

# 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](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](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

### 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

#### 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

## 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

### 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

## 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**
- 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.

#### 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 Spectrum	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	-

## 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:
  - $[k_1, k_2] \in \mathbb{R}^2[[\max(\min(k_1, k_2), \min(data.Srange).. \min(\max(k_1, k_2), \max(data.Srange))) \in data.Srange]$
  - 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 $[\max(\min(k_1, k_2), \min(data.Srange).. \min(\max(k_1, k_2), \max(data.Srange))) \in data.Srange \Rightarrow \text{RANGE\_OUTSIDE\_BOUNDS}]$

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 OUT-SIDE BOUNDS
ApplyMask	data	masked data	SIZE MIS-MATCH
ModifyMask	vertex list	mask2D	RANGE OUT-SIDE 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 $size(mask) \neq size(data) \Rightarrow$ 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 $[x_i, y_i] \notin [0..size(data_x), 0..size(data_y)] \Rightarrow$ 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 $size(mask) \neq size(data) \Rightarrow$ 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 $[x_i, y_i, k_i] \notin [0..size(data_x), 0..size(data_y), 0..size(data_k)] \Rightarrow$ 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 $[max(minC, min(data.data)..maxC, max(data.data))]$ $\notin$ $data.Srange \Rightarrow$ 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- persion & [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
- `exception`:



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

## 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 $data \notin \mathbb{R}^{X \times Y} \mid Imcal \notin \mathbb{R} \Rightarrow \text{WRONG\_DATA\_TYPE}$
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   dispersion & [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 MISMATCH	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:

## 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.