ExtrudeMask1D | slice, size(data) | mask3d | SIZE MISMATCH |
| ApplyMask3D | data | masked data | SIZE MISMATCH |
| ModifyMask3D | vertex list | mask3d | RANGE OUTSIDE BOUNDS |

21.4 Semantics

This module allows the user to extract portions of a 3D dataset for further analysis with other modules.

21.4.1 State Variables

- mask3D, $\forall value \in mask, value \in \{True, False\}, size(mask3D) = size(data)$, mask of boolean values representing the desired mask from the user

21.4.2 Access Routine Semantics

CreateMask3D():

- input
 - vertex list: $[x_i, y_i, k_i], x_i, y_i, k_i \in \mathbb{N}$, a list of (x, y, k) ordered pairs of indices to access an array of size(data)
 - size(data): \mathbb{N}^3 , the size of the data to which the mask and vertex list refers
- transition: Creates mask
- output: mask2D
- exception:

| Exception | Condition |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| RANGE OUTSIDE BOUNDS | The user tried to select a mask with a vertex outside the data boundaries $[x_i, y_i, k_i] \notin [0..size(data_x), 0..size(data_y), 0..size(data_k)] \Rightarrow$ RANGE_OUTSIDE_BOUNDS |

ExtrudeMask2D():

- input
 - mask2D: **mask2D**
 - size(data): \mathbb{N}^3 , the size of the data to which the mask and vertex list refers
- transition: Creates mask3D from mask2D by extruding it along the third dimension
- output: mask3D
- exception:

| Exception | Condition |
|---------------|--------------------------------------------------------------------------------------------------------------------------------|
| SIZE MISMATCH | The size of the data is not the same as the size of the mask $size(mask) \neq size(data) \Rightarrow \text{SIZE_MISMATCH}$ |

ExtrudeMask1D():

- input
 - slice: **slice**
 - size(data): \mathbb{N}^3 , the size of the data to which the mask and vertex list refers
- transition: Creates mask3D from slice by extruding it along the two extra dimensions
- output: mask3D
- exception:

| Exception | Condition |
|---------------|--------------------------------------------------------------------------------------------------------------------------------|
| SIZE MISMATCH | The size of the data is not the same as the size of the mask $size(mask) \neq size(data) \Rightarrow \text{SIZE_MISMATCH}$ |

ApplyMask3D():

- input
 - data: **Spectrum Image**
- transition:
- output: Masked data, **Spectrum Image**

- exception:

| Exception | Condition |
|---------------|--------------------------------------------------------------------------------------------------------------------------------|
| SIZE MISMATCH | The size of the data is not the same as the size of the mask $size(mask) \neq size(data) \Rightarrow \text{SIZE_MISMATCH}$ |

ModifyMask3D():

- input
 - vertex list: $[x_i, y_i, k_i], x_i, y_i, k_i \in \mathbb{N}$, a list of (x, y, k) ordered pairs of indices to access an array of size(data)
 - size(data): \mathbb{N}^3 , the size of the data to which the mask and vertex list refers
- transition: Creates mask
- output: mask3D
- exception:

| Exception | Condition |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| RANGE OUTSIDE BOUNDS | The user tried to select a mask with a vertex outside the data boundaries $[x_i, y_i, k_i] \notin [0..size(data_x), 0..size(data_y), 0..size(data_k)] \Rightarrow \text{RANGE_OUTSIDE_BOUNDS}$ |

22 MIS of Display 1D Spectrum Module

22.1 Module

Disp1D

22.2 Uses

- Data 1D Spectrum
- Plotting library

22.3 Syntax

22.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|------|------|-----------------------|------------|
| plot | data | axis1D, event handler | - |

22.4 Semantics

This module plots 1D spectrum data and allows event handling (*eg*, to slice the spectrum).

22.4.1 State Variables

- Spectrum axis: **axis1D** containing the plotted data and **event handler**

22.4.2 Access Routine Semantics

plot():

- input:
 - data: **Spectrum**
- transition: create axis and plot data on axis, initialize event handler for axis
- output:
 - axis1D: **axis1D**
 - event handler: **axis1D**
- exception: N/A

23 MIS of Display 2D Image Module

23.1 Module

Disp2D

23.2 Uses

- **Data 1D Spectrum**
- **Plotting library**

23.3 Syntax

23.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|----------------|-----------------------|--------------------------|----------------|
| plot | data | axis2D, event handler | - |
| AddScalebar | - | - | NO CALIBRATION |
| ChangeContrast | [minC, maxC], data | - | OUT OF RANGE |

23.4 Semantics

This module plots 2D image data and allows event handling (*eg*, to create masks on the image).

23.4.1 State Variables

- Image axis: **axis2D** containing the plotted data and **event handler**

23.4.2 Access Routine Semantics

plot():

- input:
 - data: **Image**
- transition: create axis and plot data on axis, initialize event handler for axis
- output:
 - axis2D: **axis2D**
 - event handler: **axis2D**
- exception: N/A

AddScalebar():

- input: N/A
- transition: Add scalebar to Image axis
- output: N/A
- exception:

| Exception | Condition |
|----------------|-------------------------------------------------------------------------------------------------------------------------------|
| NO CALIBRATION | No calibration exists in the image, so a scalebar cannot be added $\nexists data.Imcal \Rightarrow \text{NO_CALIBRATION}$ |

ChangeContrast():

- input:
 - $[minC, maxC], \in \mathbb{R}^2$, the minimum and maximum contrast to stretch the colourscale to
 - data: **Image**
- transition: Change the contrast of the displayed image
- output: N/A
- exception:

| Exception | Condition |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| OUT OF RANGE | The user tried to select a contrast range of values which was wholly outside the data's intensity limits $[max(minC, min(data.data)..maxC, max(data.data))]$ \notin $data.Srange \Rightarrow \text{OUT_OF_RANGE}$ |

24 MIS of Display 3D Spectrum Image Module

24.1 Module

Disp3D

24.2 Uses

- Data
- Plotting library
- 2D image plot
- 1D spectrum plot

24.3 Syntax

24.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|------|------|-------------------------|------------|
| plot | data | figure3d, event handler | - |

24.4 Semantics

This module arranges the elements of the 1D and 2D display modules to suit a 3D dataset, and allows connection of the different axes (through event handling) such that within one figure, all axes refer to the same dataset.

24.4.1 State Variables

- figure3d: **figure** containing image plot, spectrum plot, mask plot, colourbar, and image contrast histogram
- image plot: **axis2D** for plotting images extracted from **slicing** the spectrum axis
- spectrum plot: **axis1D** for plotting spectra extracted from **masks** on the image axis
- mask plot: **axis2D**
- colourbar axis: colourbar **axis** for image plot
- image contrast axis: histogram **axis** for image plot

24.4.2 Access Routine Semantics

plot():

- input:
 - data: **Image**
- transition: create axis and plot data on axis, initialize event handler for axis
- output:
 - figure3D: contains **axis1D**, **axis2D**
 - event handler for **axis1D**
 - event handler for **axis2D**
- exception: N/A

25 MIS of Data 1D Spectrum Module

25.1 Template Module

Spectrum

25.2 Uses

- Array data structure

25.3 Syntax

25.3.1 Types

Spectrum

25.3.2 Exported Access Programs

| Name | In | Out | Exceptions |
|------|----------------------------------------------------------------------|-----|----------------------------------------|
| init | data, (Srange (dis- person & [index, value])), Slabel, Sunit | - | WRONG DATA TYPE, LENGTH MISMATCH |

25.4 Semantics

This module contains the abstract data type Spectrum, including the following state variables.

25.4.1 State Variables

- $SRange$: \mathbb{R}^K
- $data$: \mathbb{R}^K
- $index$: \mathbb{Z}
- $value$: \mathbb{R}
- $dispersion$: \mathbb{R}
- $Slabel$: str
- $Sunit$: str
- $metadata$: $dict$

25.4.2 Access Routine Semantics

`init()`: `init` initializes a `Spectrum` object.

- input:
 - *data*: intensity values, $\in \mathbb{R}^K$
 - *Srange*: spectral axis values, $\in \mathbb{R}^K$
 - *dispersion*: difference between neighbouring channels along the spectral axis, \mathbb{R}
 - *index*: location on the spectral axis at which *value* is, \mathbb{Z}
 - *value*: value of the spectral axis (in spectral axis units) at the location given by *index*, \mathbb{R}
 - *Slabel*: spectrum label, the name for the spectral axis (*e.g.* Energy, Wavelength), *str*
 - *Sunit*: spectrum units, the units which the spectral axis uses (*e.g.* eV, nm), *str*
- transition: Creates all state variables
- output: N/A [You actually have an output for a constructor. If you look at slide 19 of the MISContinued slides, you'll see an example of an ADT. You output the object here and then it can be an input for another access program. —SS]
- exception:

| Exception | Condition |
|------------------|----------------------------------------------------------------------------------------------------------|
| WRONG DATA TYPE | Any of the input data are the wrong type |
| LENGTH MIS-MATCH | The length of <i>Srange</i> is not the same as the length of <i>data</i> $len(Srange) \neq len(data)$ |

26 MIS of Data 2D Image Module

26.1 Template Module

Image

26.2 Uses

- Array data structure

26.3 Syntax

26.3.1 Types

Image

26.3.2 Exported Access Programs

| Name | In | Out | Exceptions |
|------|-----------------------|-----|-----------------------------------------|
| init | data, Imcal, metadata | - | WRONG DATA TYPE, WRONG DIMENSIONS |

26.4 Semantics

This module contains the abstract data type Spectrum, including the following state variables.

26.4.1 State Variables

- data: $\mathbb{R}^{X \times Y}$
- Imcal: \mathbb{R}
- metadata: dict

26.4.2 Access Routine Semantics

init(): init initializes an Image object.

- input:
 - *data*: intensity values, $\in \mathbb{R}^{X \times Y}$
 - *Imcal*: image calibration values (*e.g.* number of nm per pixel), $\in \mathbb{R}$
 - *metadata*: dictionary containing extra information about the source of the image (*e.g.* experimental parameters)
- transition: Creates all state variables
- output: N/A
- exception:

| Exception | | Condition |
|----------------|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| WRONG TYPE | DATA | The input data are not real numbers or the Imcal value is not a real float $data \notin \mathbb{R}^{X \times Y} Imcal \notin \mathbb{R} \Rightarrow \text{WRONG_DATA_TYPE}$ |
| WRONG SIONS | DIMEN- | The input data is not 2D $size(data) \notin \mathbb{N}^2 \Rightarrow \text{WRONG_DIMENSIONS}$ |

27 MIS of Data 3D Spectrum Image Module

27.1 Template Module

SI

27.2 Uses

- Array Data Structure

27.2.1 Types

Spectrum Image

27.2.2 Exported Access Programs

| Name | In | Out | Exceptions |
|------|---------------------------------------------------------------------------------------|-----|-----------------------------------------|
| init | data, Srange disper- sion & [index, value], Slabel, Sunit, Imcal, metadata | - | WRONG DATA TYPE, WRONG DIMENSIONS |

27.3 Semantics

This module holds spectrum image data (a 3D dataset) and associated calibrations and other related information.

27.3.1 State Variables

- $data: \mathbb{R}^{X \times Y \times K}$
- $Imcal: \mathbb{R}$

- *dispersion*: \mathbb{R}
- *Srange*: \mathbb{R}^K
- *index*: \mathbb{Z}
- *value*: \mathbb{R}
- *Slabel*: string
- *Sunit*: string
- *metadata*: dict

27.3.2 Access Routine Semantics

init

- input:
 - *data*: intensity values, $\in \mathbb{R}^{X \times Y \times K}$
 - *Srange*: spectral axis values, $\in \mathbb{R}^K$
 - *dispersion*: difference between neighbouring channels along the spectral axis, \mathbb{R}
 - *index*: location on the spectral axis at which *value* is, \mathbb{Z}
 - *value*: value of the spectral axis (in spectral axis units) at the location given by *index*, \mathbb{R}
 - *Slabel*: spectrum label, the name for the spectral axis (*e.g.* Energy, Wavelength), *str*
 - *Sunit*: spectrum units, the units which the spectral axis uses (*e.g.* eV, nm), *str*
 - *Imcal*: image calibration values (*e.g.* number of nm per pixel), $\in \mathbb{R}$
 - *metadata*: dictionary containing extra information about the source of the image (*e.g.* experimental parameters)
- transition: Initialize all state variables
- output: N/A
- exception:

| Exception | Condition |
|------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| WRONG DATA TYPE | Any of the input data are the wrong type $(data \notin \mathbb{R}^{X \times Y \times K}) \vee (Srange \notin \mathbb{R}^K) \vee (dispersion \notin \mathbb{R}) \vee (index \notin \mathbb{Z}) \vee (value \notin \mathbb{R}) \vee (Slabel \notin str) \vee (Sunit \notin str) \vee (Imcal \notin \mathbb{R}) \Rightarrow \text{WRONG_DATA_TYPE}$ |
| LENGTH MIS-MATCH | The length of Srange is not the same as the length of data's spectral axis $len(Srange) \neq size(data)[2] \Rightarrow \text{LENGTH_MISMATCH}$ |
| WRONG DATA TYPE | The input data are not real numbers or the Imcal value is not a real float $data \notin \mathbb{R}^{X \times Y} \vee Imcal \notin \mathbb{R} \Rightarrow \text{WRONG_DATA_TYPE}$ |
| WRONG DIMENSIONS | The input data is not 2D $size(data) \notin \mathbb{N}^2 \Rightarrow \text{WRONG_DIMENSIONS}$ |

28 MIS of Array Data Structure Module

28.1 Template Module

Array

28.2 Uses

N/A

28.3 Syntax

28.3.1 Type

- Array

28.3.2 Exported Access Programs

| Name | In | Out | Exceptions |
|-------------|-------|-------|------------|
| CreateArray | data | Array | - |
| ModifyArray | Array | Array | - |

28.4 Semantics

This module holds the array structure and functions for performing various calculations on arrays.

28.4.1 State Variables

- Array: \mathbb{C}^N , $\dim(N) \in \mathbb{N}$

28.4.2 Access Routine Semantics

CreateArray():

- input: data, \mathbb{C}^N
- transition: Create array variable
- output: Array, \mathbb{C}^N
- exception: N/A

ModifyArray():

- input: Array, \mathbb{C}^N
- transition: Modify array by some operation, including but not limited to, addition, subtraction, multiplication, division, *etc.*
- output: Array, \mathbb{C}^N
- exception: N/A

29 MIS of Plotting Library Module

29.1 Module

Plotting

29.2 Uses

- Hardware Hiding Module

29.3 Syntax

29.3.1 Exported Access Programs

| Name | In | Out | Exceptions |
|------|------|--------|------------|
| plot | data | window | - |

29.4 Semantics

This module is the basis for plotting 1D and 2D data and handling events such as mouse clicks and keyboard presses.

29.4.1 State Variables

- figure
- axis1D
- axis2D
- event handler

29.4.2 Environment Variables

- window: 2D on-screen display of plot figure

29.4.3 Access Routine Semantics

plot():

- input: data, $\mathbb{R}^K | \mathbb{R}^{X \times Y}$
- transition: Creates a figure to display the input data, with a 1D plot axis for 1D data or a 2D plot axis for 2D data. Provides handling for events such as mouse clicks or keyboard key presses and options to format the display.
- output: window
- exception:

[Great work. There is too much in here for me to go over everything, but I am confident that you are on the right track with your documentation. Hopefully maintaining the documentation with the code will not be too difficult. I look forward to your feedback in the future to see how easy/hard it is to keep the documentation in sync. —SS]

References

- [1] D. M. Hoffman and P. A. Strooper, *Software Design, Automated Testing, and Maintenance: A Practical Approach*. New York, NY, USA: International Thomson Computer Press, 1995.
- [2] C. Ghezzi, M. Jazayeri, and D. Mandrioli, *Fundamentals of Software Engineering*. Upper Saddle River, NJ, USA: Prentice Hall, 2nd ed., 2003.