# Guest Observer Handbook for FIFI-LS Data Products

*Release: FIFI-LS Data Handbook Rev. G*

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Part I

Introduction

This guide describes the data produced by the SOFIA/FIFI-LS data reduction pipeline (Redux) for guest investigators. The FIFI-LS observing modes are described in the SOFIA Observer’s Handbook, available from the Proposing and Observing page on the SOFIA website.

This handbook applies to FIFI-LS Redux version 2.3.0.

Part II

SI Observing Modes Supported

1 FIFI-LS Instrument Information

FIFI-LS has two separate and independent grating spectrometers with common fore-optics feeding two large Ge:Ga detector arrays (16 x 25 pixels each). The wavelength ranges of the two spectral channels are 42 – 110 microns and 110 – 210 microns, referred to as the BLUE and RED channels, respectively.

Multiplexing takes place both spectrally and spatially. An image slicer redistributes 5 x 5 pixel spatial fields-of-view (approximately diffraction-limited in each wave band) along the 1 x 25 pixel entrance slits of the spectrometers. Anamorphic collimator mirrors help keep the spectrometer compact in the cross-dispersion direction. The spectrally dispersed images of the slits are anamorphically projected onto the detector arrays, to independently match spectral and spatial resolution to detector size, thus enabling instantaneous coverage over a velocity range of ~ 1500 to 3000 km/s around selected FIR spectral lines, for each of the 25 spatial pixels (“spaxels”).

The detectors are read out with integrating amplifiers: at each pixel a current proportional to the incident flux charges a capacitor. The resulting voltage is sampled at about 256Hz. After a certain number of read-outs (the ramp length),
the capacitors are reset to prevent saturation. Thus, the data consist of linearly rising ramps for which the slope is proportional to the flux. See Fig. 2 for an illustration of the read-out sequence.

2 FIFI-LS Observing Modes

Symmetric chop mode, also known as nod-match-chop mode, is the most common observing mode. In this mode, the telescope chops symmetrically to its optical axis, with a matched telescope nod to remove background. A typical observation sequence will cycle through the A nod position and the B nod position in an ABBA pattern.

Most observations will be taken using symmetric chop mode. However, if the object is very bright, the efficiency is improved by observing in an asymmetric chopping mode. This mode typically consists of two map positions and one off-position per nod-cycle (an AAB pattern, where the B position contains only empty sky). Asymmetric chopping may also be used if an object’s size requires a larger chop throw than is possible with symmetric chopping.

Occasionally, for very bright targets, it may be advantageous to take data with no chopping at all. This mode, called total power mode, may be taken with either symmetric or asymmetric nodding for sky subtraction, or with no nods at all.

For extended targets, total power observations may also be taken in on-the-fly (OTF) scanning mode. In this mode, the telescope is continuously scanned across the target, at a speed calculated for minimal smearing within a single ramp. Each ramp is then treated as if it were a separate observation (A nod), with its own position coordinates. The sky position (B nod) may be observed separately, before or after the OTF scan, similar to the asymmetric nodding method. The sky position is not scanned.

At each chop and nod position (on- and off-position), it is common to step the grating through a number of positions before each telescope move. These additional grating scans effectively increase the wavelength coverage of the observation. Note, however, that grating scans are not used with the OTF mode, due to the continuous telescope motion.

Part III

Algorithm Description

3 Overview of Data Reduction Steps

This section will describe, in general terms, the major algorithms used to reduce a FIFI-LS observation. See Fig. 4 for a flow chart showing how these algorithms fit together.

4 Reduction Algorithms

The following subsections detail each of the data reduction pipeline steps outlined in the flowchart above.
Fig. 2: FIFI-LS readout sequence

Frequencies of pattern generator output lines:

CLK 8192 Hz
SYNC 256 Hz
RCRES 256 Hz / (ramps per complete chop cycle)
CHOP 256 Hz / (ramps per fundamental chop cycle)
MOVE_GRAT 256 Hz / [(ramps per complete chop cycle)x(chop cycles per grating step)]

Pattern generator clock frequency: 4 x 8192 Hz (CLK and everything else in pattern generator derived from this)

Digital multiplexer clock frequency: 64 x 8192 Hz (PLL-generated inside WRE from CLK)

Chopper signal sampling frequency (both x nd y): 2048 Hz = CLK/4, will produce 2 x 8 = 16 samples per 1/256 s ramp sampling interval which will be mapped onto 16 out of 18 "pixels" of one fake detector column
Fig. 3: The geometry of chopping and nodding in the symmetric chop mode (left) and the asymmetric mode (right).

Fig. 4: Processing steps for FIFI-LS data. The blue box describes an overview of the steps and the white box contains the actual steps carried out.
4.1 Split Grating and Chop

A single FIFI-LS raw FITS file contains the data from both chop positions (on and off) for each grating step used in a single nod position. FIFI-LS records its grating positions in “inductosyn” units. These are long integer values that are used to convert the data to a micron scale in the wavelength calibrate step.

The raw FIFI-LS data consist of a header (metadata describing the observation) and a table of voltage readings from the detector pixels. Each data section contains one frame, i.e. simultaneous readouts of all detector pixels and chopper values.

The data header is sent before each frame. The following 8 unsigned 16-bit words contain the header information.

- Word 0: The word #8000 marks the start of the header.
- Word 1: The low word of the 32-bit frame counter.
- Word 2: The high word of the 32-bit frame counter.
- Word 3: The flag word. Bit 0 is the chopper signal. Bit 1 is the detector (0=red, 1=blue). Unused bits are fixed to 1 to recognize this flag word.
- Word 4: The sample count as defined in the timing diagrams (see Fig. 2). This count gets advanced at every sync pulse and reset at every long sync pulse.
- Word 5: The ramp count as defined in the timing diagrams. This counter gets advanced with a long sync pulse and reset by RCRES.
- Word 6: The scan index
- Word 7: A spare word (for now used as “end of header”: #7FFF).

Only columns 3, 4, and 5 are used in the split grating/chop step. The following shows example header values for a raw RED FIFI-LS file:

```
columns:
  0  1  2  3  4  5  6  7
---------------------------
32768 28160 15  1  0  0  89 32767
32768 28161 15  1  1  0  89 32767
32768 28162 15  1  2  0  89 32767
32768 28163 15  1  3  0  89 32767
32768 28164 15  1  4  0  89 32767
32768 28165 15  1  5  0  89 32767
32768 28166 15  1  6  0  89 32767
32768 28167 15  1  7  0  89 32767
32768 28168 15  1  8  0  89 32767
32768 28169 15  1  9  0  89 32767
32768 28170 15  1 10  0  89 32767
32768 28171 15  1 11  0  89 32767
...```

Column 3 is all ones, indicating that the data is for the RED channel, column 4 counts the readouts from 0 to 31, and column 5 indicates the ramp number.

Where each chop and grating position starts and stops in the raw data table is determined using the header keywords RAMPLN_[B,R], C_CYC_[B,R], C_CHOPLN, G_PSUP_[B,R], G_PSDN_[B,R] keywords. A RED data example is as follows:

```
RAMPLN_R= 32 / number of readouts per red ramp
C_CHOPLN= 64 / number of readouts per chop position
```

(continues on next page)
Here, \( C_{\text{CHOPLN}} / \text{RAMPLN}_R \) is \( 64 / 32 = 2 \); therefore, there are 2 ramps per chop.

Each chop switch index is determined using the 5th column in the header. It is chop 0 if the value is odd and chop 1 if the value is even. Grating scan information determines how that chop phase is split up into separate extensions using the following formula:

\[
\text{binsize} = \frac{\text{nreadout} \times \text{ramplength}}{\text{nstep} \times \text{choplength}}
\]

where \( \text{nreadout} \) is the total number of readouts (frames) in the file, \( \text{ramplength} \) is determined by the appropriate \text{RAMPLN} keyword, \( \text{nstep} \) is the number of grating steps (\( \text{G_PSDN} + \text{G_PSUP} \)), and \( \text{choplength} \) is the number of readouts per chop position (\( \text{C_CHOPLN} \)).

The binary data section is comprised of 468 signed 16-bit words: one each for 25 spaxels, plus one control value, times 18 spectral channels ("spexels"). The spaxels are read out one spectral channel at a time. Spectral channel zero of all 25 pixels are read out, and then a chopper value (analog readout from the secondary mirror) is recorded; then the next channel of all the pixels is read out, and then the next chopper value, and so on, through all the spectral channels. The chopper values are discarded during pipeline processing. Of the 18 spectral channels, channel 0 is the CRE resistor row and row 17 is the blind CRE row ("dummy channels"). These two channels are discarded; the other 16 channels are considered valid spexels.

The first step in the data reduction pipeline is to split out the data from each grating scan position into separate FITS image extensions, and to save all grating positions from a single chop position into a common file. For example, if there are five grating scans per chop, and two chop positions, then a single one-extension input raw FITS file will be reorganized into two files (chop 0 and chop 1) with 5 extensions each. For total power mode, there is only one chop position, so there will be one output file, with one extension for each grating step. Each extension in the output FITS files contains the data array corresponding to the grating position recorded in its header (keyword \text{INDPOS}). Hereafter, in the pipeline, until the Combine Grating Scans step, each grating scan is handled separately.

For OTF mode data, an additional binary table is attached to the FITS file, recording the telescope position at each readout sample. These positions are calculated from the telescope speed keywords in the FITS header (\text{OBSLAMV} and \text{OBSBETV}, for RA and Dec speeds in arcsec/s, respectively). Readouts taken before and after the telescope scanning motion are also identified using the \text{OTFSTART} and \text{TRK_DRTN} header keywords. These readouts are flagged in the \text{SCANPOS} table for removal from consideration in later pipeline steps.

### 4.2 Fit Ramps

The flux measured in each spatial and spectral pixel is reconstructed from the readout frames by fitting a line to the voltage ramps. The slope of the line corresponds to the flux value.

Before fitting a line to a ramp, some likely bad frames are removed from the data. The chopper values (in the 26th spaxel position), the first ramp from each spaxel, the first 2-3 readouts per ramp, and the last readout per ramp are all removed before fitting.

Optionally, the flux in the first (empty) spectral pixel may be subtracted from all other spexels in its associated spaxel, as a correction for detector readout bias. The dummy channels in the first and last spectral pixels are then removed from the flux array; they are not propagated through the rest of the pipeline.

A ramp may be marked as saturated if it does not have its highest peak in the last readout of the ramp. If this occurs, the readout before the highest peak is removed before fitting, along with any readouts after it. This ensures that the slope is not contaminated by any non-linearity near the saturation point.

Typically, multiple ramps are taken at each chop position. After the slope of each ramp is derived, the slopes are combined with a robust weighted mean. This final averaged value is recorded as the flux for the pixel and the error
on the mean is recorded as the error on the flux for that pixel. After this pipeline step, there is a flux value for each spatial and spectral pixel, recorded in a 25 x 16 data array in a separate FITS image extension for each grating scan. The error values are recorded in a separate 25 x 16 array, in another FITS image extension. The extensions are named with a suffix indicating the grating scan number. For example, for two grating scans, the output will have extensions FLUX_G0, STDDEV_G0, FLUX_G1, and STDDEV_G1.

For OTF data, each ramp represents a different sky position, so separate ramps are not averaged together, but are propagated through the pipeline as a data cube. The flux and error data arrays have dimension 25 x 16 x N\textsubscript{ramp}, where N\textsubscript{ramp} is the number of ramps for which the telescope motion was nominal. In the SCANPOS table attached to the FITS file, the telescope positions for each ramp are calculated from an average over the positions for the readouts in the ramp, and propagated forward for later use in spatial calibration.

Some pixels in the data array may be set to not-a-number (NaN). These are either known bad detector pixels, or pixels for which the ramp fits did not have sufficient signal-to-noise. These pixels will be ignored in all further reduction steps.

![Image of flux array from a single grating scan in the RED channel, at the chop 0 position in nod A after fitting ramps, flattened into a 25 x 16 array. The spectral dimension runs along the y-axis. The data was taken in symmetric chopping mode.](image)

Fig. 5: The flux array from a single grating scan in the RED channel, at the chop 0 position in nod A after fitting ramps, flattened into a 25 x 16 array. The spectral dimension runs along the y-axis. The data was taken in symmetric chopping mode.
4.3 Subtract Chops

To remove instrument and sky background emission, the data from the two chop positions must be subtracted. For A nods in symmetric mode, chop 1 is subtracted from chop 0. For B nods in symmetric mode, chop 0 is subtracted from chop 1. All resulting source flux in the symmetric chop-subtracted data should therefore be positive, so that the nods are combined only by addition. In asymmetric mode, chop 1 is subtracted from chop 0 regardless of nod position.

This pipeline step produces one output file for each pair of input chop files. In total power mode, no chop subtraction is performed.

![Fig. 6: The same flux array as in Fig. 5, with the corresponding chop 1 subtracted.](image)

4.4 Combine Nods

After the chops are subtracted, the nods must be combined to remove residual background.

In symmetric chopping mode, the A nods are paired to adjacent B nods. In order to match a given A nod, a B nod must have been taken at the same dither position (FITS header keywords DLAM_MAP and DBET_MAP), and with the same grating position (INDPOS). The B nod meeting these conditions and taken nearest in time to the A nod (keyword DATE-OBS) is added to the A nod.

In asymmetric mode, a single B nod may be subtracted from multiple A nods. For example, in an AAB pattern the B nod is combined with each preceding A nod. The B nods in this mode need not have been taken at the same dither position as the A nods, but the grating position must still match. The matching B nod taken nearest in time is subtracted from each A nod.

Optionally, in asymmetric mode, the nearest B nods before and after the A nod may be combined before subtracting from the A nod, either by averaging them, or by linearly interpolating their values to the time of the A nod observation.
In some cases, this may reduce background artifacts resulting from changes in the sky background between the A and B nod observations.

This pipeline step produces an output file for each input A nod file, containing the chop- and nod-combined flux and error values for each grating scan.

Fig. 7: The chop-subtracted symmetric mode nod A flux array, with the corresponding nod B added.

4.5 Wavelength Calibrate

The wavelength calibrate step calculates wavelength values in microns for each of the spectral pixels in each grating scan, based on the known grating position, a model of the optical geometry of the instrument, and measurements of the positions of known spectral lines. The optics within FIFI-LS tend to drift with time and therefore the FIFI-LS team updates the wavelength solution every year. The wavelength equation (below) is stored in a script, while all relevant constants are stored in a reference table, with an associated date of applicability.

The wavelength ($\lambda$) for the pixel at spatial position $i$ and spectral position $j$ is calculated from the equation:

\[
\phi_i = 2\pi \left( \frac{ISF_{ind} + ISOFF_i}{24} \right)
\]

\[
\delta_j = [j - 8.5] \times PS + sign[j - QOFF] \times [j - QOFF]^2 \times QS
\]

\[
g_i = g_0 \times cos\left(\frac{SlitPos_i - NP}{a}\right)
\]

\[
\lambda_{ij} = 1000 \frac{g_i}{m} [\sin (\phi_i - \gamma) + \sin (\phi_i + \gamma + \delta_j)]
\]

where:

**VERIFY THAT THIS IS THE CORRECT REVISION BEFORE USE**
\( ind \): the input inductosyn position
\( m \): the spectral order of the observation (1 or 2)

are inputs that depend on the observation settings, and

\( ISF \): inductosyn scaling factor
\( PS \): pixel scale, in radians
\( QOFF \): offset of quadratic pixel scale part from the “zero” pixel, in pixels
\( QS \): quadratic pixel scale correcting factor, in radians/pixel^2
\( g_0 \): grating constant
\( NP \): slit position offset
\( a \): slit position scale factor
\( \gamma \): offset from Littrow angle

are constants determined by the FIFI-LS team, and

\( ISOFF_i \): offset of the home position from grating normal in inductosyn units for the \( i \)th spaxel
\( SlitPos_i \): slit position of the \( i \)th spaxel

are values that depend on the spatial position of the pixel, also determined by the FIFI-LS team. The spaxels are ordered from 1 to 25 spatially as follows:

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
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with corresponding slit position:
Note that each spectral pixel has a different associated wavelength, but it also has a different effective spectral width. This width \((d\lambda/dp)\) is calculated from the following equation:

\[
d\lambda_{ij}/dp = 1000 \frac{g_i}{m} [PS + 2 \times \text{sign} (j - QOFF) \times (j - QOFF) \times QS] \cos (\phi_i + \gamma + \delta_j)
\]

where all variables and constants are defined above.

In order to propagate consistent values throughout the pipeline, all flux values are now divided by the spectral bin width in frequency units:

\[
d\nu_{ij}/dp = (c/\lambda^2)(d\lambda_{ij}/dp)
\]

The resulting flux density values (units \(\text{ADU/sec/Hz}\)) are propagated throughout the rest of the pipeline.

The wavelength values calculated by the pipeline for each pixel are stored in a new 25 x 16 array in an image extension for each grating scan (extension name LAMBDA_Gi for grating scan \(i\)).

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<thead>
<tr>
<th>Slit position</th>
<th>Spaxel</th>
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4.6 Spatial Calibrate

The locations of the spaxels are not uniform across the detector, due to the optics not being perfectly aligned. See Fig. 8 for a plot of the average of the center of each spaxel location, as measured in the lab. This location is slightly different at each wavelength. These spaxel positions are determined by the FIFI-LS team and recorded in a look-up table.

![Pixel position (sky) including red-blue offset](image)

Fig. 8: Average fitted spaxel positions in arcsecond offsets from the center of the detector. The red dots indicate the positions for the RED channel; blue dots indicate the BLUE channel.

For a particular observation in standard chop-nod modes, the recorded dither offsets in arcseconds are used to calculate the x and y coordinates for the pixel in the $i$th spatial position and the $j$th spectral position using the following formulae:

$$x_{ij} = ps(xpos_{ij} + dx) + d\lambda cos(\theta)\cdot d\beta sin(\theta)$$
\[ y_{ij} = ps(y_{pos,ij} + dy) + d\lambda \sin(\theta) + d\beta \cos(\theta) \]

where \( ps \) is the plate scale in arcseconds/mm (FITS header keyword PLATSCAL), \( d\lambda \) is the right ascension dither offset in arcseconds (keyword DLAM_MAP), \( d\beta \) is the declination dither offset in arcseconds (keyword DBET_MAP), \( d\theta \) is the detector angle, \( x_{pos,ij} \) and \( y_{pos,ij} \) are the fitted spaxel positions in mm for pixel \( i,j \), and \( dx \) and \( dy \) are the spatial offsets between the primary array (usually BLUE), used for telescope pointing, and the secondary array (usually RED). The \( dx \) and \( dy \) offsets also take into account a small offset between the instrument boresight and the telescope boresight, for both the primary and secondary arrays. By default, the coordinates are then rotated by the detector angle (minus 180 degrees), and the \( y \)-coordinates are inverted in order to set North up and East left in the final coordinate system:

\[
\begin{align*}
    x'_{ij} &= -x_{ij}\cos(\theta) + y_{ij}\sin(\theta) \\
    y'_{ij} &= x_{ij}\sin(\theta) + y_{ij}\cos(\theta)
\end{align*}
\]

The pipeline stores these calculated \( x \) and \( y \) coordinates for each spaxel in two 25 element arrays for each grating scan (extensions XS_Gi and YS_Gi for grating scan \( i \)).

For OTF data, the process is the same as described above, except that each ramp in the input data has its own DLAM_MAP and DBET_MAP value, recorded in the SCANPOS table, rather than in the primary FITS header. The output spatial coordinates match the number of spaxels and ramps in the flux data, which has dimensions 25 x 16 x \( N_{ramp} \), such that the XS_Gi and YS_Gi extensions have dimensions 25 x 1 x \( N_{ramp} \).

### 4.7 Apply Flat

In order to correct for variations in response among the individual pixels, the FIFI-LS team has generated flat field data that correct for the differences in spatial and spectral response across the detector. There is a normalized spatial flat field for each of the RED and BLUE channels, which specifies the correction for each spaxel. This correction may vary over time. There is also a set of spectral flat fields, for each channel, order, and dichroic, over the full wavelength range for the mode, which specifies the correction for each spaxel.

In order to apply the flat fields to the data, the pipeline interpolates the appropriate spectral flat onto the wavelengths of the observation, for each spaxel, then multiplies the value by the appropriate spatial flat. The flux is then divided by this correction value. The updated flux and associated error values are stored in the FLUX_Gi and STDDDEV_Gi extensions.

### 4.8 Combine Grating Scans

Up until this point, all processing has been done on each grating scan separately. The pipeline now combines the data from all grating scans, in order to fill in the wavelength coverage of the observation.

Due to slight variations in the readout electronics, there may be additive offsets in the overall flux level recorded in each grating scan. To correct for this bias offset, the pipeline calculates the mean value of all pixels in the overlapping wavelength regions for each grating scan. This value, minus the mean over all scans, is subtracted from each grating scan, in order to set all extensions to a common bias level.

For standard chop/nod modes, the pipeline sorts the data from all grating scans by their associated wavelength values in microns, and stores the result in a single data array with dimensions 25 x (16 * \( N_{scan} \)), where \( N_{scan} \) is the total number of grating scans in the input file. Note that the wavelengths are still irregularly sampled at this point, due to the differing wavelength solutions for each grating scan and spatial pixel. All arrays in the output FITS file (FLUX, STDDEV, LAMBDA, XS, and YS) now have dimensions 25 x (16 * \( N_{scan} \)).

For the OTF mode, only a single grating scan exists. The output FLUX, STDDEV, XS, and YS arrays for this mode have dimensions 25 x 16 x \( N_{ramp} \). Since the wavelength solution does not depend on the sky position, the LAMBDA array has dimensions 25 x 16.
4.9 Telluric Correct

Telluric correction is the process of attempting to correct an observed spectrum for absorption by molecules in the earth’s atmosphere, in order to recover the intrinsic (“exo-atmospheric”) spectrum of the source. The atmospheric molecular components (primarily water, ozone, CO2) can produce both broad absorption features that are well resolved by FIFI-LS and narrow, unresolved features. The strongest absorption features are expected to be due to water. Because SOFIA travels quite large distances during even short observing legs, the water vapor content along the line of sight through the atmosphere can vary substantially on fairly short timescales during an observation. Therefore, observing a “telluric standard,” as is usually done for ground-based observations, will not necessarily provide an accurate absorption correction spectrum. For this reason, telluric corrections of FIFI-LS data rely on models of the atmospheric absorption, as provided by codes such as ATRAN, in combination with the estimated line-of-sight water vapor content (precipitable water vapor, PWV) provided by the water vapor monitor (WVM) aboard SOFIA. Currently, the WVM does not generate PWV values that are inserted into the FITS headers of the FIFI-LS data files. It is expected that these values may become available in the future, and at that point the PWV values will be used to generate telluric correction spectra.

Currently, correction spectra are generated using PWV values derived from observations of telluric lines made with FIFI-LS during the set-up period at the start of observing legs and after changes of altitude. Experience has shown that these provide better corrections than simply using the expected value for the flight altitude and airmass, particularly in regions with deep, sharp features (e.g. near 63 microns). However, changes of PWV during flight legs are not monitored and this may cause inaccuracies if the value changes rapidly. Furthermore, accurate correction of spectral lines in the vicinity of narrow telluric absorption features is problematic even with the use of good atmospheric models and knowledge of the PWV. This is due to the fact that the observed spectrum is the result of a multiplication of the intrinsic spectrum by the telluric absorption spectrum, and then a convolution of the product with the instrumental profile, whereas the correction derived from a model is the result of the convolution of the theoretical telluric absorption spectrum with the instrumental profile. The division of the former by the latter does not necessarily yield the correct
Fig. 10: Example spectral flux from the center spaxel for a single dither position. The red circles and green diamonds represent two different grating scans. The gray line indicates the combined flux array, after bias correction.
Fig. 11: The full 25 x 32 flux array, after combining two grating scans.
results, and the output spectrum may retain telluric artifacts after telluric correction.

A set of ATRAN models appropriate for a range of altitudes, zenith angles, and PWV values has been generated for pipeline use. In the telluric correction step, the pipeline selects the model closest to the observed altitude, zenith angle, and PWV value and smooths the transmission model to the resolution of the observed spectrum, interpolates the transmission data to the observed wavelength at each spexel, and then divides the data by the transmission model. Very low transmission values result in poor corrections, so any pixel for which the transmission is less than 60% (by default) is set to NaN. For reference, the smoothed, binned transmission data is attached to the FITS file as a 25 x (16 * N_{scan}) data array (extension ATRAN). The original unsmoothed data is attached as well, in the extension UNSMOOTHED_ATRAN.

Since the telluric correction may introduce artifacts, or may, at some wavelength settings, produce flux cubes for which all pixels are set to NaN, the pipeline also propagates the uncorrected flux cube through the remaining reduction steps. The telluric-corrected cube and its associated error are stored in the FLUX and STDDEV extensions. The uncorrected cube and its associated error are stored in the UNCORRECTED_FLUX and UNCORRECTED_STDDEV extensions.

**4.10 Flux Calibrate**

Flux calibration of FIFI-LS data is carried out via the division of the instrumental response, as recorded in response files appropriate for each grating setting, wavelength range, and dichroic. The response values have units of ADU/s/Hz/Jy and are derived from observations of “flux standards.” At the wavelengths at which FIFI-LS operates, there are very few stars bright enough to yield high signal-to-noise data useful for flux calibration purposes. Therefore, observations of asteroids, planets, and planetary moons are used, along with models of such objects, to derive the response curves. Since the observed fluxes of such solar system objects vary with time, the models must be generated for the time of each specific observation. To date, observations of Mars have been used as the primary flux calibration source. Predicted total fluxes for Mars across the FIFI-LS passband at the specific UT dates of the observations have been generated using the model of Lellouch and Amri.\(^1\) Predicted fluxes at several frequencies have been computed and these have then been fit with blackbody curves to derive values at a large number of wavelength points. The deviations of the fits from the input predictions are much less than 1%. After the models have been generated, the telluric-corrected spectra of the standards, in units of ADU/s/Hz, are divided by the theoretical spectra, in Jy. The results are smoothed and then fit with a polynomial to derive response functions (ADU/s/Hz/Jy) that can then used to flux calibrate the telluric-corrected spectra of other astronomical sources (see Fig. 13).

The pipeline stores a set of response functions for each channel and dichroic value. To perform flux calibration, it selects the correct response function for each input observation, interpolates the response onto the wavelengths of each spexel, and divides the flux by the response value to convert it to physical units (Jy/pixel). From this point on, the data products are considered to be Level 3 (FITS keyword PROCSTAT=LEVEL_3). For reference, the resampled response data is attached to the FITS file as a 25 x (16 * N_{scan}) data table in the first FITS extension (column RESPONSE). Flux calibration is applied to both the telluric-corrected cube and the uncorrected cube. The estimated systematic error in the flux calibration is recorded in the CALERR keyword in the FITS header, as an average fractional error. At this time, flux calibration is expected to be good to within about 5-10% (CALERR \leq 0.1).\(^2\)

---

2. Earlier versions of this pipeline (prior to v1.3.2) propagated the systematic error on the flux calibration in the STDDEV and ERROR arrays in the output products. As of v1.3.2, the calibration error is only propagated in the FITS header keyword CALERR.
Fig. 12: The telluric-corrected flux array. Some pixels are set to NaN due to poor atmospheric transmission at those wavelengths. The cutoff level was set to 80% for this observation, for illustrative purposes.
Fig. 13: Response fits overplotted on telluric-corrected data, with model spectra divided out. Data shown was taken in 2015-2019 for the blue channel order 2, blue channel order 1, and red channel. Plots on the left are from an older filter set; plots on the right are for data taken with an updated filter set.
4.11 Correct Wave Shift

Due to the motion of the earth with respect to the local standard of rest, the wavelengths of features in the spectra of astronomical sources will appear to be slightly shifted, by different amounts on different observation dates. In order to avoid introducing a broadening of spectral features when multiple observations obtained over different nights are combined, the wavelength calibration of FIFI-LS observations must be adjusted to remove the barycentric wavelength shift. This shift is calculated as an expected wavelength shift \( d\lambda/\lambda \), from the radial velocity of the earth with respect to the sun and the sun with respect to the local standard of rest, on the observation date, toward the RA and Dec of the observed target. This shift is recorded in the header keyword BARYSHFT, and applied to the wavelength calibration in the LAMBDA field as:

\[
\lambda' = \lambda + \lambda(d\lambda/\lambda)
\]

Since the telluric absorption lines do not change with the motion of the earth, the barycentric wavelength shift cannot be applied to non-telluric-corrected data. Doing so would result in a spectrum in which both the intrinsic features and the telluric lines are shifted. Therefore, the unshifted wavelength calibration is also propagated in the output file, in the extension UNCORRECTED_LAMBDA.

4.12 Resample

Finally, the pipeline resamples the flux for each spatial and spectral pixel onto a regular 3D grid (right ascension, declination, and wavelength). This step combines the spatial information from all input nod-combined dither positions into a single output map. See Fig. 14 for an overview of the resampling algorithm.

Fig. 14: Overview of the resampling algorithm. Given a cloud of irregularly spaced data points, the algorithm assigns values to voxels of a regular grid by fitting data points in a local cloud with a low-order polynomial function.
Grid Size

The pipeline first determines the maximum and minimum wavelengths and spatial offsets present in all input files, from all dither positions for the observation. For OTF data, the scan positions for each ramp in each input file are also considered. The full range of sky positions and wavelengths observed sets the range of the output grid.

The spacing of the output grid in the wavelength dimension (dw) is set by the desired oversampling. By default, in the wavelength dimension, the pipeline samples the average expected spectral FWHM for the observation (Table 1) with 8 output pixels.

The spacing in the spatial dimensions (dx) is fixed for each channel at 1.5 arcseconds in the BLUE and 3.0 arcseconds in the RED. These values are chosen to ensure an oversampling of the spatial FWHM by at least a factor of three.

For example, for the RED observation in the figures above, the expected spectral FWHM at the central wavelength is 0.13 um, so sampling this FWHM with 8 pixels creates a grid with a spectral width of 0.016 um. Given a min and max wavelength of 157.27 um and 158.48 um, the output grid will sample the full range of wavelengths with 76 spectral pixels. Since it is a RED channel observation, the spatial scale will be 3.0 arcseconds. If the range of x offsets is -41.0 to 57.74 and the range of y offsets is -43.9 to 36.9, then the output spatial grid will have dimensions 33 x 27, with an oversampling of the FWHM (using the interpolated value at 157.876 um of 15.6 arcseconds) of 5.2. The full output cube then is 33 x 27 x 76 (nx x ny x nw).

In the spatial dimensions, the flux in each pixel represents an integrated flux over the area of the pixel. Since the pixel width changes after resampling, the output flux must be corrected for flux conservation. To do so, the resampled flux is multiplied by the area of the new pixel ($dx^2$), divided by the intrinsic area of the spaxel (approximately 36 arcseconds$^2$ for BLUE, 144 arcseconds$^2$ for RED).

<table>
<thead>
<tr>
<th>Channel/Order</th>
<th>Wavelength (um)</th>
<th>Spectral Resolution ($d\lambda/\lambda$)</th>
<th>Spatial Resolution (arcsec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blue Order 1</td>
<td>70</td>
<td>545</td>
<td>6.9</td>
</tr>
<tr>
<td>Blue Order 1</td>
<td>80</td>
<td>570</td>
<td>7.9</td>
</tr>
<tr>
<td>Blue Order 1</td>
<td>90</td>
<td>628</td>
<td>8.9</td>
</tr>
<tr>
<td>Blue Order 1</td>
<td>100</td>
<td>720</td>
<td>9.9</td>
</tr>
<tr>
<td>Blue Order 1</td>
<td>110</td>
<td>846</td>
<td>11.0</td>
</tr>
<tr>
<td>Blue Order 1</td>
<td>120</td>
<td>1005</td>
<td>12.0</td>
</tr>
<tr>
<td>Blue Order 2</td>
<td>45</td>
<td>947</td>
<td>5.9</td>
</tr>
<tr>
<td>Blue Order 2</td>
<td>50</td>
<td>920</td>
<td>6.2</td>
</tr>
<tr>
<td>Blue Order 2</td>
<td>65</td>
<td>1415</td>
<td>7.3</td>
</tr>
<tr>
<td>Blue Order 2</td>
<td>70</td>
<td>1772</td>
<td>7.7</td>
</tr>
<tr>
<td>Red</td>
<td>120</td>
<td>747</td>
<td>11.9</td>
</tr>
<tr>
<td>Red</td>
<td>140</td>
<td>939</td>
<td>13.9</td>
</tr>
<tr>
<td>Red</td>
<td>160</td>
<td>1180</td>
<td>15.8</td>
</tr>
<tr>
<td>Red</td>
<td>180</td>
<td>1471</td>
<td>17.7</td>
</tr>
<tr>
<td>Red</td>
<td>200</td>
<td>1813</td>
<td>19.6</td>
</tr>
</tbody>
</table>

Algorithm

For each pixel in the 3D output grid, the resampling algorithm finds all flux values with assigned wavelengths and spatial offsets within a fitting window, typically 0.5 times the spectral FWHM in the wavelength dimension, and 3 times the spatial FWHM in the spatial dimensions. For the spatial grid, a larger fit window is typically necessary than for the spectral grid, since the observation setup usually allows more oversampling in wavelength than in space.

Then, a low-order 3D polynomial surface is fit to all the good data points within the window. The fit is weighted by the error on the flux, as calculated by the pipeline, and a Gaussian function of the distance of the input data value from the grid location. The distance weighting function may be held constant for each output pixel, or it may optionally be
allowed to vary in scale and shape in response to the input data characteristics. This adaptive smoothing kernel may help in preserving peak flux values for bright, compact flux regions, but may overfit the input data in some sparsely sampled observations (see Fig. 15).

The output flux value for this algorithm is the value of the fit polynomial surface, evaluated at the grid location, and the associated error is the error on the fit (see Fig. 16).

Output grid locations for which there was insufficient input data for stable polynomial fits are set to NaN. The threshold for how much output data is considered invalid is a tunable parameter, but it is typically set to eliminate most edge effect artifacts from the final output cube.

For some types of observations, especially undithered observations of point sources for which the spatial FWHM is undersampled, the polynomial surface fits may not return good results. In these cases, it is beneficial to use an alternate resampling algorithm. In this algorithm, the master grid is determined as above, but each input file is resampled with polynomial fits in the wavelength dimension only. Then, for each wavelength plane, the spatial data is interpolated onto the grid, using radial basis function interpolation. Areas of the spatial grid for which there is no data in the input file are set to NaN. The interpolated cubes are then mean-combined, ignoring any NaNs, to produce the final output cube.

For either algorithm, the pipeline also generates an exposure map cube indicating the number of observations of the source that were taken at each pixel (see Fig. 17). These exposure counts correspond to the sum over the projection of the detector field of view for each input observation onto the output grid. The exposure map may not exactly match the valid data locations in the flux cube, since additional flagging and pixel rejection occurs during the resampling algorithms.

**Uncorrected Flux Cube**

Both the telluric-corrected and the uncorrected flux cubes are resampled in this step, onto the same 3D grid. However, the telluric-corrected cube is resampled using the wavelengths corrected for barycentric motion, and the uncorrected cube is resampled using the original wavelength calibration. The spectra from the uncorrected cube will appear slightly shifted with respect to the spectra from the telluric-corrected cube.

**Output Data**

The pipeline stores the resampled data as a 3D FITS image extension with extension name FLUX. The associated error is stored in a separate extension, with the name ERROR. The non-telluric-corrected cubes are stored in UNCORRECTED_FLUX and UNCORRECTED_ERROR extensions, respectively. The output wavelengths and x and y coordinates are stored in WAVELENGTH, X, and Y extensions.

For reference, a model of the atmospheric transmission spectrum, smoothed to the resolution of the observation, and the instrumental response curve used in flux calibration are also attached to the FITS file in 1D extensions called TRANSMISSION and RESPONSE.

Finally, an unsmoothed transmission spectrum is attached in a 2D image extension called UNSMOOTHED_TRANSMISSION. This extension will have size $N_{\text{trans}} \times 2$, where $N_{\text{trans}}$ is the number of data points in the spectrum, the first row is the wavelength array, and the second row is the transmission fraction. This spectrum may be useful for further analysis of the data (e.g. for determining the total flux in an emission line).

The final output from the pipeline is a FITS file with 11 image extensions:

- **FLUX**: The $nx \times ny \times nw$ cube of flux values.
- **ERROR**: The associated error values on the flux (also $nx \times ny \times nw$).
- **UNCORRECTED_FLUX**: The $nx \times ny \times nw$ cube of flux values that have not been corrected for atmospheric transmission.
- **UNCORRECTED_ERROR**: The associated error values on the uncorrected flux (also $nx \times ny \times nw$).
- **WAVELENGTH**: The wavelength values associated with each plane of the cube ($nw$).
- **X**: The x-coordinates of the data, in arcsecond offsets from the base position ($nx$).
- **Y**: The y-coordinates of the data, in arcsecond offsets from the base position ($ny$).
- **TRANSMISSION**: The atmospheric transmission model ($nw$).
- **RESPONSE**: The instrumental response curve ($nw$).
- **EXPOSURE_MAP**: The exposure map ($nx \times ny \times nw$).
- **UNSMOOTHED_TRANSMISSION**: The unsmoothed atmospheric transmission model ($N_{\text{trans}} \times 2$).
Fig. 15: Comparison of a non-adaptive (left), adaptively scaled (middle), and adaptively shaped and scaled (right) smoothing kernel for the above target, using a baseline smoothing radius corresponding to the spatial beam size. The top row shows the spatial slice at wavelength 157.83 um, locked to a common display scale. The bottom row shows the distance weights used by the resampling algorithm at the wavelength slice shown, also locked to a common display scale. Distance weights correlate with the size of the kernel used and the number of input pixels within the fit window. The plot below compares the spectral slice at pixel x,y = 14, 15 for the three resampled versions: green is non-adaptive, blue is adaptively scaled, and purple is adaptively shaped and scaled.
Fig. 16: The final output flux cube. The image on the left is a spatial slice at wavelength 157.83 um. The plot on the right is a spectral slice at pixel x,y = 14, 15, near the peak of the source.

Fig. 17: Exposure map of input dither positions, corresponding to the above flux cube. Values range from 0 (purple, near the edges) to 108 (yellow, near the center).
Part IV

Data products

5 Filenames

FIFI-LS output files from Redux are named according to the convention:

FILENAME = F####_FI_IFS_AOR-ID_CHANNEL_Type_FN1[-FN2].fits,

where #### is the four-digit SOFIA flight number, FI is the instrument identifier, IFS specifies that it is integral field spectroscopy data, AOR-ID is the AOR identifier for the observation, CHANNEL is either BLU or RED, Type is three letters identifying the product type (listed in the table below), and FN1 is the file number corresponding to the input file. FN1-FN2 is used if there are multiple input files for a single output file, where FN1 is the file number of the first input file and FN2 is the file number of the last input file.

6 Pipeline Products

The following table lists all intermediate products generated by Redux for FIFI-LS, in the order in which they are produced. The product type is stored in the primary FITS header of the file, under the keyword PRODTYPE. By default, the scan_combined, flux_calibrated, and resampled products are saved.3

Table 2: Final and intermediate data products

<table>
<thead>
<tr>
<th>Step</th>
<th>Product Type</th>
<th>Proc. status</th>
<th>File code</th>
<th>Saved</th>
<th>Extensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Split</td>
<td>grating_chop_split</td>
<td>LEVEL_2</td>
<td>CP0, CP1</td>
<td>N</td>
<td>Nscan image extensions:</td>
</tr>
<tr>
<td>Grating /</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>FLUX_Gi for i=0...Nscan-1</td>
</tr>
<tr>
<td>Chop</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fit</td>
<td>ramps_fit</td>
<td>LEVEL_2</td>
<td>RP0, RP1</td>
<td>N</td>
<td>2 Nscan image extensions:</td>
</tr>
<tr>
<td>Ramps</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>FLUX_Gi, STDDEV_Gi for i=0...Nscan-1</td>
</tr>
<tr>
<td>Subtract</td>
<td>chop_subtracted</td>
<td>LEVEL_2</td>
<td>CSB</td>
<td>N</td>
<td>2 Nscan image extensions:</td>
</tr>
<tr>
<td>Chops</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>FLUX_Gi, STDDEV_Gi for i=0...Nscan-1</td>
</tr>
<tr>
<td>Combine</td>
<td>nod_combined</td>
<td>LEVEL_2</td>
<td>NCM</td>
<td>N</td>
<td>2 Nscan image extensions:</td>
</tr>
<tr>
<td>Nods</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>FLUX_Gi, STDDEV_Gi for i=0...Nscan-1</td>
</tr>
</tbody>
</table>

3 Earlier versions of this pipeline (prior to v2.3.0) stored intermediate data as binary FITS tables, rather than image extensions. Refer to earlier revisions of this manual for more information.
<table>
<thead>
<tr>
<th>Step</th>
<th>Product Type</th>
<th>Proc. status</th>
<th>File code</th>
<th>Saved</th>
<th>Extensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lambda Calibrate</td>
<td>wavelength_calibrated</td>
<td>LEVEL_2</td>
<td>WAV</td>
<td>N</td>
<td>3 $N_{\text{scan}}$ image extensions: FLUX$_i$, STDDEV$_i$, LAMBDA$<em>i$ for $i=0\ldots N</em>{\text{scan}}-1$</td>
</tr>
<tr>
<td>Spatial Calibrate</td>
<td>spatial_calibrated</td>
<td>LEVEL_2</td>
<td>XYC</td>
<td>N</td>
<td>5 $N_{\text{scan}}$ image extensions: FLUX$_i$, STDDEV$_i$, LAMBDA$_i$ XS$_i$, YS$<em>i$ for $i=0\ldots N</em>{\text{scan}}-1$</td>
</tr>
<tr>
<td>Apply Flat</td>
<td>flat_fielded</td>
<td>LEVEL_2</td>
<td>FLF</td>
<td>N</td>
<td>7 $N_{\text{scan}}$ image extensions: FLUX$_i$, STDDEV$_i$, LAMBDA$_i$ XS$_i$, YS$_i$, FLAT$_i$, FLATERR$<em>i$ for $i=0\ldots N</em>{\text{scan}}-1$</td>
</tr>
<tr>
<td>Combine Scans</td>
<td>scan_combined</td>
<td>LEVEL_2</td>
<td>SCM</td>
<td>Y</td>
<td>5 image extensions: FLUX, STDDEV, LAMBDA, XS, YS</td>
</tr>
<tr>
<td>Telluric Correct</td>
<td>telluric_corrected</td>
<td>LEVEL_2</td>
<td>TEL</td>
<td>N</td>
<td>9 image extensions: FLUX, STDDEV, UNCORRECTED_FLUX, UNCORRECTED_STDDEV, LAMBDA, XS, YS, ATRAN, UNSMOOTHED_ATRAN</td>
</tr>
<tr>
<td>Flux Calibrate</td>
<td>flux_calibrated</td>
<td>LEVEL_3</td>
<td>CAL</td>
<td>Y</td>
<td>10 image extensions: FLUX, STDDEV, UNCORRECTED_FLUX, UNCORRECTED_STDDEV, LAMBDA, XS, YS, ATRAN, RESPONSE, UNSMOOTHED_ATRAN</td>
</tr>
</tbody>
</table>

continues on next page
<table>
<thead>
<tr>
<th>Step</th>
<th>Product Type</th>
<th>Proc. status</th>
<th>File code</th>
<th>Saved</th>
<th>Extensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Correct Wave Shift</td>
<td>wavelength_shifted</td>
<td>LEVEL_3</td>
<td>WSH</td>
<td>N</td>
<td>11 image extensions: FLUX, STDDEV, UNCORRECTED_FLUX, LAMBDA, UNCORRECTED_LAMBDA, UNCORRECTED_LAMBDA, XS, YS, ATRAN, RESPONSE, UNSMOOTHED_ATRAN</td>
</tr>
<tr>
<td>Spatial Resample</td>
<td>resampled</td>
<td>LEVEL_4</td>
<td>WXY</td>
<td>Y</td>
<td>11 image extensions: FLUX, ERROR, UNCORRECTED_FLUX, UNCORRECTED_ERROR, WAVELENGTH, X, Y, TRANSMISSION, RESPONSE, EXPOSURE_MAP, UNSMOOTHED_TRANSMISSION</td>
</tr>
</tbody>
</table>

### 7 Data Format

All files produced by the pipeline are multi-extension FITS files, for which the primary HDU contains only the primary header, and all data is contained in separate extensions.

For standard chop/nod modes, all output extensions are FITS image extensions. Pipeline steps prior to the Combine Scans step output one extension of each type for each of $N_{\text{scan}}$ grating scans performed. Intermediate flux and error data for all steps after the Fit Ramps step are 2D arrays (spaxel x spexel); the final product contains 3D spectral cubes (RA x Dec x wavelength).

For the OTF mode, intermediate data files produced by pipeline steps prior to the Spatial Calibrate step additionally contain a binary table holding sky position data for each scan position (extension SCANPOS_G0). Intermediate flux and error data in this mode are 3D cubes (spaxel x spexel x scan position). The final product is identical to other modes.