

User requirements for the visualization of spectral data from the Herschel/SPIRE imaging Fourier transform spectrometer

Issue 0.5

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1 Scope

This note specifies user requirements for the visualization of spectral data from the SPIRE imaging Fourier transform spectrometer. The ICC extension work packages provide effort to develop software tailored to visualizing 1D spectral data, creating 3D hyperspectral data cubes, and visualizing 3D hyperspectral data cubes (section 3). Detailed user requirements are specified to guide the work under these work packages (section 4). It may also be useful to consider interfaces to software dealing with 2D image processing (section 5). Requirements for spectral analysis are spelled out in the shape of informal use cases to guide the search for suitable 3rd party or external software to analyze and interpret spectral and hyperspectral data (section 6).

2 Reference documents

<i>ID</i>	<i>Document title</i>	<i>Document reference number</i>	<i>Issue</i>	<i>Date</i>
RD1	HCSS Data Processing Use Case Definitions	HERSCHEL-HSC-DOC-0480	1.2	April 6, 2006
RD2	HCSS-SPIRE Statement of Work for iteration 11			April 2007
RD3	1. Statement of Work for Blue Sky Spectroscopy			October 2005

3 Work package descriptions

Descriptions are from RD2, the *HCSS-SPIRE Statement of Work for iteration 11* and RD3, the *Statement of Work for Blue Sky Spectroscopy*.

WP 6.3.1.1: SPIRE Spectral Visualization Tools, iteration 11, Apr – Sep 07

HCSS-SPIRE Statement of Work for iteration 11

SPIRE contains an imaging Fourier transform spectrometer and the resulting level 1 products contain multiple spectra relating to each of the SPIRE detectors. The SPIRE spectral visualization tool will allow users to inspect the contents of the level 1 products, isolating individual spectra and pixels and the associated metadata.

Activities for this iteration:

1. Define requirements for SPIRE spectral visualisation tool(s)
2. Provide inputs for HCSS URD and DP use-case document reflecting high-level requirements/use-cases extracted from (1)
3. Define the architecture of the tool(s)
4. Implement and test the tool(s)
5. Provide user and developer documentation and test harnesses for the module

This work package will deliver

1. Document listing requirements for SPIRE spectral visualisation tool(s)
2. Inputs for HCSS URD and DP use-case document reflecting high-level requirements/use-cases extracted from (1)
3. Document describing the architecture and design of the Spectral Visualisation Tools
4. Inputs for the DP ADD extracted from (3)
5. Software, user and developer documentation and test harnesses for the tool(s)

WP 6.3.1.2: SPIRE Cube Dataset Visualization Tools, iteration 12, Oct 07 – Mar 08

Statement of Work for Blue Sky Spectroscopy

After aggregating several SPIRE spectral datasets to a spectral cube, the SPIRE spectral cube can be visualized with the Herschel CubeView Tool. The Graphical User Interface SPIRECubeDataset will provide access to the Herschel CubeView Tool in order to visualize SPIRE spectral cubes.

This should be updated when the Statement of Work for the next iterations is prepared. See the scenario outline below.

WP 6.6.1.1: SPIRE FTS to Cube (Basic Module), iteration 11, Apr – Sep 07

HCSS-SPIRE Statement of Work for iteration 11

The SPIRE spectral observations are arranged to provide spatial coverage of an area of the sky as well as spectral information. The basic module will spectrally and spatially re-

sample measured spectral datasets into a level 2 spectral data cube containing a uniformly sampled spectral image.

Activities during this iteration:

1. Document requirements for the module.
2. Provide inputs for HCSS URD and DP use-case document reflecting high-level requirements/use-cases extracted from (1)
3. Design of architecture of the Module
4. Implementation and test of the Module
5. Provision of user and developer documentation and test harnesses for the module
6. Participation in integration testing within the DP system

This work package will deliver

1. Document listing requirements for the module
2. Inputs for HCSS URD and DP use-case document reflecting high-level requirements/use-cases extracted from (1)
3. Document describing the architecture and design of the Source Extraction Module
4. Inputs for the DP ADD extracted from (3)
5. Software, user and developer documentation and test harnesses for the module

WP 6.6.1.2: SPIRE FTS to Cube (Advanced Module), iteration 12/13, Oct 07 – Sep 08

Statement of Work for Blue Sky Spectroscopy

The SPIRE FTS will measure a different spectrum from the same point in the sky depending on the pixel making the measurement. This is due to instrument characteristics such as vignetting, off-axis effects, physical differences between bolometers, channel fringes, etc. The advanced module will account for such systematic differences between pixels to increase the scientific validity of the derived level 2 spectral data cube.

This should be updated when the Statement of Work for the next iterations is prepared. See the scenario outline below.

WP 6.6.1.3: SPIRE FTS to Cube (User Tool), iteration 14/15, Oct 08 – Sep 09

Statement of Work for Blue Sky Spectroscopy

The User Tool will be a Graphical User Interface to provide astronomers with efficient and intuitive access to the Basic and Advanced Cube Generation Modules.

This should be updated when the Statement of Work for the next iterations is prepared. See the scenario outline below.

4 User Requirements for the Herschel/SPIRE imaging FTS

The SPIRE team has to decide where to direct the effort that has become available through the extended ICC work packages. Two scenarios seem currently possible. They are summarized below:

Scenario A: Herschel-wide integration of spectral cube viewing

Spectrum Visualization tools will be developed specific to SPIRE in coordination with the other instrument teams to work towards a homogeneous look & feel. The Basic Cube Module creates a spatially and spectrally re-gridded cube which can be viewed with the SPIRE Cube Visualization tools. The latter will be developed in coordination with the other instrument teams to work towards a homogeneous look & feel.

The Advanced Cube Module combines SPIRE and PACS cubes into one Herschel cube and allows for visualization in SPIRE, PACS, and HIFI tools. THIS WILL REQUIRE EFFORT FROM SPIRE AND PACS. A Cube User Tool will provide a convenient GUI application to allow users to create SPIRE cubes, combine them with PACS cubes, visualize SPIRE, PACS, and HIFI cubes, and store the created cubes. THIS WILL REQUIRE EFFORT FROM SPIRE, PACS, HIFI, AND THE CSDT.

Advantages:

- User-friendly.
- The SPIRE team can work with the other teams towards a Herschel-wide integration of hyperspectral visualization.

Risks:

- Many interfaces to PACS and HIFI are required which are not well established.
- The scope of this undertaking may be beyond our means – depending on what other teams contribute, such as CSDT, instrument teams, Key Programs.

Scenario B: Focus on SPIRE cube generation and visualization

Spectrum Visualization tools will be developed specific to SPIRE in coordination with the other instrument teams to work towards a homogeneous look & feel. The Basic Cube Module creates a spatially and spectrally re-gridded cube which can be viewed with the SPIRE Cube Visualization tools. The latter will be developed in coordination with the other instrument teams to work towards a homogeneous look & feel.

The Advanced Cube Module improves on the quality of the data when resampling data into a hyperspectral cube by taking detailed instrument characterization into account. A Cube User Tool will provide a convenient GUI application to allow users to create,

visualize, and store SPIRE cubes in coordination with the other instrument teams to work towards a homogeneous look & feel.

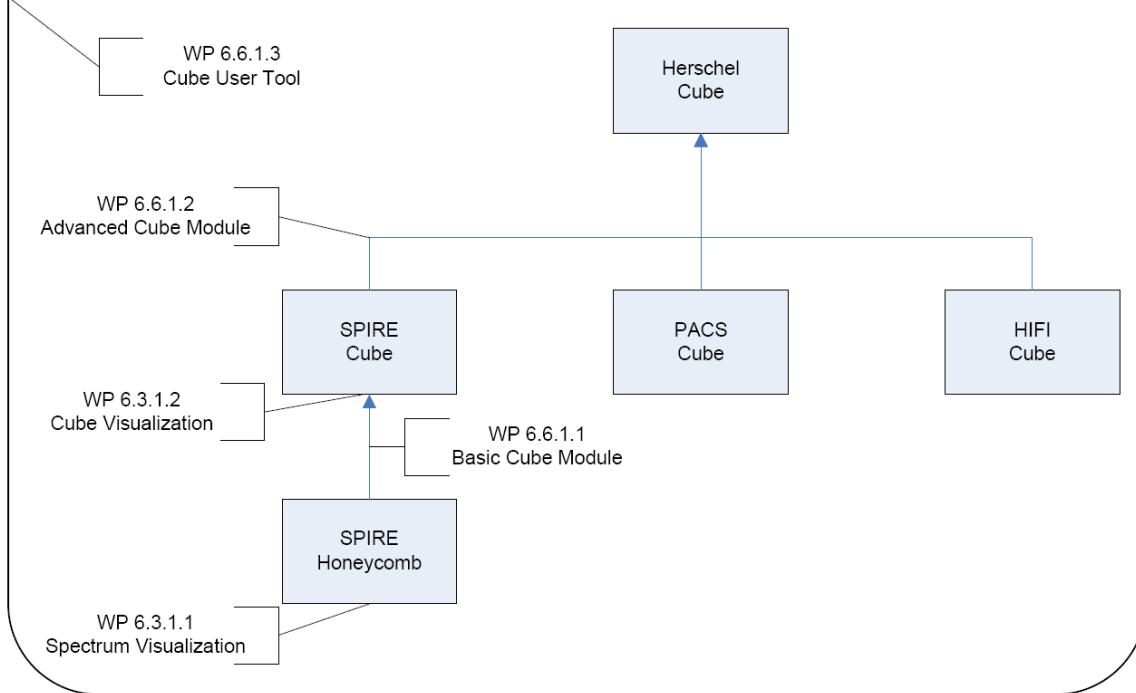
Advantages:

- Minimal interfaces to other development teams allows us to develop efficiently.

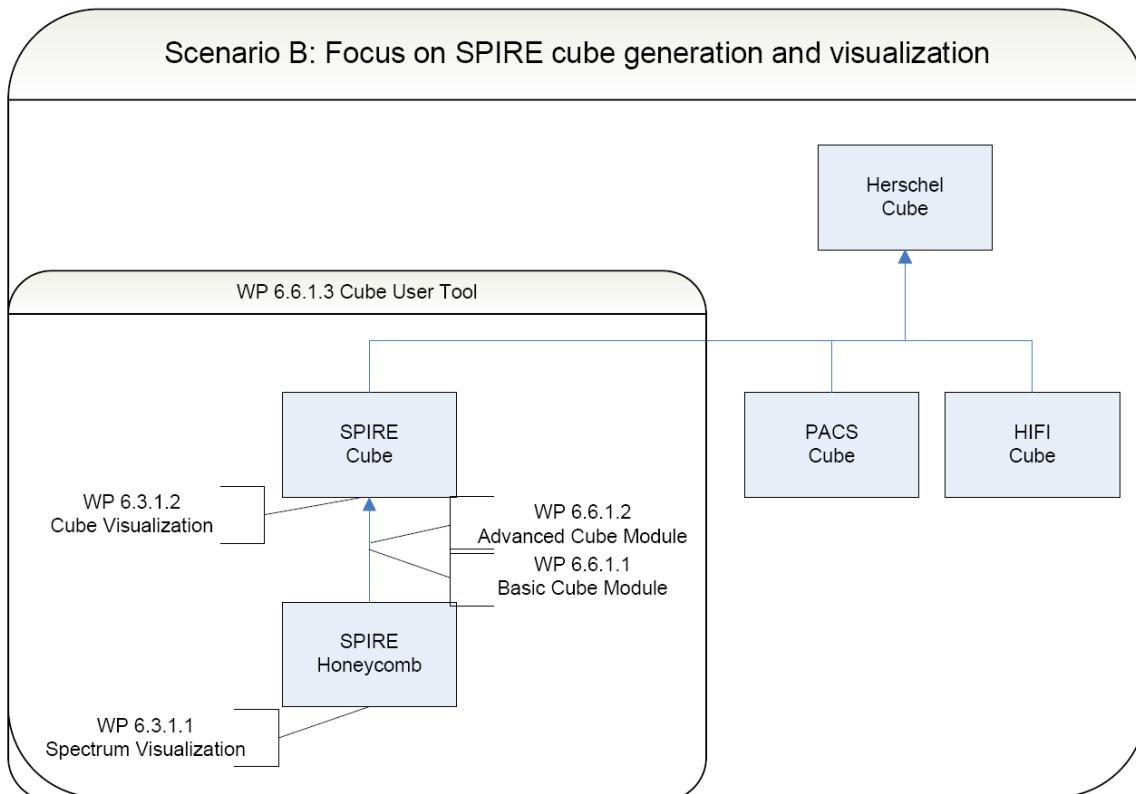
Risks:

- SPIRE cubes cannot easily be used in visualization tools from PACS and HIFI.
- Visualization tools for SPIRE/PACS/HIFI cubes will present themselves differently to users.

Scenario A: Herschel-wide integration of spectral cube viewing



Scenario B: Focus on SPIRE cube generation and visualization



WP 6.3.1.1: SPIRE Spectral Visualization Tools, iteration 11, Apr – Sep 07

The user will be able to visualize spectral data from one observation (one 1D spectrum per pixel per scan) in the following ways:

1. Select one or several pixels from SSW and SLW, which are presented in their honeycomb configuration, and select one or several scans to display one or several 1D spectra plus metadata. There should be no limitation on the number of pixels that can be selected at the same time.
2. Select to co-add spectra from several or all scans and display the resulting average 1D spectra and standard deviations/error bars per pixel plus metadata. Here is an interface to spectral arithmetic that should be dealt with separately (cf. HIFI's SpectrumArithmetics).
3. The display tool for 1D spectra will be based on PlotXY task and will provide common display functionality such as PlotStyle, ColourModel, Zoom, Pan and Move control, Search, Range Scale, Export, Print, Legend, Colour box, Axis, Axis labels. This should be coordinated with the other instrument teams.
4. Multiple spectra can either be displayed in multiple windows or they can be overplotted. This should be coordinated with the other instrument teams.
5. Select a spectral band on the wave axis to fill the pixels of the two honeycombs with a greyscale or color schemes (silly fashion statement).

WP 6.3.1.2: SPIRE Cube Dataset Visualization Tools, iteration 12, Oct 07 – Mar 08

The user will be able to visualize a 3D hyperspectral cube (2D image plus 1D spectrum) in the following ways:

1. Show a 2D image in various configurations such as B/W or with specific color schemes.
2. Select a spectral band on the wave axis from which to calculate the 2D image.
3. Select one or several pixels with the mouse to display one or several 1D spectra in the same way as the SPIRE spectral visualization tool (cf. WP 6.3.1.1).
4. Co-add a set of selected spectra and display the resulting average 1D spectrum with a standard deviation envelope in the same way as the SPIRE spectral visualization tool (cf. WP 6.3.1.1).
5. Scenario A: Layer/Overplot spectral cubes (from SPIRE and HIFI).
6. Is a 3D representation of a SPIRE cube useful/required?

WP 6.6.1.1: SPIRE FTS to Cube (Basic Module), iteration 11, Apr – Sep 07

The user will be able to create a spectral data cube from one or several observations, e.g. from spectral maps:

1. Spatial re-sampling: Re-grid the spectral information that has been measured during one or several observations by pixels in a honeycomb configuration onto an equidistantly spaced grid in angles of right ascension/declination. This will take into account the variations in beam-size as a function of wavelength. The user will have control over the spacing of the grid.
2. Spectral re-sampling I: Re-sample the spectral information onto a wavescale that is equidistantly sampled in wavenumber. The user will have control over the spacing of the wavenumber grid.
3. Spectral re-sampling II: Re-sample the spectral information onto a wavescale that is equidistantly sampled in wavelength. The user will have control over the spacing of the wavelength grid.
4. Combine spectral cubes from the SPIRE short and long wavelength arrays into one single spectral cube.

WP 6.6.1.2: SPIRE FTS to Cube (Advanced Module), iteration 12/13, Oct 07 – Sep 08

1. Scenario A: Combine spectral cubes from SPIRE and PACS into one single spectral cube that is compatible with the SPIRE, PACS, and HIFI cubes.
2. Scenario B: Optimize the FTS to Cube Basic Module to increase accuracy and/or efficiency of resampling algorithms.

WP 6.6.1.3: SPIRE FTS to Cube (User Tool), iteration 14/15, Oct 08 – Sep 09

1. Scenario A: A GUI-enabled application will allow users to conveniently load Herschel spectral data, create spectral cubes from SPIRE and PACS data (see WP 6.6.1.1 and WP 6.6.1.2), visualize spectral cubes from Herschel (see WP 6.3.1.2), and store spectral cubes.
2. Scenario B: A GUI-enabled application will allow users to conveniently load SPIRE spectral data, create (see WP 6.6.1.1 and WP 6.6.1.2), visualize (see WP 6.3.1.2), and store SPIRE hypercubes.

5 User Requirements for the interfaces of spectral data from SPIRE

It is not quite clear at this point whether the following is required and if so, how they map onto the work packages.

1. Slice from a spectral region

A SPIRE or PACS/SPIRE spectral cube provides an interface to photometry through a function `imageFromCube(lowWaveEdge, highWaveEdge)` which returns a 2d image from a spectral cube, integrating the power in a band specified by the two parameters `lowWaveEdge` and `highWaveEdge`. The resulting image can then be fed into photometric analysis routines such as source extraction, flux per source, etc. PD: Who can spell out this etc.?

NB: This function will produce misleading results when used for individual lines measured by SPIRE because the flux is hidden in the ripples of the instrumental line shape. See next point ...

2. Slice from a line position

A SPIRE or SPIRE/HIFI spectral cube provides an interface to line-oriented work through a function `imageFromCube(line center)` which returns a 2d image from a spectral cube, integrating the flux of a line at a given frequency which can then be fed into photometric analysis routines such as source extraction, etc. PD: Who can spell out this etc.?

3. Drill out a SPIRE spectrum

An individual spectrum can be extracted from a SPIRE spectral cube and used in a single point spectral analysis. A function `spectrumFromCube(x,y)` returns a SPIRE spectrum data product at the sky position (x,y) from a SPIRE spectral cube.

4. Drill out a cross-instrument spectrum

Individual spectra can be extracted from cross-instrument spectral cubes and used in a single point spectral analysis. A function `spectrumFromCube(x,y)` returns HIFI/PACS/SPIRE spectrum data products at the sky position (x,y) from a cross-instrumental spectral cube (one to three windows or overplotted).

6 Requirements for spectral analysis

The following outlines requirements on any down-stream tools that could be used to analyze spectral data from SPIRE:

6.1 Line information

1. Signal-to-noise ratio for the detection of a specific line
“Is there a line at a given frequency?”
2. Position of a line
“What is the frequency and error bar of a line?”
3. Flux of a line
“What is the flux and error bar of this line?”
4. Width of a line
“What is the width and error bar of this line?”
5. Amplitude of a line
“What is the amplitude and error bar of this line?”
6. Continuum value at a line position
“What would the continuum value and corresponding error be if the line weren't there?”
7. Line information for a given spectral range
“What are the SNR's, positions, and fluxes of all the lines in the band?”
8. Line information for a specified set of lines
“What are the SNR's, positions, and fluxes of the lines that I am interested in (e.g. only CO transitions)?”
9. Store line information
“Save the derived information in a Line List data product.”

6.2 Continuum information

1. Values of the best fit for a parametrized spectral model
“What are the parameters values where my parameterized model best matches the measured spectrum?”
NB: Uses something similar to IDL's MPFITFUN from the HCSS's herschel.ia.numeric.toolbox.fit package
2. Goodness of fit for a given spectral profile
“How well does this specific model fit the measured spectrum?”
NB: This is an atomic function to allow for the implementation of a self-made model-fitting scheme.

7 HCSS context

Applicable use cases from the HCSS Data Processing Use Case Definitions, issue 1.2 [RD1]:

UCF-IA: Perform Interactive Analysis

UCF-PLOT: Plot 1d Data Artefact

UCF-IMAGE: Display Image of a Data Artefact

I think, there should also be a use case to reflect the automated processing of data with a pipeline rather than interactively. The use case

UCF-SPG: Perform Standard Product Generation

does not reflect this functionality as it refers only to the production of level 1 data by the scientific product analysts and not astronomers. Will there be an additional use case for an astronomer to process data in a pipeline rather than interactively?

Also, I assume there will be a UCF-CUBE to cover the visualization of 3d data.

From looking more closely at the use cases 1 – 3 I take the following conclusions for spectral processing and visualization:

Data processing is broken down into the following steps:

- select data
- select task(s) and set task parameters
- execute
- visualize (optional)
- serialize (optional)
- Visualization gives users access to the following tools:
 - select color schemes
 - zoom
 - scale
 - annotate
 - change units
 - overplot
 - error bars (1d only)