SpectrumImageAnalysisPy

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1 Revision History

Date	Version	Notes
Date 1	1.0	Notes
Date 2	1.1	Notes

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2 Reference Material

This section records information for easy reference.

2.1 Table of Units

Throughout this document SI (Système International d'Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the SI name.

symbol	**unit**	**SI**
nm	length	nanometre
eV	energy	electron volt

[Only include the units that your SRS actually uses —SS]

2.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units. The choice of symbols was made to be consistent with the heat transfer literature and with existing documentation for solar water heating systems. The symbols are listed in alphabetical order.

symbol	**unit**	**description**
A_C	m^2	coil surface area
A_{in}	m^2	surface area over which heat is transferred in

[Use your problems actual symbols. The si package is a good idea to use for units. —SS]

Table 1: **Revision History**

Date	**Version**	**Notes**
Date 1	1.0	Notes
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2.3 Abbreviations and Acronyms

symbol	description
3D	Three-dimensional
A	Assumption
CL	Cathodoluminescence Spectroscopy
DD	Data Definition
EELS	Electron Energy Loss
EELS	Electron Energy Loss Spectroscopy
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
PS	Physical System Description
PSF	Point Spread Function
R	Requirement
SI	Spectrum Image
SRS	Software Requirements Specification
STEM	Scanning Transmission Electron Microscope
SEM	Scanning Electron Microscope
SpectrumImageAnalysisPy	[put your program name here —SS]
T	Theoretical Model

[Add any other abbreviations or acronyms that you add —SS]

3 Introduction

[This SRS template is based on **??**. It will get you started, but you will have to make changes. Any changes to section headings should be approved by the instructor, since that implies a deviation from the template. Although the bits shown below do not include type information, you may need to add this information for your problem. —SS]

[Feel free to change the appearance of the report by modifying the LaTeX commands. —SS]

[If you are documenting a family of models, you can start from this same template, but you will have to add a section for variabilities. For program families you should look at **??**. You should be able to do one document that captures the commonality analysis and the requirements. —SS]

3.1 Purpose of Document

This document details the requirements of the software SpectrumImageAnalysisPy.

3.2 Scope of Requirements

The scope of the requirements for the software SpectrumImageAnalysisPy is limited to the import; removal of instrumentation artifacts; visualization and navigation through; and the export of EELS and CL spectrum imaging data.

3.3 Characteristics of Intended Reader

The reader of this document should have an understanding of spectrum imaging techniques, particularly EELS and the data processing methods used to remove effects of the acquisition system from the data acquired. A basic knowledge of convolution theory will be helpful to the reader and an understanding of the characteristics of 3D datasets. The reader should understand EELS and CL, as relevant to the sections of the document.

3.4 Organization of Document

4 General System Description

This section identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

4.1 System Context

Use of the software SpectrumImageAnalysisPy infers the following responsibilities on the part of the user, and confers the following responsibilities from the program.

- User Responsibilities:
  - Provide the correct input data to the program;
  - Be capable of interacting with the software via a mouse and keyboard;
  - Have the necessary dependencies for the program installed;
  - Judge the quality of the output data is sufficient for the application, or change the processing steps performed;
- SpectrumImageAnalysisPy Responsibilities:
  - Check the inputs for the correct data type and size
  - Display the data and graphical user interface for the user to interact with
  - Respond to user commands as appropriate, including visualization and data processing commands
  - Export data in the correct file format(s)

4.2 User Characteristics

The end user of SpectrumImageAnalysisPy should be familiar with the concept of a spectrum image and an understanding of what the data represents and the appropriate actions needed to process spectrum images and extract useful information. A basic familiarity with programming is expected. An understanding of the spectro-microscopy technique (CL or EELS) used to generate the data will be beneficial, but is not strictly required.

4.3 System Constraints

The software must be able to read .dm3 and .dm4 files for EELS data import, and .h5 files for CL data import.

5 Specific System Description

This section first presents the problem description, which gives a high-level view of the problem to be solved. This is followed by the solution characteristics specification, which presents the assumptions, theories, definitions and finally the instance models. [Add any project specific details that are relevant for the section overview. —SS]

5.1 Problem Description

SpectrumImageAnalysisPy is a software to allow users to import, process, navigate, and export spectrum image data.

5.1.1 Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

- Spectrum Image
- Point Spread Function (PSF)
- Sample

5.1.2 Physical System Description

The physical system of SpectrumImageAnalysisPy, as shown in Figure ?, includes the following elements:

PS1: Sample under study.

PS2: STEM equipped with EEL spectrometer. [Find an image/schematic of Titan —Author]

PS3: SEM or STEM equipped with CL collection system. [Find an image/schematic of SEM-CL system —Author]

[A figure here may make sense for most SRS documents —SS]

5.1.3 Goal Statements

Given the [inputs —SS], the goal statements are:

GS1: Read in a three-dimensional dataset

GS2: Display a three-dimensional dataset to allow the user to interact with it and navigate all three dimensions

GS3: Provide processing options including: normalization and deconvolution for EELS SI; normalization and background subtraction for a CL SI

GS4: Extract slices from the dataset as desired by the user and communicated through the user interface

5.2 Solution Characteristics Specification

The instance models that govern SpectrumImageAnalysisPy are presented in Subsection 5.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

5.2.1 Assumptions

This section simplifies the original problem and helps in developing the theoretical model by filling in the missing information for the physical system. The numbers given in the square brackets refer to the theoretical model [T], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

A1: The EELS data can be described as the convolution of the "real" spectrum of the sample with the response of the microscope and spectrometer system function. The microscope and spectrometer system typically causes broadening in the peaks of the "real" spectrum.

A2: Fluctuations in the intensity of the EELS signal are due to changes in the beam current as collected by the spectrometer.

A3: A subtraction can be performed to remove the contributions of the dark signal and the substrate signal from the sample signal.

A4: The spectrometer wavelength sensitivity can be accurately modelled by experimental reference data.

5.2.2 Theoretical Models

This section focuses on the general equations and laws that SpectrumImageAnalysisPy is based on. [Modify the examples below for your problem, and add additional models as appropriate. —SS]

Number	T1
Label	**Conservation of thermal energy**
Equation	$-\nabla \cdot \mathbf{q} + g = \rho C \frac{\partial T}{\partial t}$
Description	The above equation gives the conservation of energy for transient heat transfer in a material of specific heat capacity C ($\mathrm{J\,kg^{-1}\,°C^{-1}}$) and density ρ ($\mathrm{kg\,m^{-3}}$), where $\mathbf{q}$ is the thermal flux vector ($\mathrm{W\,m^{-2}}$), g is the volumetric heat generation ($\mathrm{W\,m^{-3}}$), T is the temperature (°C), t is time (s), and ∇ is the gradient operator. For this equation to apply, other forms of energy, such as mechanical energy, are assumed to be negligible in the system (A**??**). In general, the material properties (ρ and C) depend on temperature.
Source	http://www.efunda.com/formulae/heat_transfer/conduction/overview_cond.cfm
Ref. By	GD**??**

5.2.3 General Definitions

This section collects the laws and equations that will be used in deriving the data definitions, which in turn are used to build the instance models. [Some projects may not have any content for this section, but the section heading should be kept. —SS] [Modify the examples below for your problem, and add additional definitions as appropriate. —SS]

Number	GD1
Label	**Newton's law of cooling**
SI Units	$\mathrm{W\,m^{-2}}$
Equation	$q(t) = h\Delta T(t)$
Description	Newton's law of cooling describes convective cooling from a surface. The law is stated as: the rate of heat loss from a body is proportional to the difference in temperatures between the body and its surroundings. $q(t)$ is the thermal flux ($\mathrm{W\,m^{-2}}$). h is the heat transfer coefficient, assumed independent of T (A**??**) ($\mathrm{W\,m^{-2}\,°C^{-1}}$). $\Delta T(t) = T(t) - T_{\text{env}}(t)$ is the time-dependent thermal gradient between the environment and the object (°C).
Source	(**?**, p. 8)
Ref. By	DD1, DD**??**

Detailed derivation of simplified rate of change of temperature

[This may be necessary when the necessary information does not fit in the description field. —SS]

5.2.4 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given. [Modify the examples below for your problem, and add additional definitions as appropriate. —SS]

Number	DD1
Label	**Heat flux out of coil**
Symbol	q_C
SI Units	$\mathrm{W\,m^{-2}}$
Equation	$q_C(t) = h_C(T_C - T_W(t))$, over area A_C
Description	T_C is the temperature of the coil (°C). T_W is the temperature of the water (°C). The heat flux out of the coil, q_C ($\mathrm{W\,m^{-2}}$), is found by assuming that Newton's Law of Cooling applies (A**??**). This law (GD1) is used on the surface of the coil, which has area A_C ($\mathrm{m^2}$) and heat transfer coefficient h_C ($\mathrm{W\,m^{-2}\,°C^{-1}}$). This equation assumes that the temperature of the coil is constant over time (A**??**) and that it does not vary along the length of the coil (A**??**).
Sources	**?**
Ref. By	IM2

5.2.5 Instance Models

This section transforms the problem defined in Section 5.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 5.2.4 to replace the abstract symbols in the models identified in Sections 5.2.2 and 5.2.3.

The goals [reference your goals —SS] are solved by [reference your instance models —SS]. [other details, with cross-references where appropriate. —SS] [Modify the examples below for your problem, and add additional models as appropriate. —SS]

Number	IM1
Label	**Normalization to the integral**
Input	k_1 k_2 $I(x_i, y_j, E_k)$ The input is constrained such that $k_1 >= 0$, and $k_2 <= N$
Output	$I_{norm}(x_i, y_j, E_k) = \frac{I(x_i,y_j,E_k)}{\sum_{E_k=k_1}^{E_k=k_2} I(x_i,y_j,E_k)}$
Description	$I(x_i, y_j, E_k)$ is the 3D spectrum image, user input k_1: Index of beginning of spectrum range (spectrum axis), user input k_2: Index of end of spectrum range (spectrum axis), user input K: Last index along the spectral axis x_i: Pixel index along first spatial axis y_j: Pixel index along second spatial axis $I_{norm}(x_i, y_j, E_k)$: Spectrum image with each individual pixel normalized independently along the spectral axis
Sources	**?**
Ref. By	IM**??**

Number	IM2
Label	**Normalization to one channel**
Input	k_1 $I(x_i, y_j, E_k)$
Output	$I_{norm}(x_i, y_j, E_k) = \frac{I(x_i,y_j,E_k)}{I(x_i,y_j,E_{k=k_0})}$
Description	$I(x_i, y_j, E_k)$ is the 3D spectrum image, user input k_0: Index of the channel to normalize the spectrum to, user input x_i: Pixel index along first spatial axis y_j: Pixel index along second spatial axis $I_{norm}(x_i, y_j, E_k)$: Spectrum image with each individual pixel normalized to one channel (eg, a peak maximum) independently along the spectral axis
Sources	**?**
Ref. By	IM**??**

Derivation of ...

[May be necessary to include this subsection in some cases. —SS]

5.2.6 Data Constraints

Tables 2 and 4 show the data constraints on the input and output variables, respectively. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable. The column for software constraints restricts the range of inputs to reasonable values. The constraints are conservative, to give the user of the model the flexibility to experiment with unusual situations. The column of typical values is intended to provide a feel for a common scenario. The uncertainty column provides an estimate of the confidence with which the physical quantities can be measured. This information would be part of the input if one were performing an uncertainty quantification exercise.

The specification parameters in Table 2 are listed in Table 3.

Table 2: Input Variables

Var	Physical Constraints	Software Constraints	Typical Value	Uncertainty
L	$L > 0$	$L_{\text{min}} \leq L \leq L_{\text{max}}$	1.5 m	10%

(*) [you might need to add some notes or clarifications —SS]

Table 3: Specification Parameter Values

Var	**Value**
L_{min}	0.1 m

Table 4: Output Variables

Var	**Physical Constraints**
T_W	$T_{\text{init}} \leq T_W \leq T_C$ (by A??)

5.2.7 Properties of a Correct Solution

A correct solution must exhibit [fill in the details —SS]

6 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

6.1 Functional Requirements

R1: Accept and read the following as Spectrum Image inputs:

- 3D data array
- File in format *.dm3 containing 3D data array
- File in format *.h5 containing 3D data array

R2: Accept and read the following as Spectrum inputs:

- 1D data array
- File containing 1D data array in *.csv format

R3: Verify that the data input is of the correct dimensionality and composed of Real numbers

R4: Accept user input to select a spectral range and extract (x,y) slices averaged over the selected spectral range and display the (x,y) slice as an image. The software should also export this image to an image file, as desired by the user.

R5: Accept user input to define an area on an (x,y) image display and extract a spectrum averaged over selected pixels. The software should also export this spectrum as a *.csv file, as desired by the user.

R6: Given a 1D spectrum array and an integer number, the software should perform that number of deconvolution iterations on a 3D EELS dataset using the 1D spectrum array as a reference of the system response. The software should display the output of the deconvolution for navigation by the user. Output of the deconvolution algorithm will be validated by an expert user.

R7: The software should be able to normalize a 3D spectrum image upon user command: either to an integrated portion of a chosen range along the spectral axis or to a single chosen channel.

R8: [It isn't always required, but often echoing the inputs as part of the output is a good idea. —SS]

R9: [Calculation related requirements. —SS]

R10: [Verification related requirements. —SS]

R11: [Output related requirements. —SS]

6.2 Nonfunctional Requirements

[List your nonfunctional requirements. You may consider using a fit criterion to make them verifiable. —SS]

7 Likely Changes

LC1: [Give the likely changes, with a reference to the related assumption (aref), as appropriate. —SS]

8 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an "X" may have to be modified as well. Table 5 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 6 shows the dependencies of instance models, requirements, and data constraints on each other. Table 7 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

[You will have to modify these tables for your problem. —SS]

	T1	T??	T??	GD1	GD??	DD1	DD??	DD??	DD??	IM2	IM??	IM??	IM??
T1													
T??			X										
T??													
GD1													
GD??	X												
DD1				X									
DD??				X									
DD??													
DD??								X					
IM2					X	X	X				X		
IM??					X		X		X	X			X
IM??		X											
IM??		X	X				X	X	X		X		

Table 5: Traceability Matrix Showing the Connections Between Items of Different Sections

The purpose of the traceability graphs is also to provide easy references on what has to be additionally modified if a certain component is changed. The arrows in the graphs represent dependencies. The component at the tail of an arrow is depended on by the component at the head of that arrow. Therefore, if a component is changed, the components that it points to should also be changed. Figure **??** shows the dependencies of theoretical models, general definitions, data definitions, instance models, likely changes, and assumptions on each other. Figure **??** shows the dependencies of instance models, requirements, and data constraints on each other.

	IM2	IM??	IM??	IM??	5.2.6	R??	R??
IM2		X				X	X
IM??	X			X		X	X
IM??						X	X
IM??		X				X	X
R??							
R??						X	
R??					X		
R8	X	X				X	X
R??	X						
R??		X					
R??			X				
R??				X			
R10			X	X			
R??		X					
R??		X					

Table 6: Traceability Matrix Showing the Connections Between Requirements and Instance Models

	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??
T1	X																		
T??																			
T??																			
GD1		X																	
GD??			X	X	X	X													
DD1							X	X	X										
DD??			X	X						X									
DD??																			
DD??																			
IM2											X	X		X	X	X			X
IM??												X	X			X	X	X	
IM??														X					X
IM??													X					X	
LC??				X															
LC??								X											
LC??									X										
LC??											X								
LC??												X							
LC??															X				

Table 7: Traceability Matrix Showing the Connections Between Assumptions and Other Items

References

9 Appendix

[Your report may require an appendix. For instance, this is a good point to show the values of the symbolic parameters introduced in the report. —SS]

9.1 Symbolic Parameters

[The definition of the requirements will likely call for SYMBOLIC_CONSTANTS. Their values are defined in this section for easy maintenance. —SS]