Module Interface Specification for SpectrumImageAnalysisPy

Isobel Bicket

December 7, 2017

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.

Contents

	nbols, Abbreviations and Acronyms	
Intr		
	roduction	
Not	tation	
Mo	dule Decomposition	
MIS	S of Hardware Hiding Module	
6.1	Module	
6.2	Uses	
6.3	Syntax	
	6.3.1 Exported Access Programs	
6.4	Semantics	
	6.4.1 State Variables	
	6.4.2 Environment Variables	
	6.4.3 Access Routine Semantics	
MIS	S of Import csv Module	
7.1	Module	
7.2	Uses	
7.3	Syntax	
	7.3.1 Exported Access Programs	
7.4	Semantics	
	7.4.1 State Variables	
	7.4.2 Environment Variables	
	7.4.3 Access Routine Semantics	
MIS	S of Import dm3 Module	
8.1	Module	
8.2		
8.3		
-		
8.4	-	
J		
	Mo MI3 6.1 6.2 6.3 6.4 MI3 7.1 7.2 7.3 7.4 MI3 8.1 8.2 8.3	MIS of Hardware Hiding Module 6.1 Module 6.2 Uses 6.3 Syntax 6.3.1 Exported Access Programs 6.4 Semantics 6.4.1 State Variables 6.4.2 Environment Variables 6.4.3 Access Routine Semantics MIS of Import csv Module 7.1 Module 7.2 Uses 7.3 Syntax 7.3.1 Exported Access Programs 7.4 Semantics 7.4.1 State Variables 7.4.2 Environment Variables 7.4.3 Access Routine Semantics MIS of Import daccess Programs 7.4 Semantics 7.4.1 State Variables 7.4.2 Environment Variables 7.4.3 Access Routine Semantics MIS of Import dm3 Module 8.1 Module 8.2 Uses 8.3 Syntax 8.3.1 Exported Access Programs

9	MIS	of Im	port h5 Module									7
	9.1	Module	e			 						7
	9.2	Uses .				 						7
	9.3	Syntax				 						7
		9.3.1	Exported Access Programs	3		 						7
	9.4	Semant	m tics			 						7
		9.4.1	State Variables			 						7
		9.4.2	Access Routine Semantics									8
10	MIS	of Im	port rpl Module									8
	10.1	Module	e			 						8
	10.2	Uses .				 						8
	10.3	Syntax				 						8
		10.3.1	Exported Access Programs	3		 						8
	10.4	Semant	m tics			 						9
		10.4.1	State Variables			 						9
		10.4.2	Access Routine Semantics					 •				9
11	MIS	of Ex	port csv Module									9
	11.1	Module	e			 						9
	11.2	Uses .				 						9
	11.3	Syntax				 						10
		11.3.1	Exported Access Programs	8		 						10
	11.4	Semant	m tics			 						10
		11.4.1	State Variables			 						10
		11.4.2	Environment Variables			 						10
		11.4.3	Access Routine Semantics									10
12	MIS	of Ex	port h5 Module									10
	12.1	Module	e			 						10
	12.2	Uses .				 						11
	12.3	Syntax				 						11
			Exported Access Programs									11
	12.4	Semant	${ m tics}$			 						11
		12.4.1	State Variables			 						11
		12.4.2	Environment Variables			 						11
		12.4.3	Access Routine Semantics					 •				11
13	MIS	of Ex	port png Module									12
	13.1	Module	e			 						12
	13.2	Uses .				 						12
	13.3	Syntax				 						12
		•	Exported Access Programs									12

13.4	Semantics	12
	13.4.1 State Variables	12
	13.4.2 Environment Variables	13
	13.4.3 Access Routine Semantics	13
14 MIS	S of Export rpl Module	13
14.1	Module	13
14.2	Uses	13
14.3	Syntax	13
	14.3.1 Exported Access Programs	13
14.4		14
	14.4.1 State Variables	14
	14.4.2 Environment Variables	14
	14.4.3 Access Routine Semantics	14
15 MIS	S of Data Processing Richardson-Lucy Deconvolution Module	14
	Module	14
	Uses	14
		15
	· ·	15
15.4		15
		15
	15.4.2 Environment Variables	15
		15
16 MIS	S of Data Processing Normalization Module	16
	Module	16
		16
		16
		16
16.4	- · · · · · · · · · · · · · · · · · · ·	16
		17
		17
17 MIS	S of Data Processing Gain Correction Module	17
	Module	17
	Uses	17
	Syntax	17
0	17.3.1 Exported Access Programs	17
17.4	Semantics	18
	17.4.1 State Variables	18
	17.4.2 Access Routine Semantics	18

18	MIS	S of Data Processing Background Correction Module	18
	18.1	Module	18
	18.2	Uses	19
	18.3	Syntax	19
		18.3.1 Exported Access Programs	19
	18.4	Semantics	19
		18.4.1 State Variables	19
		18.4.2 Access Routine Semantics	19
19	MIS	of Data Extraction 1D Slice Module	20
	19.1	Module	20
	19.2	Uses	20
	19.3	Syntax	20
		19.3.1 Exported Access Programs	20
	19.4	Semantics	20
		19.4.1 State Variables	20
		19.4.2 Access Routine Semantics	20
20	MIS	of Data Extraction 2D Mask Module	21
	20.1	Module	21
		Uses	21
	20.3	Syntax	21
		20.3.1 Exported Access Programs	21
	20.4	Semantics	22
		20.4.1 State Variables	22
		20.4.2 Access Routine Semantics	22
21		of Data Extraction 3D Mask Module	23
		Module	
		Uses	
	21.3	Syntax	24
		21.3.1 Exported Access Programs	
	21.4	Semantics	24
		21.4.1 State Variables	24
		21.4.2 Access Routine Semantics	24
22		S of Display 1D Spectrum Module	2 6
		Module	26
		Uses	26
	22.3	Syntax	27
		22.3.1 Exported Access Programs	27
	22.4	Semantics	27
		22 4 1 State Variables	27

		22.4.2 Access Routine Semantics	27							
23		1 0	27							
	23.1		27							
	23.2	Uses	27							
	23.3	Syntax	28							
		23.3.1 Exported Access Programs	28							
	23.4	Semantics	28							
		23.4.1 State Variables	28							
			28							
24	MIS	of Display 3D Spectrum Image Module	29							
	24.1	Module	29							
	24.2	Uses	29							
	24.3	Syntax	30							
		24.3.1 Exported Access Programs	30							
	24.4		30							
		24.4.1 State Variables	30							
			30							
25	MIS of Data 1D Spectrum Module 3									
	25.1	Template Module	31							
			31							
			31							
		V	31							
		V 1	31							
	25.4		31							
	20.1		31							
			32							
26	MIS	of Data 2D Image Module	32							
			32							
		1	32							
			33							
		·	33							
		V -	33							
	26.4	·	33							
	20.1		33							
			33							
27	MIS	of Data 3D Spectrum Image Module	3 4							
•		•	34							
		•	3/							

		27.2.1 Types
		27.2.2 Exported Access Programs
	27.3	Semantics
		27.3.1 State Variables
		27.3.2 Access Routine Semantics
28	MIS	of Array Data Structure Module 36
	28.1	Template Module
	28.2	<u>Uses</u>
	28.3	Syntax
		28.3.1 Type
		28.3.2 Exported Access Programs
	28.4	Semantics
		28.4.1 State Variables
		28.4.2 Access Routine Semantics
2 9	MIS	of Plotting Library Module 37
	29.1	Module
	29.2	Uses
		Syntax
		29.3.1 Exported Access Programs
	29.4	Semantics
		29.4.1 State Variables
		29.4.2 Environment Variables
		20.4.3 Access Routino Somenties

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 SpectrumImageAnalysisPyis 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 $(c_1 \Rightarrow r_1 | c_2 \Rightarrow r_2 | ... | c_n \Rightarrow r_n)$.

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	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():

- \bullet 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 one 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 assignations 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 file system $fname \notin filesystem$
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 file system $fname \notin filesystem$
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 file system $fname \notin filesystem \Rightarrow \text{NO_FILE}$
NOT H5	The indicated file is not a *.h5 format

10 MIS of Import rpl Module

10.1 Module

 ${\bf ImportRPL}$

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 Ima	age 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 file system $fname \notin filesystem \Rightarrow \text{NO_FILE}$
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	file	FILE EXISTS
	Spectrum Image		

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 $fname \in filesystem \Rightarrow FILE_EXISTS$

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 $fname \in filesystem \Rightarrow FILE_EXISTS$

14 MIS of Export rpl Module

14.1 Module

 ${\bf ExportRPL}$

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	file	FILE EXISTS
	Spectrum Image		

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
- \bullet 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, itera-	deconvolved Spectrum	DIVIDE
	tions			BY ZERO
SIDeconvolution	Spectrum	Image,	deconvolved Spectrum	-
	PSF,	iterations,	Image	
	threads			

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: 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: 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: 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	Normalized Spectrum	DIVIDE
	Image, slice		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	\mathbf{Out}	Exceptions
GainCorrection	data, Gain Reference	Gain Corrected Spec-	DIVIDE BY ZERO,
		trum	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 $len(g(E)) \neq len(data.Srange) = 0 \Rightarrow \text{SIZE_MISMATCH}$

18 MIS of Data Processing Background Correction Module

18.1 Module

 ${\bf BkgndCorr}$

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		Exceptio	ns
BackgroundCorrection	data,	Background	Background	Cor-	SIZE	MIS-
	Refere	ence	rected Spectrum		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 $len(b(E)) \neq len(data.Srange) = 0 \Rightarrow SIZE_MISMATCH$

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
Integrate Slice	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:
 - $[k_1, k_2] \in \mathbb{R}^2 | [max(min(k_1, k_2), min(data.Srange)..min(max(k_1, k_2), max(data.Srange)))] \in data.Srange$
 - 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():

 \bullet 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
	$[x_i, y_i] \notin [0size(data_x), 0size(data_y)] \Rightarrow RANGE_OUTSIDE_BOUNDS$

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
	$[x_i, y_i] \notin [0size(data_x), 0size(data_y)] \Rightarrow RANGE_OUTSIDE_BOUNDS$

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
	$[x_i, y_i, k_i] \notin [0size(data_x), 0size(data_y), 0size(data_k)] \Rightarrow RANGE_OUTSIDE_BOUNDS$

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 $size(mask) \neq size(data) \Rightarrow SIZE_MISMATCH$

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 $size(mask) \neq size(data) \Rightarrow SIZE_MISMATCH$

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
	$[x_i, y_i, k_i] \notin [0size(data_x), 0size(data_y), 0size(data_k)] \Rightarrow RANGE_OUTSIDE_BOUNDS$

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	
${\it AddScalebar}$	-	-	NO CALIBRATION
Change Contrast	$[\min C, \max C],$	-	OUT OF RANGE
	data		

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
- ullet 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 scale bar cannot be added $\not\equiv data.Imcal \Rightarrow \text{NO_CALIBRATION}$

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 (dispersion & [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}

ullet Slabel: str

 \bullet Sunit: str

ullet $metadata:\ dict$

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 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 $data \notin \mathbb{R}^{X \times Y} Imcal \notin \mathbb{R} \Rightarrow \text{WRONG_DATA_TYPE}$
WRONG SIONS	DIMEN-	The input data is not 2D
		$size(data) \notin \mathbb{N}^2 \Rightarrow WRONG_DIMENSIONS$

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

 \bullet 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), ∈ \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}) (Srange \notin \mathbb{R}^K) (dispersion \notin \mathbb{R}) (index \notin \mathbb{Z}) (value \notin \mathbb{R}) (Slabel \notin str) (Sunit \notin str) (Imcal \notin \mathbb{R}) \Rightarrow 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	
	$data \notin \mathbb{R}^{X \times Y} Imcal \notin \mathbb{R} \Rightarrow WRONG_DATA_TYPE$	
WRONG DI- MENSIONS	- 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.