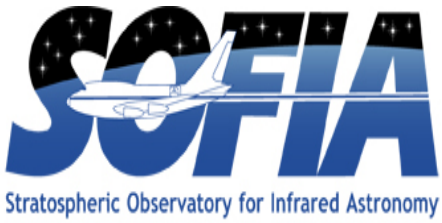

FIFI - LS Redux Pipeline Users Manual

SOF-US-HBK-OP10-2007

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SOF-US-HBK-OP10-2007

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FIFI-LS Redux User's Manual

Release : SOF-US-HBK-OP10-2007 Rev. E

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Sep 26, 2019

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Part I

Introduction

The SI Pipeline Users Manual (OP10) is intended for use by both SOFIA Science Center staff during routine data processing and analysis, and also as a reference for General Investigators (GIs) and archive users to understand how the data in which they are interested was processed. This manual is intended to provide all the needed information to execute the SI Level 2/3/4 Pipeline, and assess the data quality of the resulting products. It will also provide a description of the algorithms used by the pipeline and both the final and intermediate data products.

A description of the current pipeline capabilities, testing results, known issues, and installation procedures are documented in the SI Pipeline Software Version Description Document (SVDD, SW06, DOCREF). The overall Verification and Validation (V&V) approach can be found in the Data Processing System V&V Plan (SV01-2232). Both documents can be obtained from the SOFIA document library in Windchill at location: / Software Management Development or Verification / Pipelines (DPS).

This manual applies to FIFI-LS Redux version 2.0.0.

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.

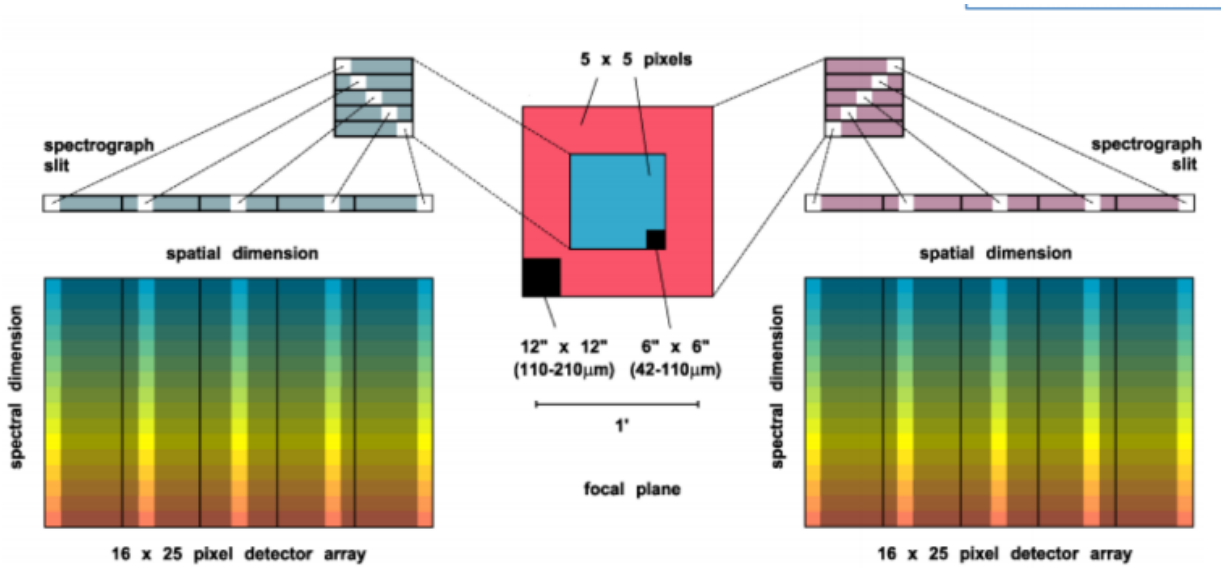


Fig. 1: The integral field unit for each channel

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 efficient 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, or with no nods at all.

At each chop and nod 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.

Part III
Algorithm Description

3 Overview of Data Reduction Steps

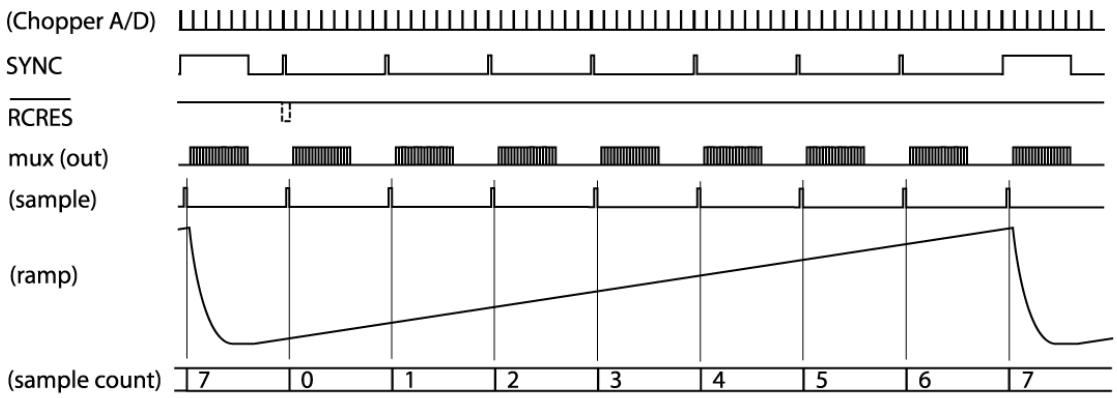
This section will describe, in general terms, the major algorithms used to reduce a FIFI-LS observation. See Fig. 4 for a flow chart showing how these algorithms fit together.

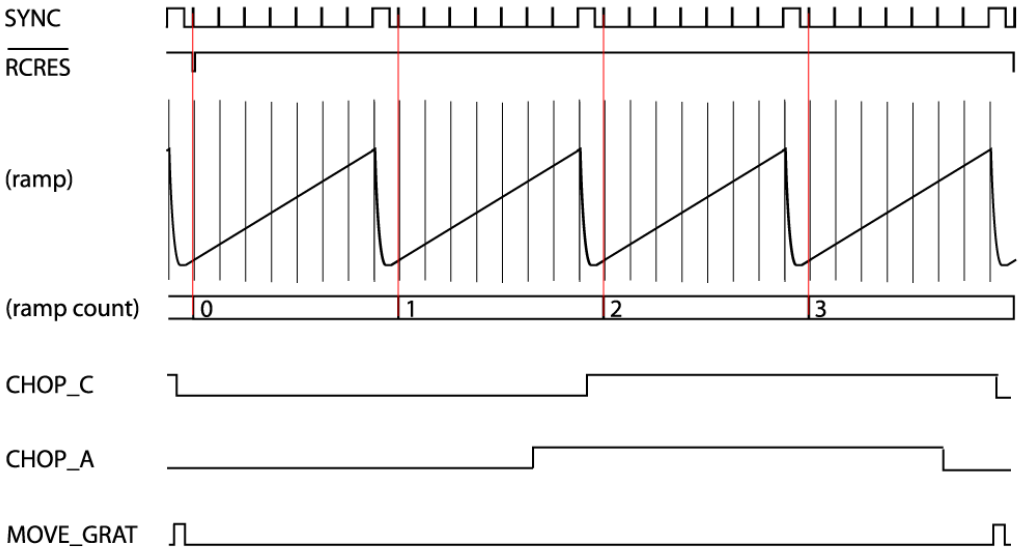
4 Reduction Algorithms

The following subsections detail each of the data reduction pipeline steps outlined in the flowchart above.

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.





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. 2: FIFI-LS readout sequence

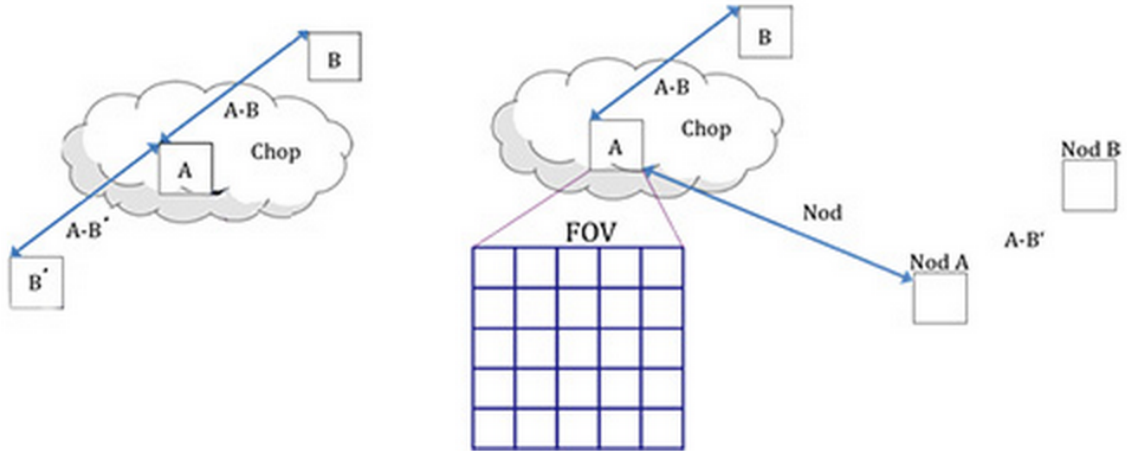


Fig. 3: The geometry of chopping and nodding in the symmetric chop mode (left) and the asymmetric mode (right).

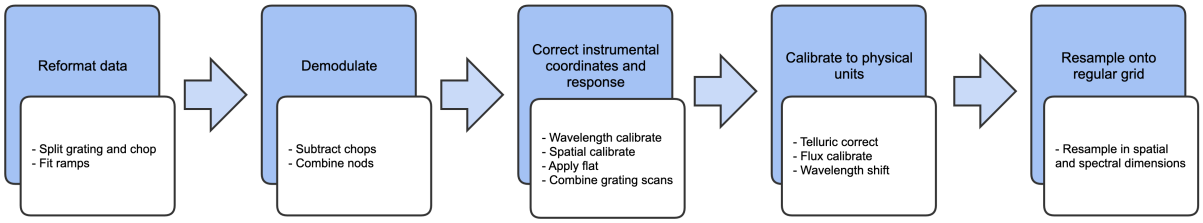


Fig. 4: Processing steps for FIFI-LS data. The blue box describes an overview of the steps and the white box contains the actual steps carried out.

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
G_PSUP_R= 5  / number of grating position up in one cycle
G_PSDN_R= 0  / number of grating position down in one cycle
```

Here, C_CHOPLN / 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:

$$binsize = (nreadout * ramplength)/(nstep * choplength)$$

where *nreadout* is the total number of readouts (frames) in the file, *ramplength* is determined by the appropriate RAMPLN keyword, *nstep* is the number of grating steps (G_PSDN + G_PSUP), and *choplength* is the number of readouts per chop position (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 tables, 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 table corresponding to the grating position recorded in its header (keyword INDPOS). Hereafter, in the pipeline, until the Combine Grating Scans step, each grating scan extension is handled separately.

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 26^{th} 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. Also, 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 5 x 5 x 18 data array in a separate FITS binary table extension for each grating scan and chop position. The error values are recorded in a separate 5 x 5 x 18 table in the same FITS extension. The table columns are named DATA and STDDEV, respectively.

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.

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.

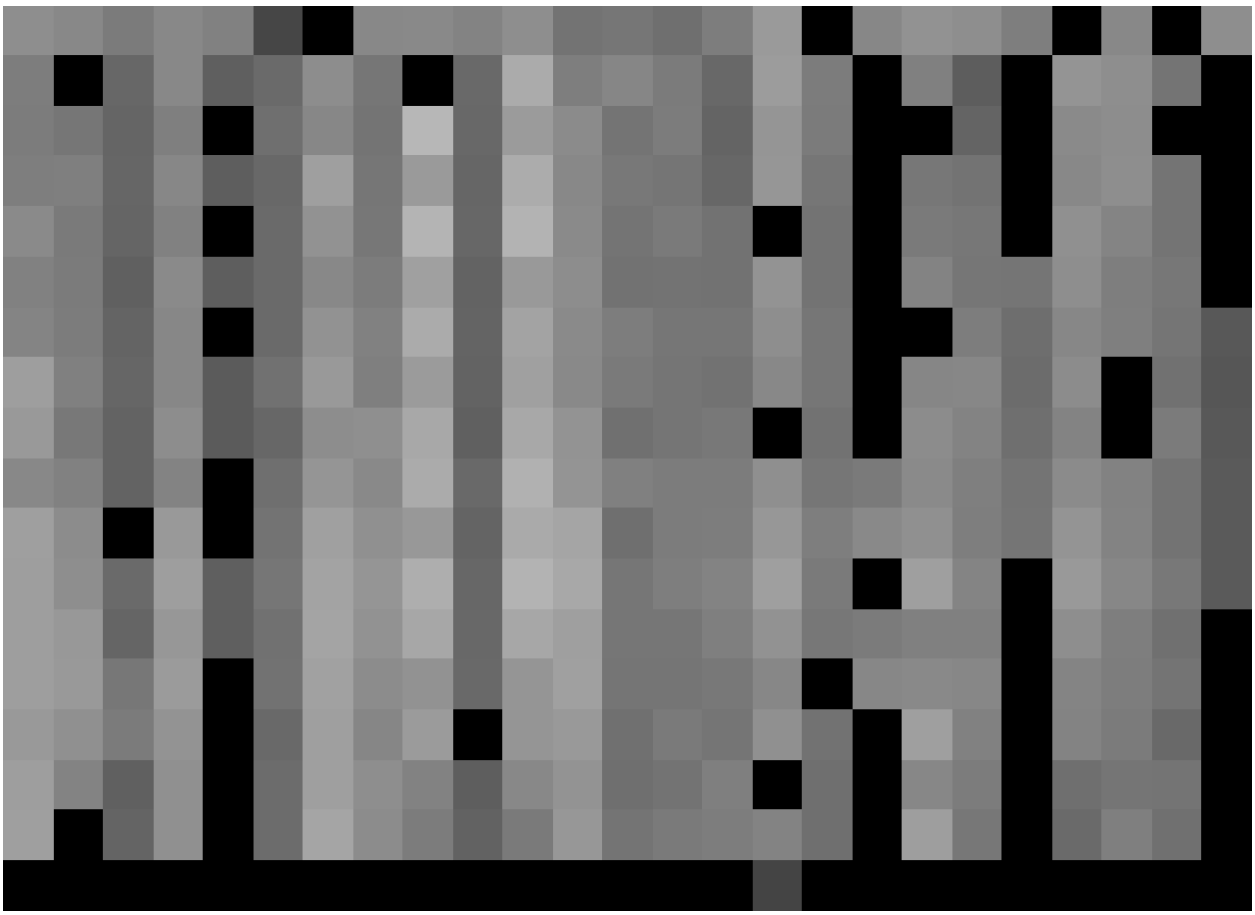


Fig. 5: The flux array from a single grating scan in the RED channel, at the chop 0 position in nod A after fitting ramps, flattened into a 25 x 18 array. The spectral dimension runs along the y-axis. The data was taken in symmetric chopping mode.

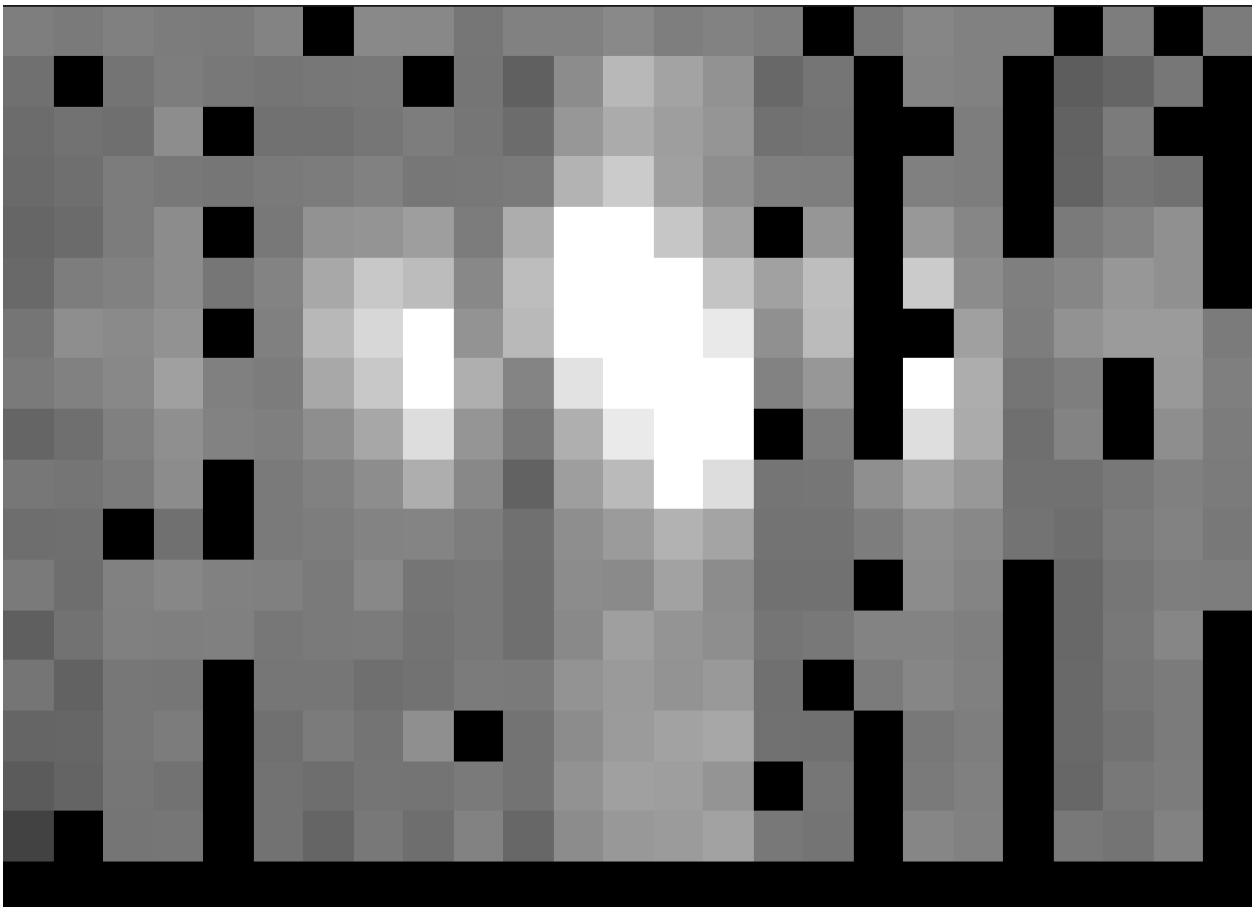


Fig. 6: The same flux array as in Fig. 5, with the corresponding chop 1 subtracted.

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 added to 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.

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.

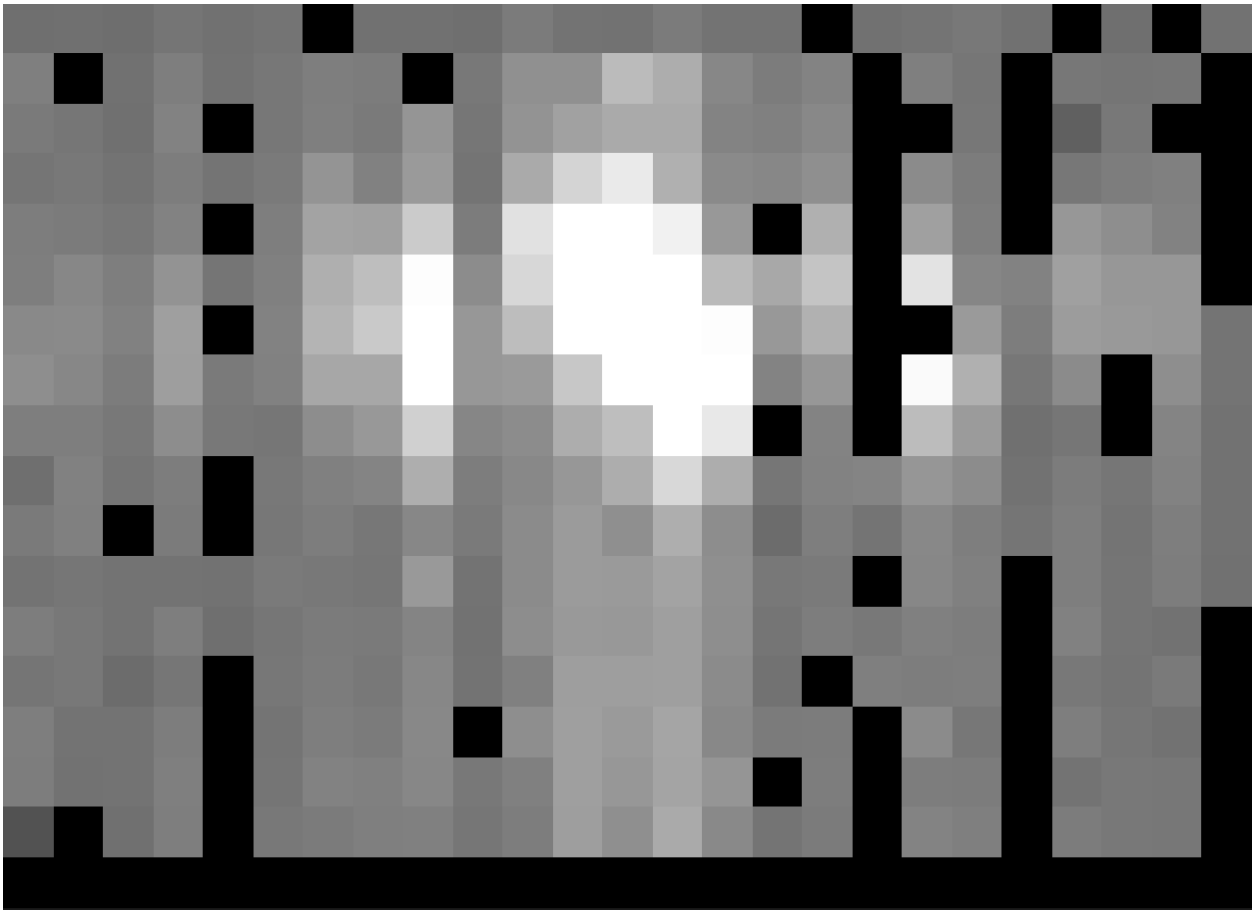


Fig. 7: The chop-subtracted nod A flux array, with the corresponding nod B added.

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 (λ) for the pixel at spatial position *i* and spectral position *j* is calculated from the equation:

$$\phi_i = 2\pi\, ISF \frac{ind + \text{ISOFF}_i}{2^{24}}$$

$$\delta_j = [j - 8.5] * PS + sign\,[j - QOFF] * [j - QOFF]^2 * QS$$

$$g_i = g_0 * \cos\left(\frac{\text{SlitPos}_i - NP}{a}\right)$$

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

where:

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

γ: 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:

1	2	3	4	5
6	7	8	9	10
11	12	13	14	15
16	17	18	19	20
21	22	23	24	25

with corresponding slit position:

Slit position	Spaxel
1	21
2	22
3	23
4	24
5	25
6	
7	16
8	17
9	18
10	19
11	20
12	
13	11
14	12
15	13
16	14
17	15
18	
19	6
20	7
21	8
22	9
23	10
24	
25	1
26	2
27	3
28	4
29	5

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:

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

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 $ADU/sec/Hz$) are propagated throughout the rest of the pipeline.

At this stage, the first and last spectral pixels (the dummy channels, top and bottom rows in Fig. 7) are removed from the flux and error arrays, so that their sizes become 5 x 5 x 16. The wavelength values and spectral widths calculated by the pipeline for each pixel are stored in a new 5 x 5 x 16 array in each grating scan table extension (columns LAMBDA and DLAMDPIX).

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.

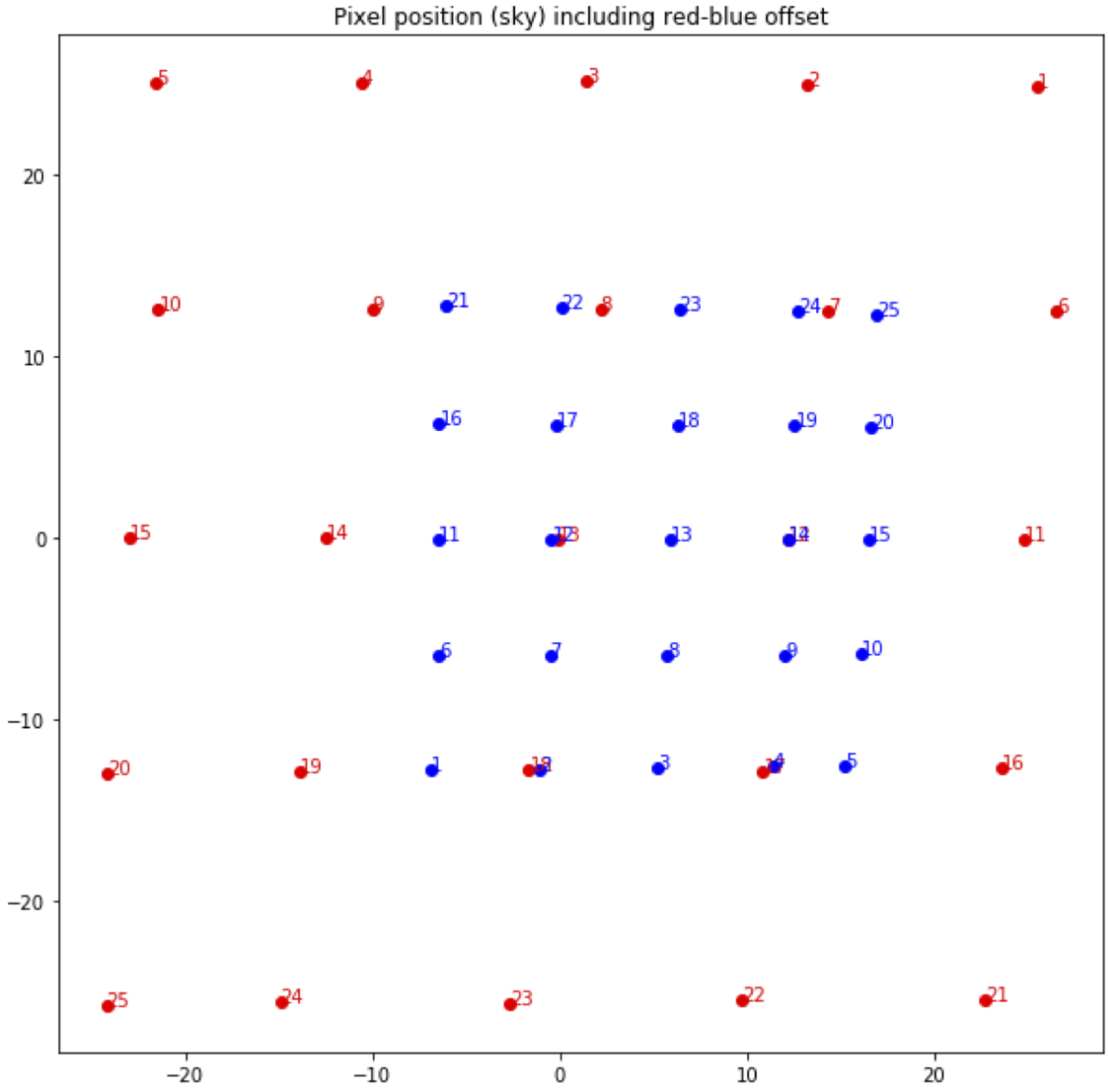


Fig. 8: Average fitted spaxel positions in arcsecond offsets from the center of the detector. The red dots indicate the positions for the RED channel; blue dots indicate the BLUE channel.

For a particular observation, 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:

$$x_{ij} = ps(xpos_{ij} + dx) + d\lambda cos(\theta)\breve{}d\beta sin(\theta)$$

$$y_{ij} = ps(ypos_{ij} + dy) + d\lambda sin(\theta) + d\beta cos(\theta)$$

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, $xpos_{ij}$ and $ypos_{ij}$ 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:

$$x'_{ij} = -x_{ij}cos(\theta) + y_{ij}sin(\theta)$$

$$y'_{ij} = x_{ij}sin(\theta) + y_{ij}cos(\theta)$$

The pipeline stores these calculated x and y coordinates in two 5 x 5 x 16 data arrays in each FITS extension table (columns XS and YS).

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 spexel.

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 spexel, then multiplies the value by the appropriate spatial flat. The flux is then divided by this correction value. The output file format does not change for this step.

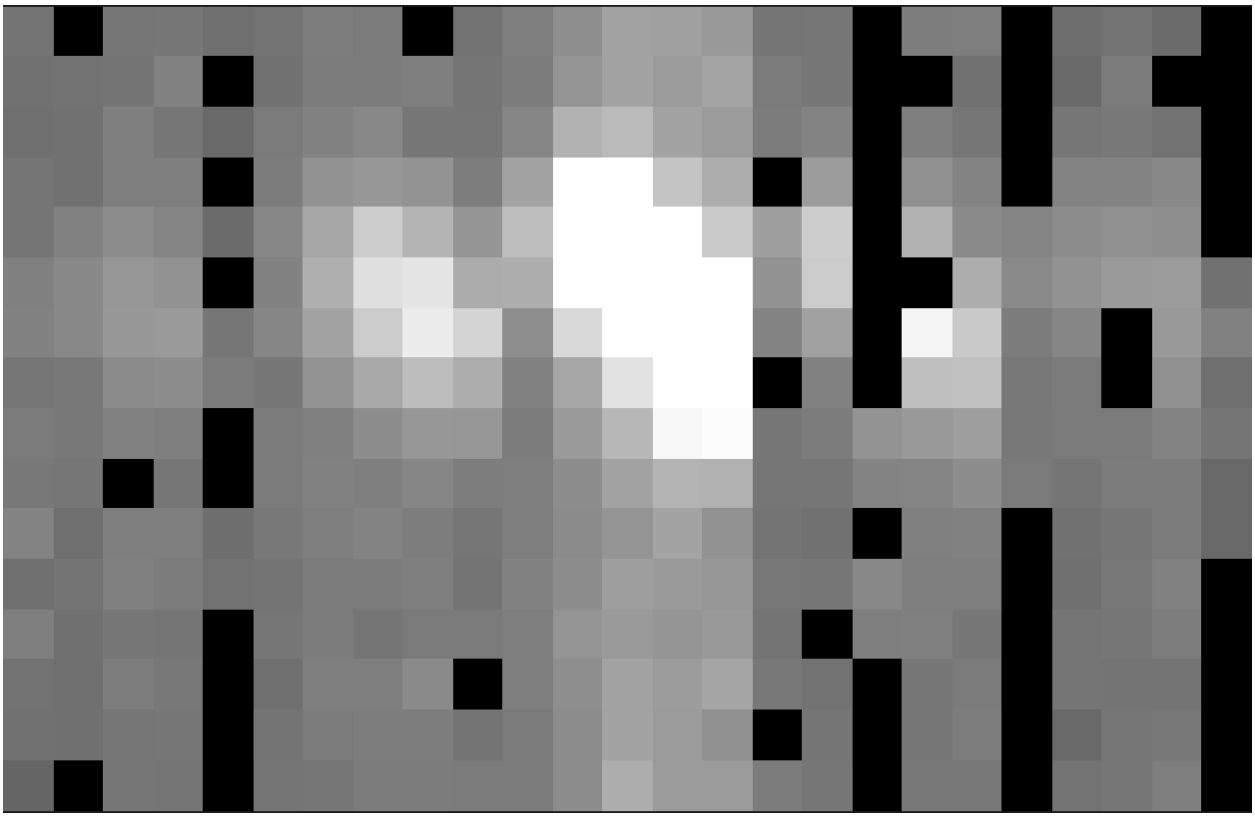


Fig. 9: The flat-corrected flux array.

4.8 Combine Grating Scans

Up until this point, all processing has been done on each grating scan extension 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.

The pipeline then 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 5 x 5 x (16 * *nscan*), where *nscan* 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 (DATA, STDDEV, LAMBDA, XS, and YS) now have dimensions 5 x 5 x (16 * *nscan*).

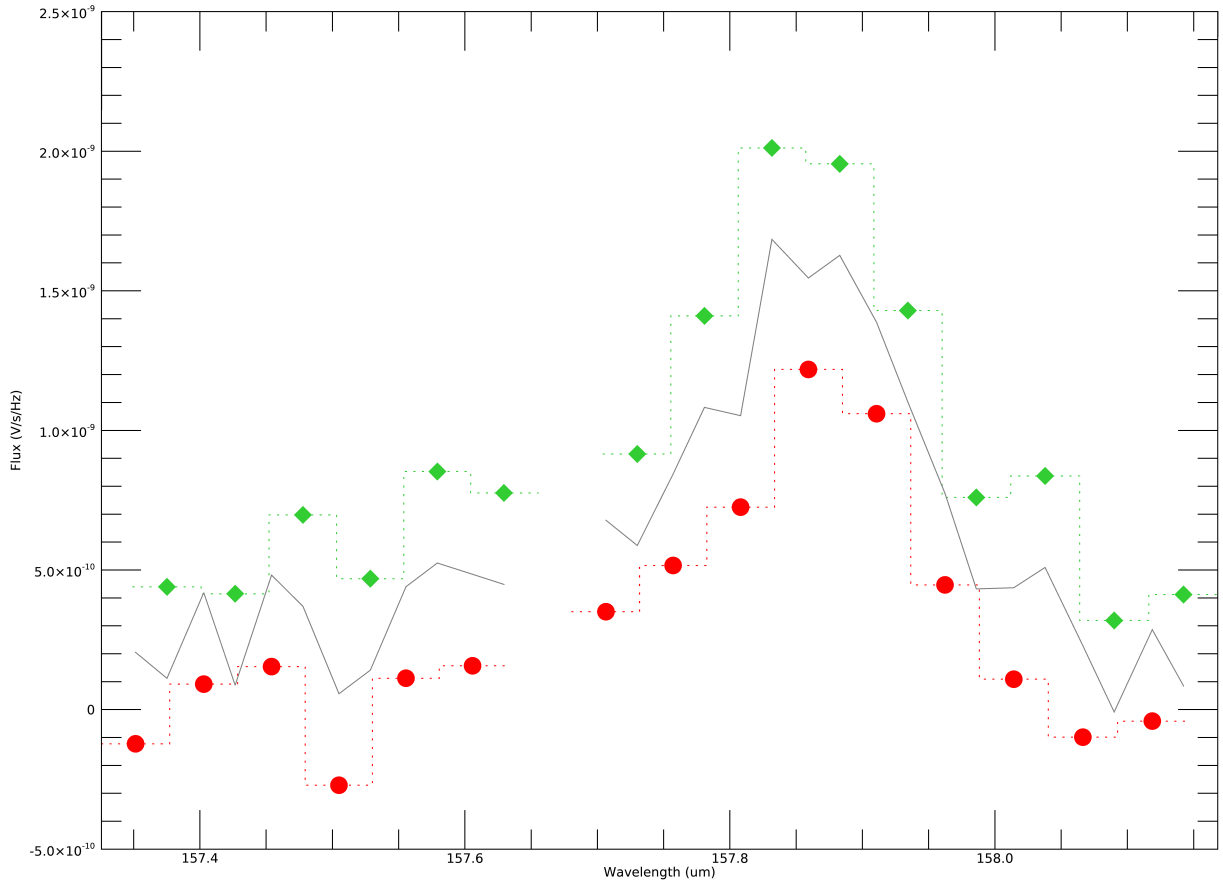


Fig. 10: Example spectral flux from the center spaxel for a single dither position. The red circles and green diamonds represents two different grating scans. The gray line indicates the combined flux array, after bias correction.

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

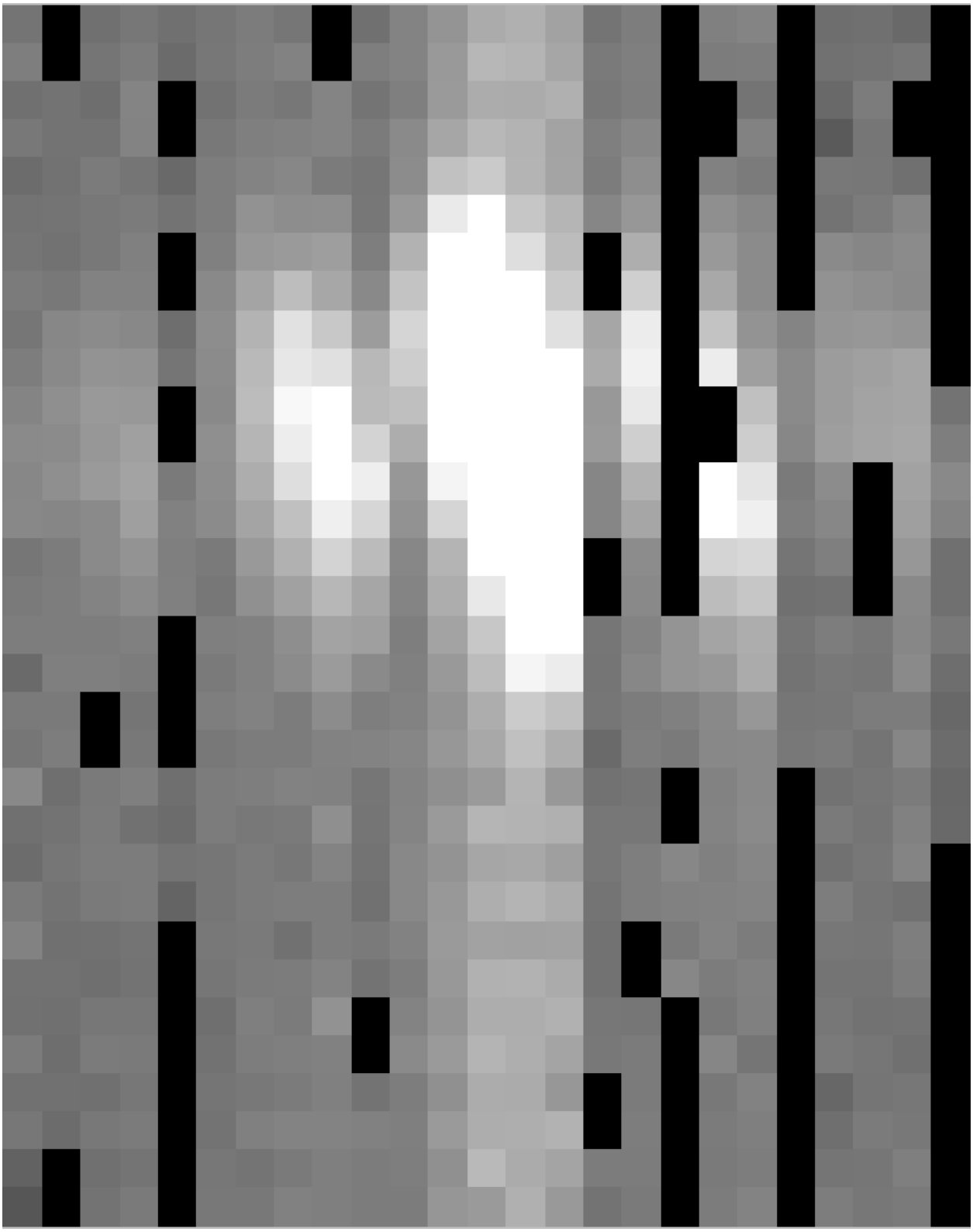


Fig. 11: The full 5 x 5 x 32 flux array, flattened to 25 x 32, after combining two grating scans.

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 relies 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. Until then, correction spectra are generated using the expected PWV value for the flight altitude and airmass appropriate for the observations. Experience with both FIFI-LS and the FORCAST instrument has shown that this method can produce reasonably accurate corrections in the vicinity of broad, shallow telluric absorption features. However, corrections in regions with deep, sharp features (e.g., near 63 microns) are extremely sensitive to the actual PWV along the line of sight. Without accurate atmospheric models and measurements of the PWV, it cannot be expected that standard models will provide reliable telluric corrections. 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 results, and the output spectrum may retain telluric artifacts after telluric correction.

A set of ATRAN models appropriate for a range of altitudes and zenith angles has been generated for pipeline use. In this step, the pipeline selects the model closest to the observed altitude and zenith angle, smooths the transmission model to the resolution of the observed spectrum, bins the transmission data to the observed wavelength and spectral width of 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 5 x 5 x (16 * *nscan*) data table in the first FITS extension (element 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 DATA and STDDEV columns of the binary table. The uncorrected cube and its associated error are stored in the UNCORRECTED_DATA and UNCORRECTED_STDDEV columns.

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).

[1] See http://www.lesia.obspm.fr/perso/emmanuel-lellouch/mars/index.php

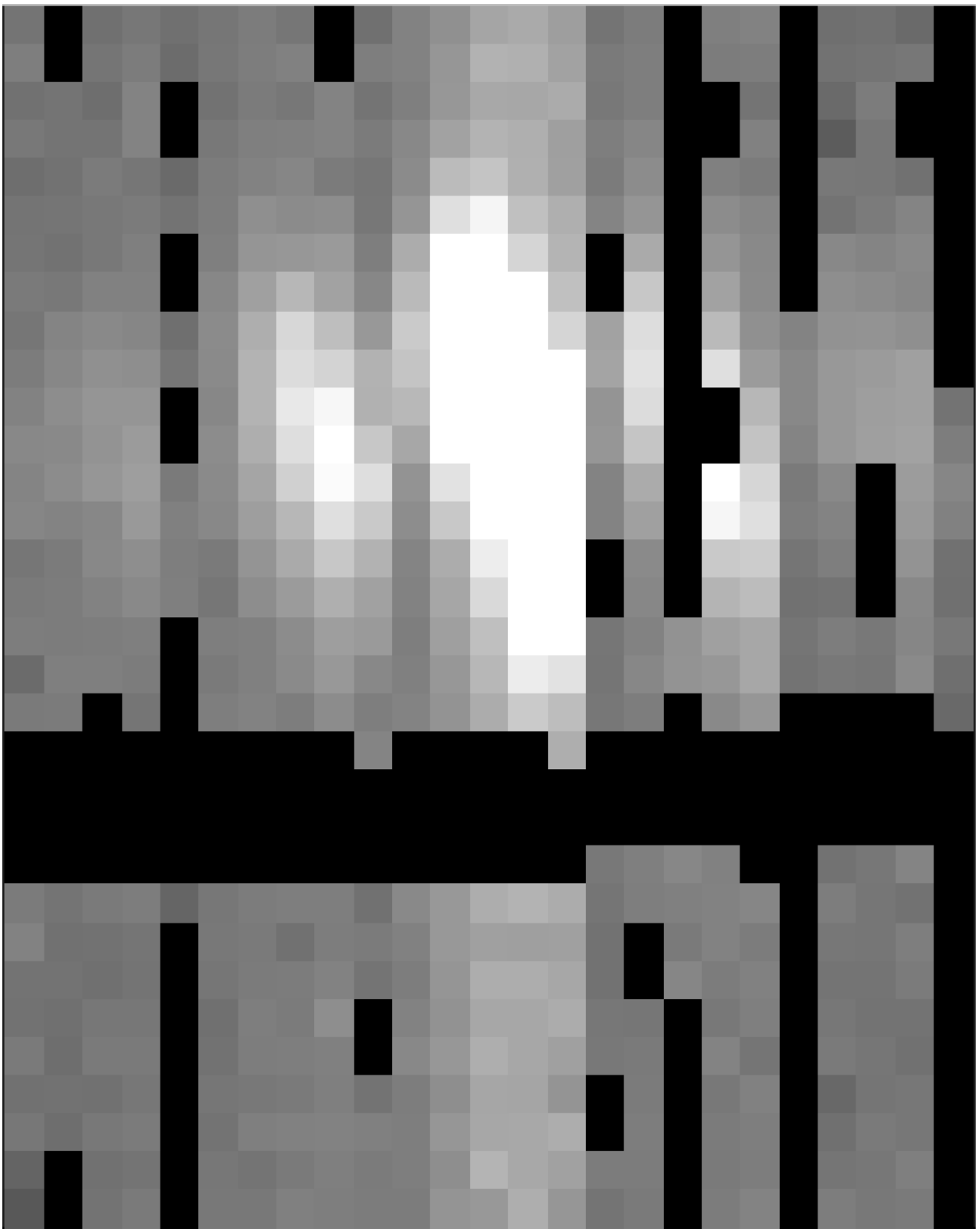


Fig. 12: The telluric-corrected flux array. Some pixels are set to NaN due to poor atmospheric transmission at those wavelengths. The cutoff level was set to 80% for this observation, for illustrative purposes.

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 5 x 5 x (16 * *nscan*) 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 ≤ 0.1).

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 field 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.

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. This sets the range of the output grid.

The spacing of the output grid is set by the desired oversampling. By default, in the wavelength dimension, the pipeline samples the average expected spectral FWHM for the observation with 8 output pixels. The spacing in the spatial dimensions (*dx*) is set by a reference spatial FWHM for the observed channel (5 arcseconds for BLUE, 10 arcseconds for RED), divided by the desired oversampling. By default, the spatial oversampling is set to 5 pixels, so that the BLUE grid spacing is 1 arcsecond and the RED grid spacing is 2 arcseconds.

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 2 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 50 x 41. The full output cube then is 50 x 41 x 75 (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

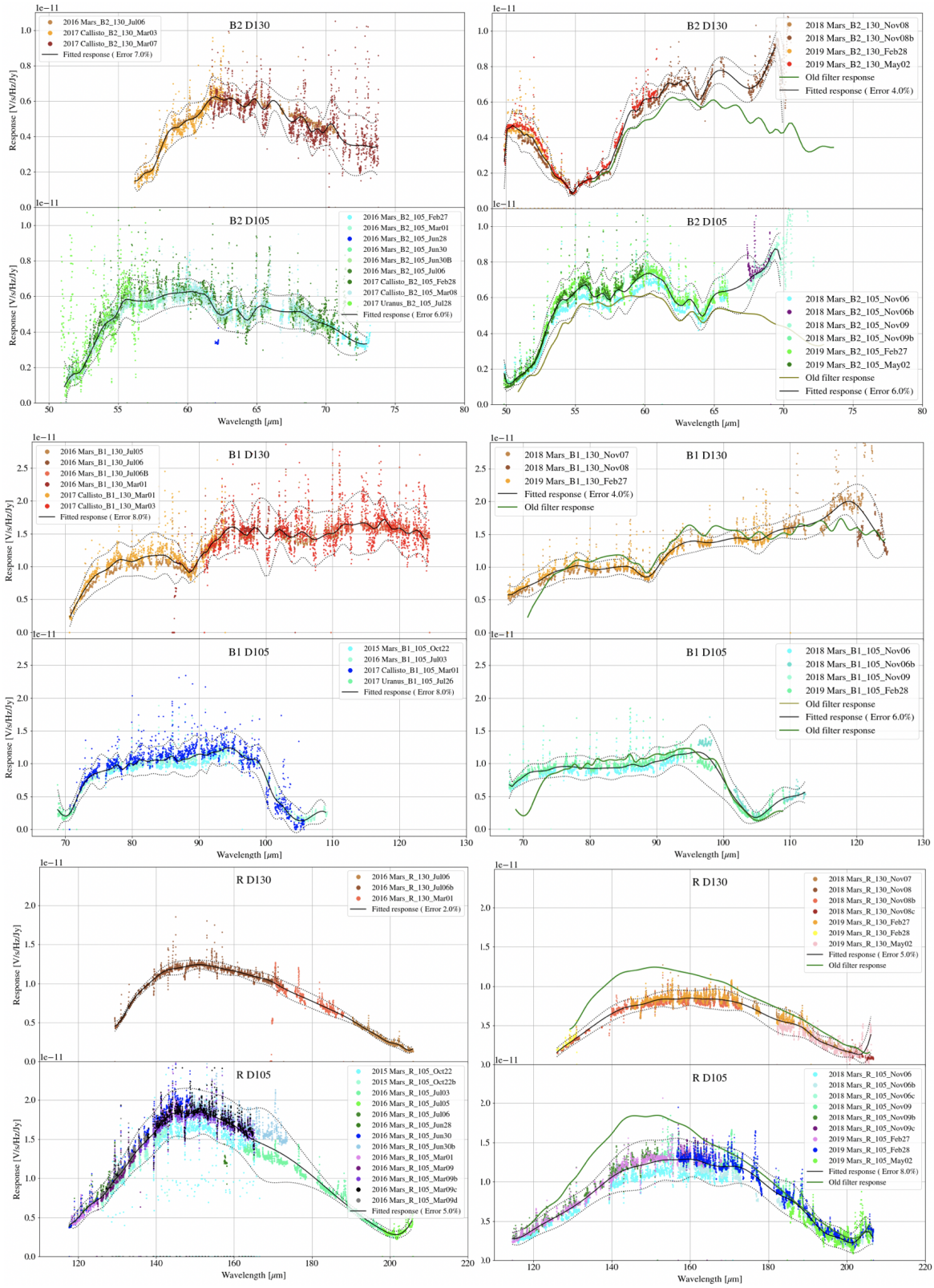


Fig. 13: Response fits overplotted on telluric-corrected data, with model spectra divided out. Data shown was taken in 2015-2019 for the blue channel order 2, blue channel order 1, and red channel. Plots on the left are from an older filter set; plots on the right are for data taken with an updated filter set.

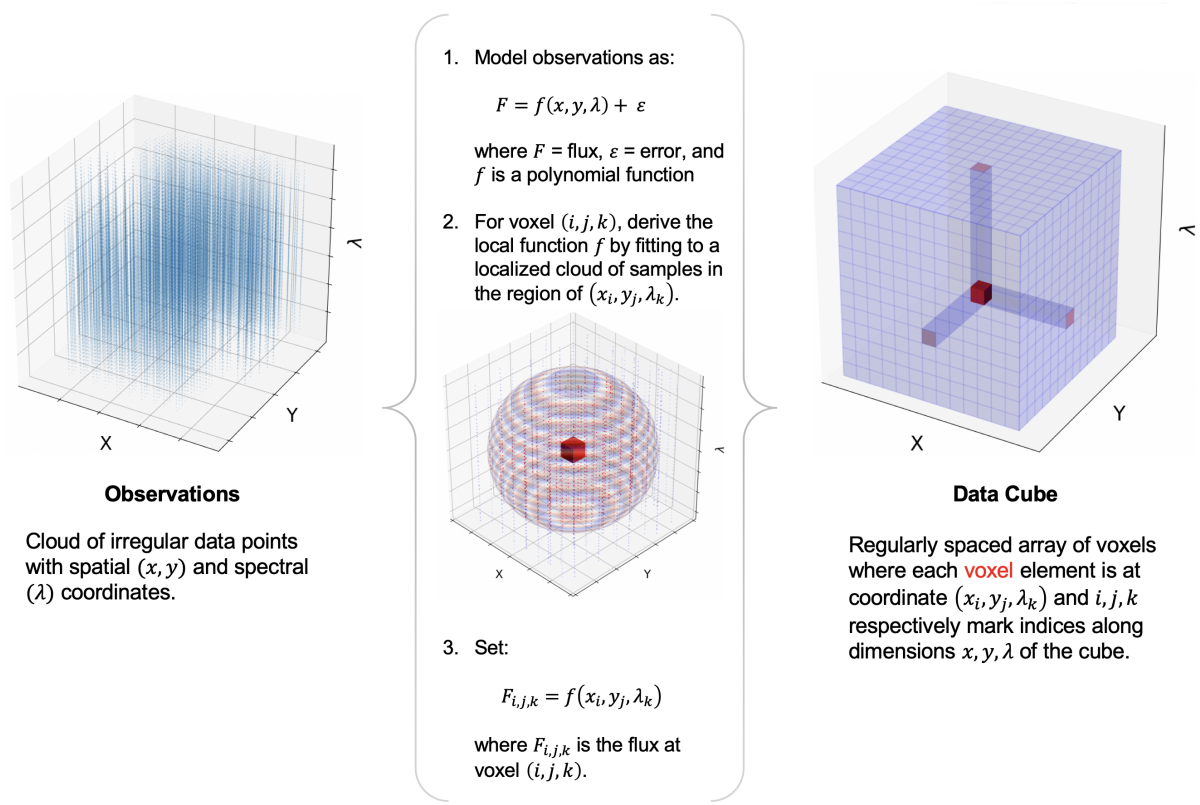


Fig. 14: Overview of the resampling algorithm. Given a cloud of irregularly spaced data points, the algorithm assigns values to voxels of a regular grid by fitting data points in a local cloud with a low-order polynomial function.

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).

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.

Outlier flux values within the window may be rejected. 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 output flux value is the value of the polynomial surface, evaluated at the grid location, and the associated error is the error on the fit.

Output grid locations for which there was insufficient input data for stable polynomial fits are set to NaN. The threshold 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. 16). 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

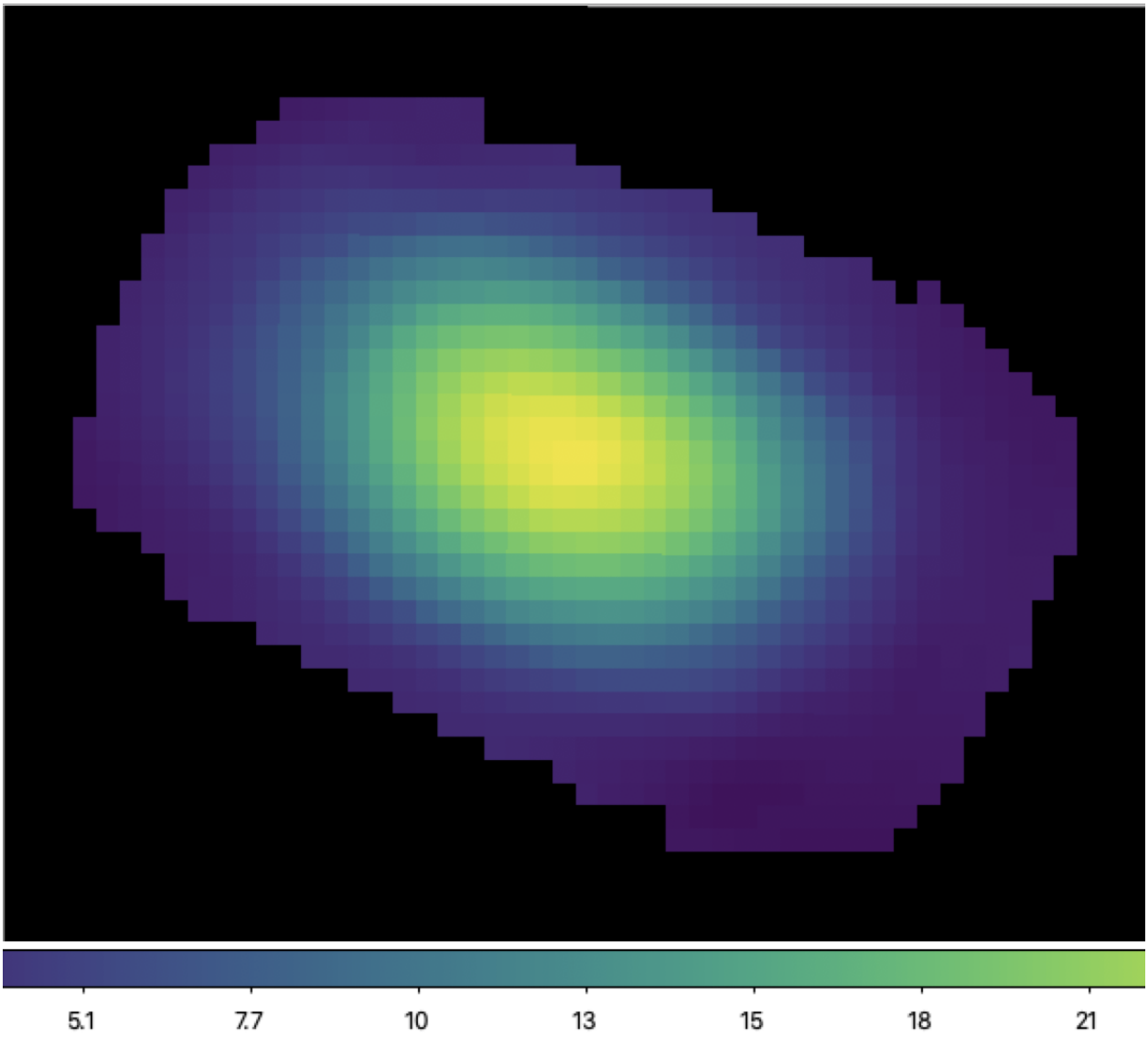
Both the telluric-corrected and the uncorrected flux cubes are resampled in this step, onto the same 3D grid. However, the telluric-corrected cube is resampled using the wavelengths corrected for barycentric motion, and the uncorrected cube is resampled using the original wavelength calibration. The 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 any 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 *ntrans* x 2, where *ntrans* 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).


5.1
7.7
10
13
15
18
21

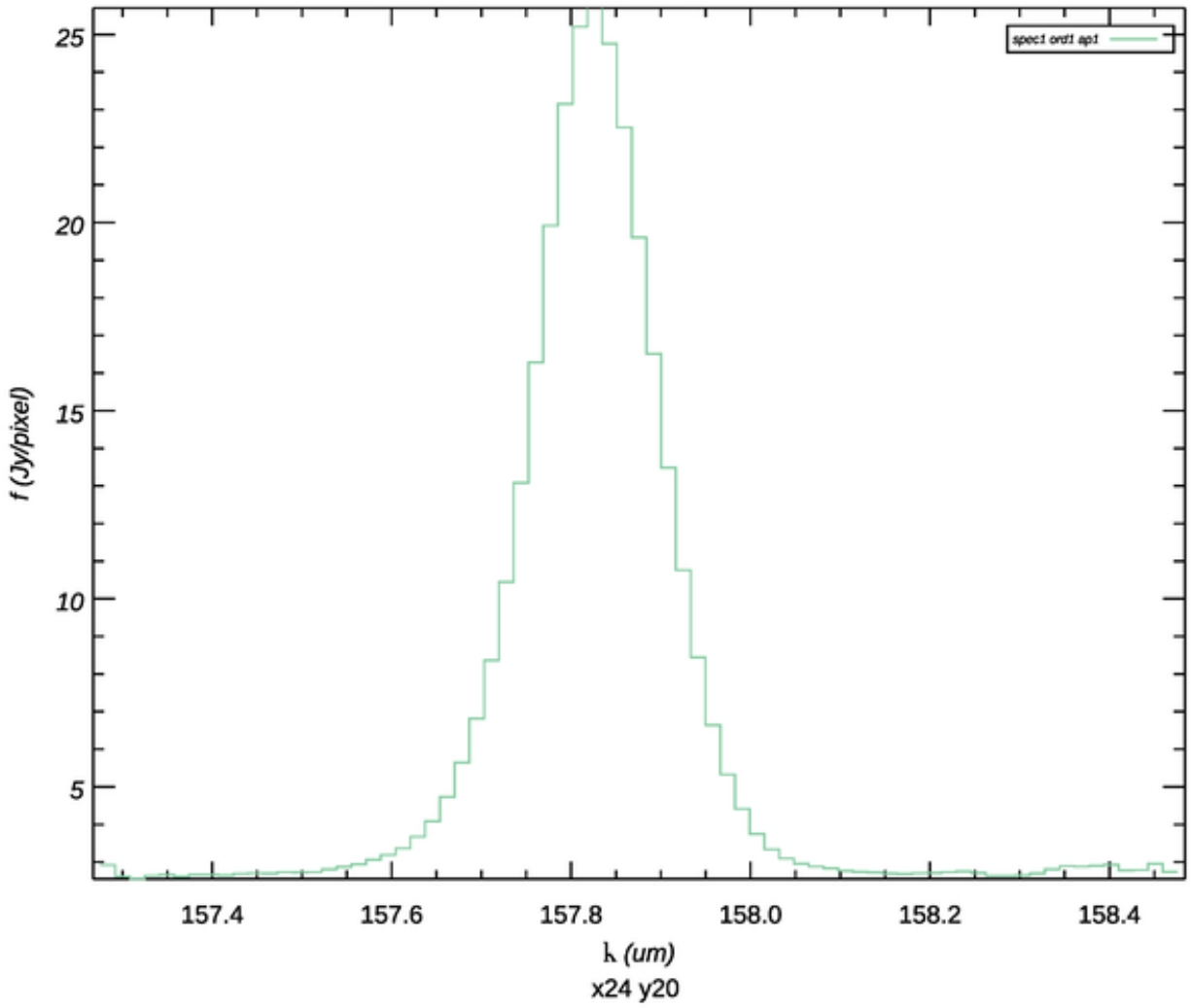


Fig. 15: The final output flux cube. The image on top is a spatial slice at wavelength 157.83 um. The plot on the bottom is a spectral slice at pixel x,y = 24, 20 (offset 7”, -4” from the base position).

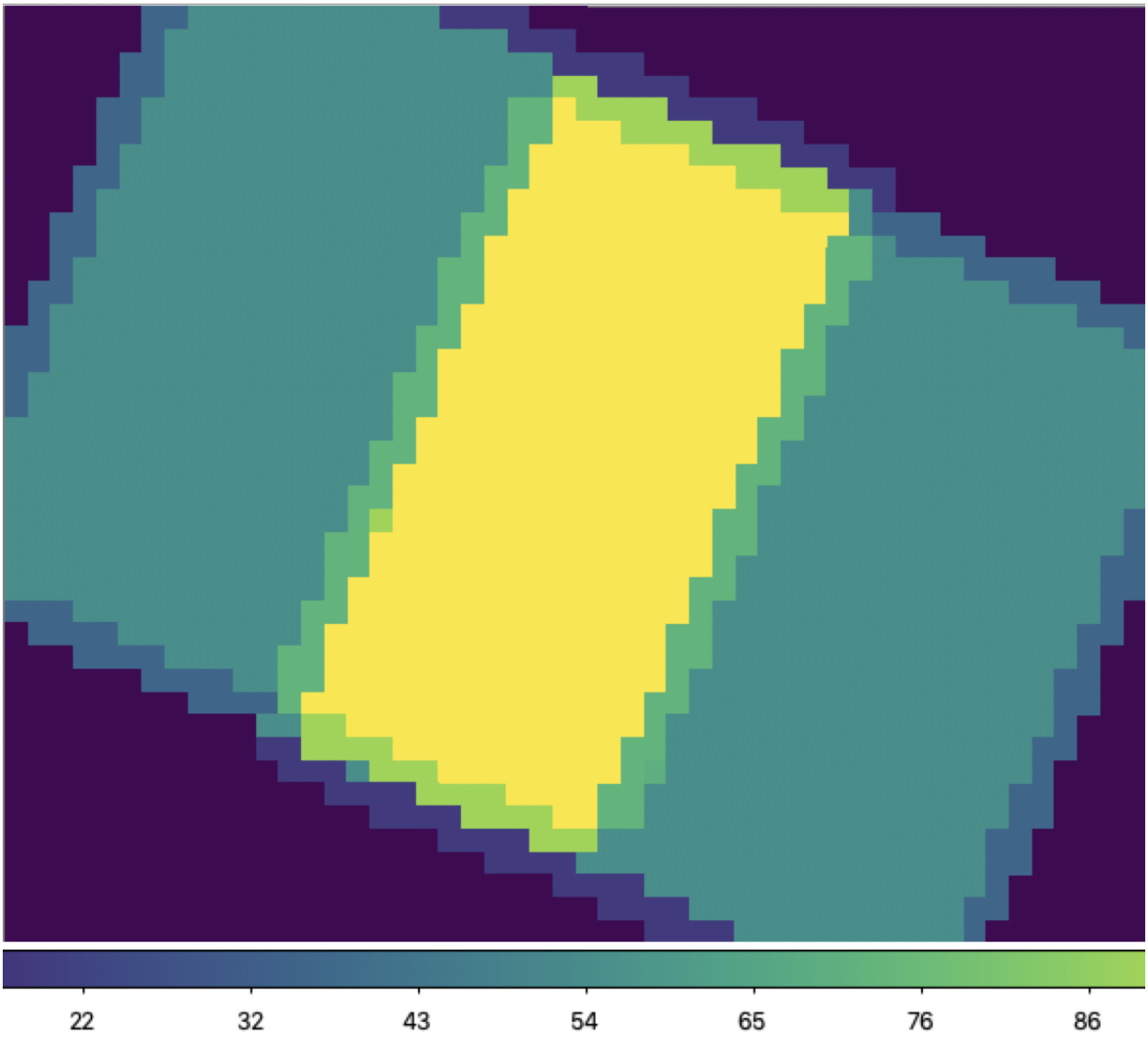


Fig. 16: Exposure map of input dither positions, corresponding to the above flux cube. Values range from 0 (purple, near the edges) to 108 (yellow, near the center).

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

- FLUX: The *nx* x *ny* x *nw* cube of flux values.
- ERROR: The associated error values on the flux (also *nx* x *ny* x *nw*).
- UNCORRECTED_FLUX: The *nx* x *ny* x *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* x *ny* x *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* x *ny* x *nw*).
- UNSMOOTHED_TRANSMISSION: The unsmoothed atmospheric transmission model (*ntrans* x 2).

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 and *resampled* products are saved. Specifying the appropriate option in either the automatic or interactive modes will save all products. Note that as of pipeline version 1.3.2, the STDDEV and ERROR extensions do not include the systematic error on the flux calibration; this is recorded separately in the FITS header keyword CALERR in the primary extension.

Table 1: Final and intermediate data products

Step	Product Type	Proc. status	File code	Saved	Extensions
Split Grating / Chop	*grating_chop_split*	LEVEL_2	CP0, CP1	N	N_{scan} binary table extensions
Fit Ramps	*ramps_fit*	LEVEL_2	RP0, RP1	N	N_{scan} binary table extensions containing DATA, STDDEV
Subtract Chops	*chop_subtracted*	LEVEL_2	CSB	N	N_{scan} binary table extensions containing DATA, STDDEV
Combine Nods	*nod_combined*	LEVEL_2	NCM	N	N_{scan} binary table extensions containing DATA, STDDEV
Lambda Calibrate	*wavelength_calibrated*	LEVEL_2	WAV	N	N_{scan} binary table extensions containing DATA, STDDEV, LAMBDA, DLAMDPIX
Spatial Calibrate	*spatial_calibrated*	LEVEL_2	XYC	N	N_{scan} binary table extensions containing DATA, STDDEV, LAMBDA, DLAMDPIX, XS, YS
Apply Flat	*flat_fielded*	LEVEL_2	FLF	N	N_{scan} binary table extensions containing DATA, STDDEV, LAMBDA, DLAMDPIX, XS, YS
Combine Scans	*scan_combined*	LEVEL_2	SCM	Y	1 binary table extension, containing DATA, STDDEV, LAMBDA, XS, YS
Telluric Correct	*telluric_corrected*	LEVEL_2	TEL	N	1 binary table extension, containing DATA, STDDEV, UNCORRECTED_DATA, UNCORRECTED_STDDEV, LAMBDA, XS, YS, ATRAN

Continued on next page

Table 1 – continued from previous page

Step	Product Type	Proc. status	File code	Saved	Extensions
Flux Calibrate	*flux_calibrated*	LEVEL_3	CAL	Y	1 binary table extension, containing DATA, STDDEV, UNCORRECTED_DATA, UNCORRECTED_STDDEV, LAMBDA, XS, YS, ATRAN, RESPONSE
Correct Wave Shift	*wavelength_shifted*	LEVEL_3	WSH	N	1 binary table extension, containing DATA, STDDEV, UNCORRECTED_DATA, LAMBDA, XS, YS, ATRAN, RESPONSE
Spatial Resample	*resampled*	LEVEL_4	WXY	Y	11 image extensions: FLUX, ERROR, UNCORRECTED_FLUX, UNCORRECTED_ERROR, WAVELENGTH, X, Y, TRANSMISSION, RESPONSE, EXPOSURE_MAP, UNSMOOTHED_TRANSMISSION

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. Before the combine scans step, all outputs will have a separate binary table extension for each grating position; the output of the combine scans and flux calibrate steps will have a single binary table extension. The binary tables contain the columns listed in the table above, along with a HEADER column. After the resampling step, the data is contained in image extensions, as listed above.

Part V
Grouping LEVEL_1 data for processing

FIFI-LS observations of a single object may dither in wavelength and/or in space. It is common to use a set of FIFI-LS observations to map out large regions of diffuse emission in a few small wavelength regions, but it is also common to use FIFI-LS to take a set of observations of a compact source over a wide range of wavelengths. As such, observations cannot simply be split on the central wavelength, or the base positions of the observation. Grouping relies on a keyword, FILEGPID, which defines a set of observations that should be reduced together to produce one final spectral map. In addition, however, observations must always be separated by detector channel, dichroic setting, nodding style (symmetric vs. asymmetric), observation type (source vs. sky flat), and the observational program ID. It may also

be desirable to group file by the observation ID (AOR-ID), but this is considered optional. This is due to the fact that, because FIFI-LS incorporates a dichroic, different AORs can have the same grating setting for one of the two detectors. In such cases, the data sets with the same settings should be combined even though the AORs are different. All of these requirements together define a set of FITS keywords that must match in order for a group of input files to be reduced together (see Table 2).

Table 2: Grouping criteria

Keyword	Data Type	Match Criterion
OBSTYPE	STR	Exact
DETCHAN	STR	Exact
DICHROIC	INT	Exact
NODSTYLE	STR	Exact
PLANID	STR	Exact
FILEGPID	STR	Exact
AOR-ID (optional)	STR	Exact

Part VI

Configuration and execution

8 Installation

The FIFI-LS pipeline is written entirely in Python. The pipeline is platform independent, but has been tested only on Linux and Mac OS X operating systems. Running the pipeline requires a minimum of 16GB RAM, or equivalent-sized swap file.

The pipeline is comprised of four separate software packages: PyFIFI, PypeUtils, PySpextool, and Redux. PyFIFI provides the data processing algorithms, with supporting libraries from PypeUtils and PySpextool. Redux is a data reduction interface package that provides interactive and batch interfaces to the pipeline algorithms.

8.1 External Requirements

To run the pipeline for any mode from the Redux interface, Python 3.6 or higher is required, as well as the following packages: numpy, scipy, matplotlib, pandas, astropy, configobj, numba, bottleneck, and joblib. Some display functions for the graphical user interface (GUI) additionally require the PyQt5, pyds9, photutils, and dill packages. All required external packages are available to install via the pip or conda package managers.

Running the pipeline interactively also requires an installation of SAO DS9 for FITS image display. See http://ds9.si.edu/ for download and installation instructions. The *ds9* executable must be available in the PATH environment variable for the pyds9 interface to be able to find and control it.

8.2 Source Code Installation

The source code for the FIFI-LS pipeline maintained by the SOFIA Data Processing Systems (DPS) team can be obtained directly from the *pyfifi*, *pyredux*, *pypeutils*, and *pyspextool* git repositories there. These repositories contains all needed configuration files, auxiliary files, and Python code to run the pipeline on FIFI-LS data in any observation mode.

After obtaining the source code, install the four Python libraries with the command:

```
python setup.py install
```

from the *pyfifi*, *pyredux*, *pypeutils*, and *pyspextool* directories. Alternately, a development installation may be performed from inside each directory with the command:

```
pip install -e .
```

After installation, the top-level pipeline interface commands should be available in the PATH. Typing:

```
redux
```

from the command line should launch the GUI interface, and:

```
redux_pipe -h
```

should display a brief help message for the command line interface.

9 Configuration

For FIFI-LS algorithms, default parameter values are defined by the Redux object that interfaces to them. These values may be overridden manually for each step, while running in interactive mode. They may also be overridden by an input parameter file, in INI format, in either interactive or automatic mode. See Appendix A for an example of an input parameter file, which contains the current defaults for all parameters.

Requirements for input header keywords are also specified in a configuration file, called *headerdef.dat*, located in the *fifi_ls/data* package directory. This table lists the keyword name, whether it is a value required to be present in the input headers, its default value, the data type of the value, and any requirements on the value range (minimum value, maximum value, or enumerated value). The table also defines how keywords from multiple input files should be combined for a single output file (e.g. take the first value, take the sum, string-concatenate, etc.). A sample of this configuration file is also given in Appendix A. All keywords present in the table will be written to output files produced by the FIFI-LS Redux pipeline.

10 Input data

Redux takes as input raw FIFI-LS FITS data files, which contain unsigned tables. The number of frames per raw data cube depends on the readout mode used to acquire the data. The FITS headers contain data acquisition and observation parameters and, combined with the pipeline configuration files, comprise the information necessary to complete all steps of the data reduction process. Some critical keywords are required to be present in the raw data in order to perform a successful grouping, reduction, and ingestion into the SOFIA archive (see Appendix A).

It is assumed that the input data have been successfully grouped before beginning reduction: Redux considers all input files in a reduction to be science files that are part of a single homogeneous reduction group, to be reduced together with the same parameters.

10.1 Auxiliary Files

In order to complete a standard reduction, the pipeline requires a number of auxiliary files to be on disk, in standard locations within the *fifi_ls/data* package directory. These files may be overridden in custom reductions, using input parameters for the relevant pipeline steps. See Table 3 for a table of all commonly used types of auxiliary files.

Table 3: Auxiliary files used by FIFI-LS reductions

Auxiliary File	File Type	Pipe Step	Comments
Bad Pixel	ASCII	Fit Ramps	Contains a list of known bad pixels
Wavelength Calibration	CSV	Lambda Calibrate	Contains wavelength calibration constants, by date
Spatial Calibration	ASCII	Spatial Calibrate	Contains spaxel position values, by date
Spatial Flat	ASCII	Apply Flat	Contains flat correction values for all 25 spaxels, by date
Spectral Flat	FITS	Apply Flat	Contains flat correction values for all spexels at all possible wavelengths
Resolution	ASCII	Telluric Correct, Resample	Contains the expected spatial and spectral resolution for all modes
ATRAN	FITS	Telluric Correct	Contains an atmospheric transmission model spectrum
Response	FITS	Flux Calibrate	Contains an instrumental response spectrum

11 Redux Usage

Redux usage is documented in the `redux` package.

11.1 Automatic Mode Execution

The DPS pipeline infrastructure runs a pipeline on previously-defined reduction groups as a fully-automatic black box. To do so, it creates an input manifest (*infiles.txt*) that contains relative paths to the input files (one per line). The command-line interface to the pipeline is run as:

```
redux_pipe infiles.txt
```

The command-line interface will read in the specified input files, use their headers to determine the observation mode, and accordingly the steps to run and any intermediate files to save. Output files are written to the current directory, from which the pipeline was called. After reduction is complete, the script will generate an output manifest (*outfiles.txt*) containing the relative paths to all output FITS files generated by the pipeline.

Optionally, in place of a manifest file, file paths to input files may be directly specified on the command line. Input files may be raw FITS files, or may be intermediate products previously produced by the pipeline. For example, this command will complete the reduction for a set of FITS files in the current directory, previously reduced through the calibration step of the pipeline:

```
redux_pipe *CAL*.fits
```

To customize batch reductions from the command line, the *redux_pipe* interface accepts a configuration file on the command line. This file may contain any subset of the full configuration file, specifying any non-default parameters for pipeline steps. An output directory for pipeline products and the terminal log level may also be set on the command line.

The full set of optional command-line parameters accepted by the *redux_pipe* interface are:

```
-h, --help            show this help message and exit
-c CONFIG, --configuration CONFIG
                      Path to Redux configuration file.
-o OUTDIR, --out OUTDIR
                      Path to output directory.
```

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```
-l LOGLEVEL, --loglevel LOGLEVEL
                      Log level.
```

11.2 Manual Mode Execution

In manual mode, the pipeline may be run interactively, via a graphical user interface (GUI) provided by the Redux package. The GUI is launched by the command:

```
redux
```

entered at the terminal prompt (Fig. 17). The GUI allows output directory specification, but it may write initial or temporary files to the current directory, so it is recommended to start the interface from a location to which the user has write privileges.

From the command line, the *redux* interface accepts an optional config file (*-c*) or log level specification (*-l*), in the same way the *redux_pipe* command does. Any pipeline parameters provided to the interface in a configuration file will be used to set default values; they will still be editable from the GUI.

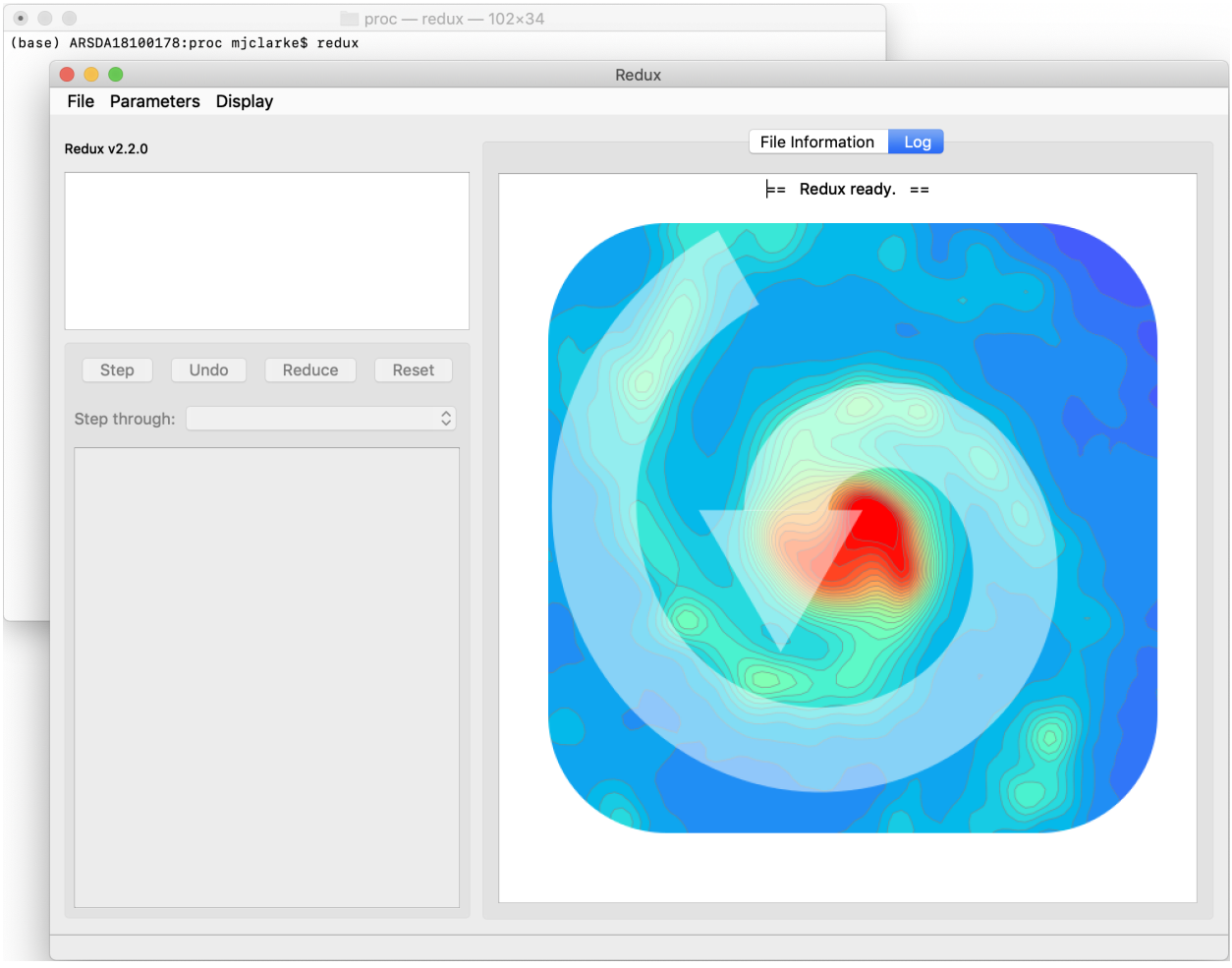

Fig. 17: Redux GUI startup.

Basic Workflow

To start an interactive reduction, select a set of input files, using the File menu (**File->Open New Reduction**). This will bring up a file dialog window (see Fig. 18). All files selected will be reduced together as a single reduction set.

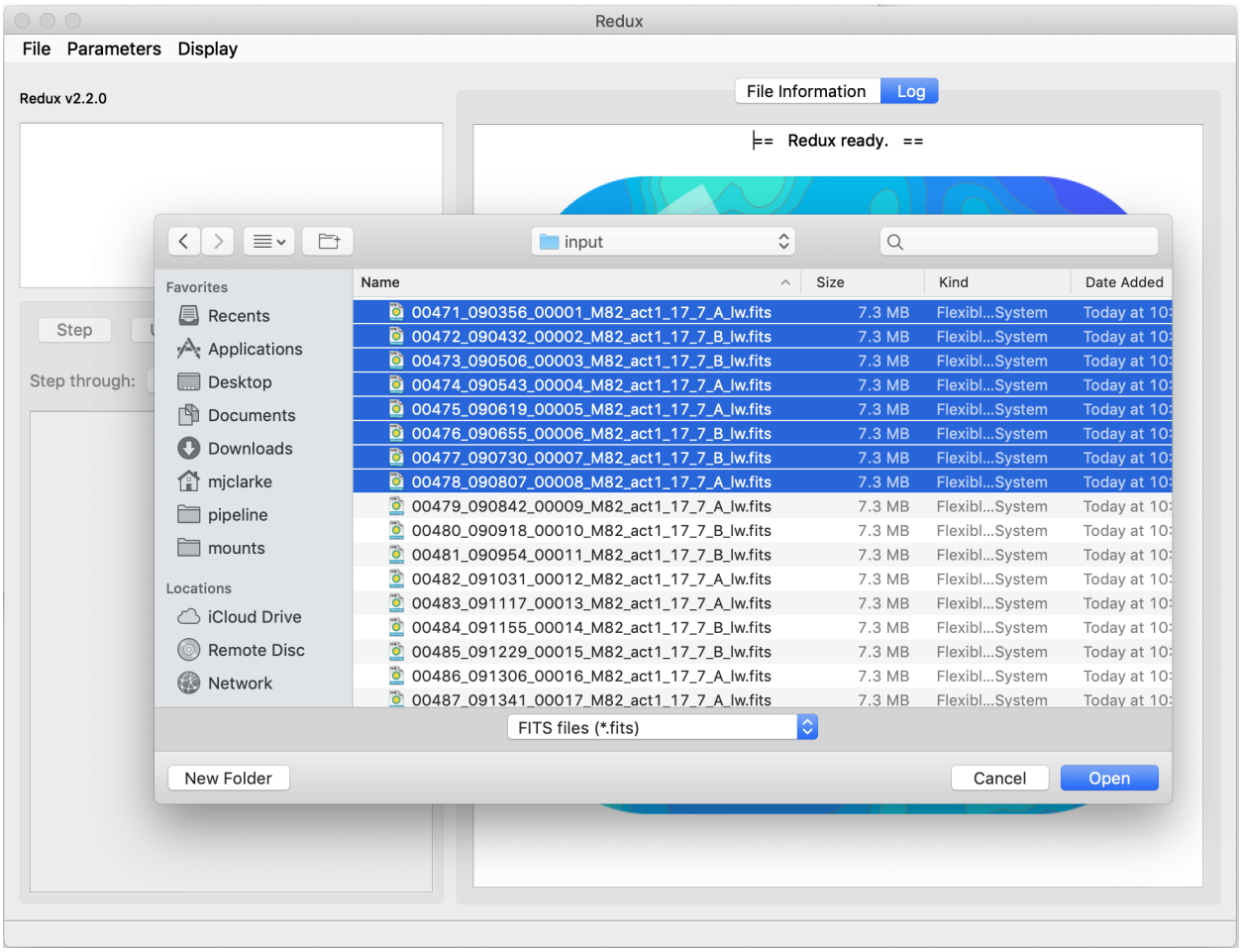

Fig. 18: Open new reduction.

Redux will decide the appropriate reduction steps from the input files, and load them into the GUI, as in Fig. 19.

Each reduction step has a number of parameters that can be edited before running the step. To examine or edit these parameters, click the **Edit** button next to the step name to bring up the parameter editor for that step (Fig. 20). Within the parameter editor, all values may be edited. Click **OK** to save the edited values and close the window. Click **Reset** to restore any edited values to their last saved values. Click **Restore Defaults** to reset all values to their stored defaults. Click **Cancel** to discard all changes to the parameters and close the editor window.

The current set of parameters can be displayed, saved to a file, or reset all at once using the **Parameters** menu. A previously saved set of parameters can also be restored for use with the current reduction (**Parameters -> Load Parameters**).

After all parameters for a step have been examined and set to the user's satisfaction, a processing step can be run on all loaded files either by clicking **Step**, or the **Run** button next to the step name. Each processing step must be run in order, but if a processing step is selected in the **Step through:** widget, then clicking **Step** will treat all steps up through the selected step as a single step and run them all at once. When a step has been completed, its buttons will be grayed out and inaccessible. It is possible to undo one previous step by clicking **Undo**. All remaining steps can be run at once

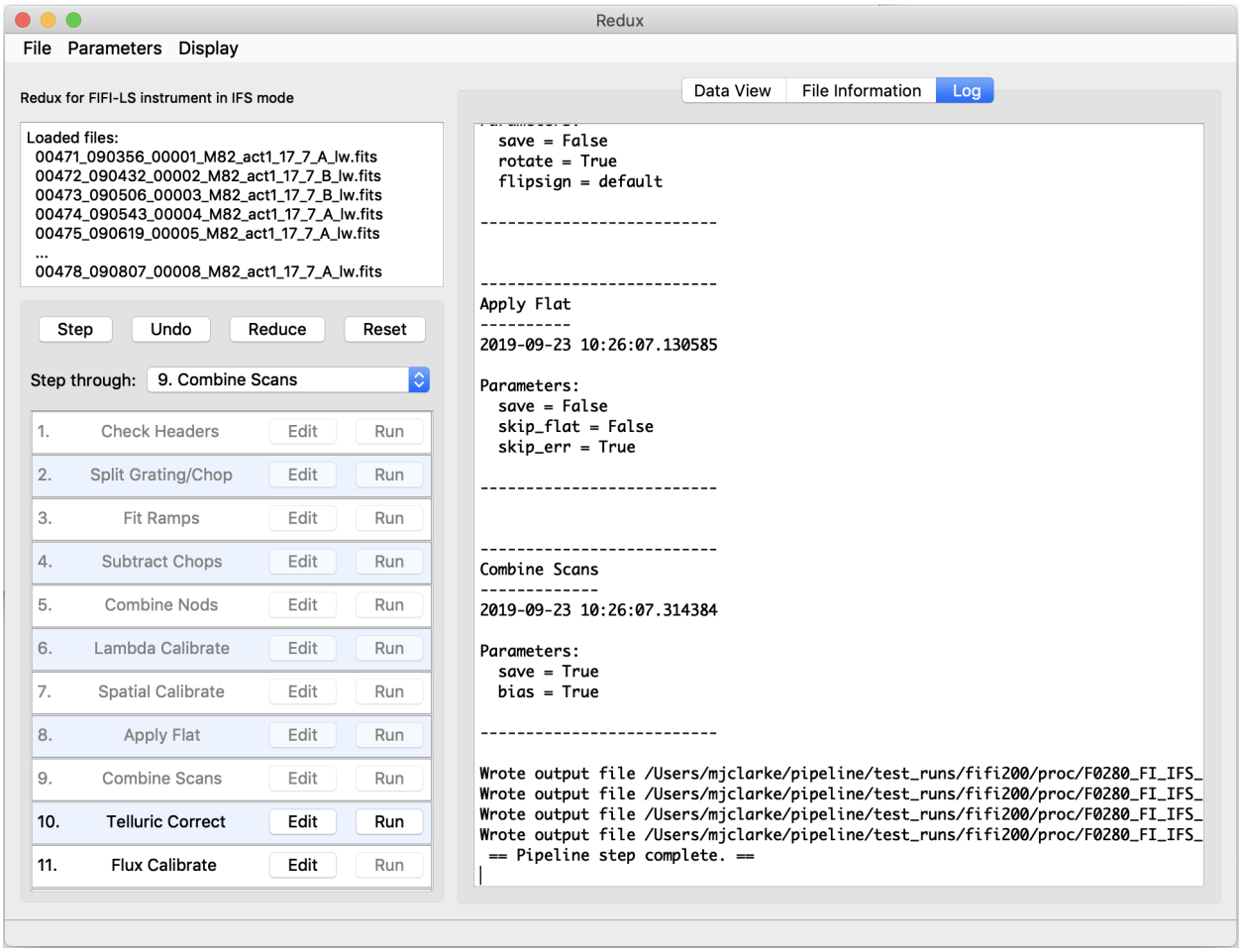

Fig. 19: Sample reduction steps. Log output from the pipeline is displayed in the **Log** tab.

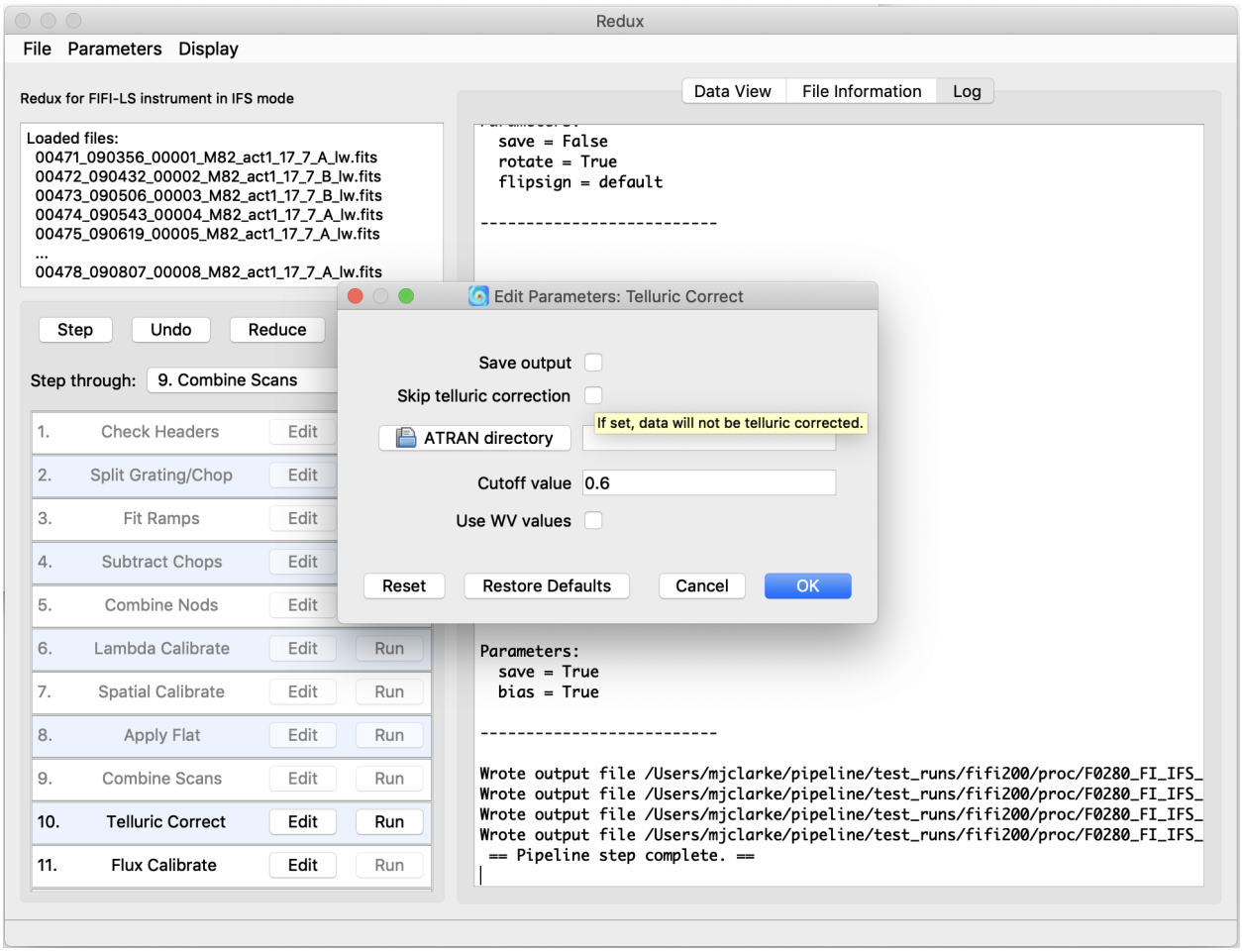

Fig. 20: Sample parameter editor for a pipeline step.

by clicking **Reduce**. After each step, the results of the processing may be displayed in a data viewer. After running a pipeline step or reduction, click **Reset** to restore the reduction to the initial state, without resetting parameter values.

Files can be added to the reduction set (**File -> Add Files**) or removed from the reduction set (**File -> Remove Files**), but either action will reset the reduction for all loaded files. Select the **File Information** tab to display a table of information about the currently loaded files (Fig. 21).

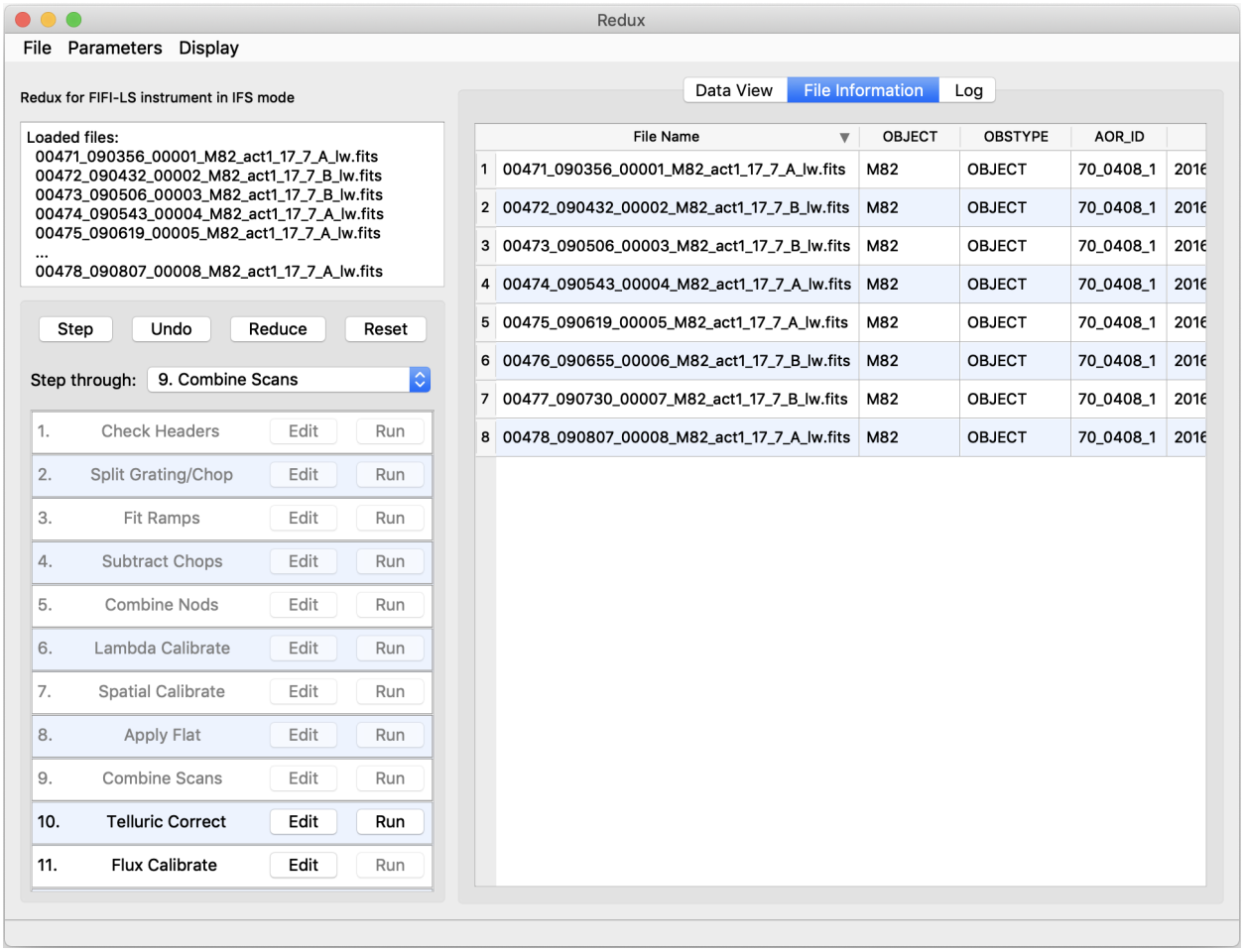

Fig. 21: File information table.

Display Features

The Redux GUI displays images for quality analysis and display (QAD) in the DS9 FITS viewer. DS9 is a standalone image display tool with an extensive feature set. See the SAO DS9 site (http://ds9.si.edu/) for more usage information.

After each pipeline step completes, Redux may load the produced images into DS9. Some display options may be customized directly in DS9; some commonly used options are accessible from the Redux interface, in the **Data View** tab (Fig. 22).

From the Redux interface, the **Display Settings** can be used to:

- Set the FITS extension to display (**First**, or edit to enter a specific extension), or specify that all extensions should be displayed in a cube or in separate frames.
- Lock individual frames together, in image or WCS coordinates.

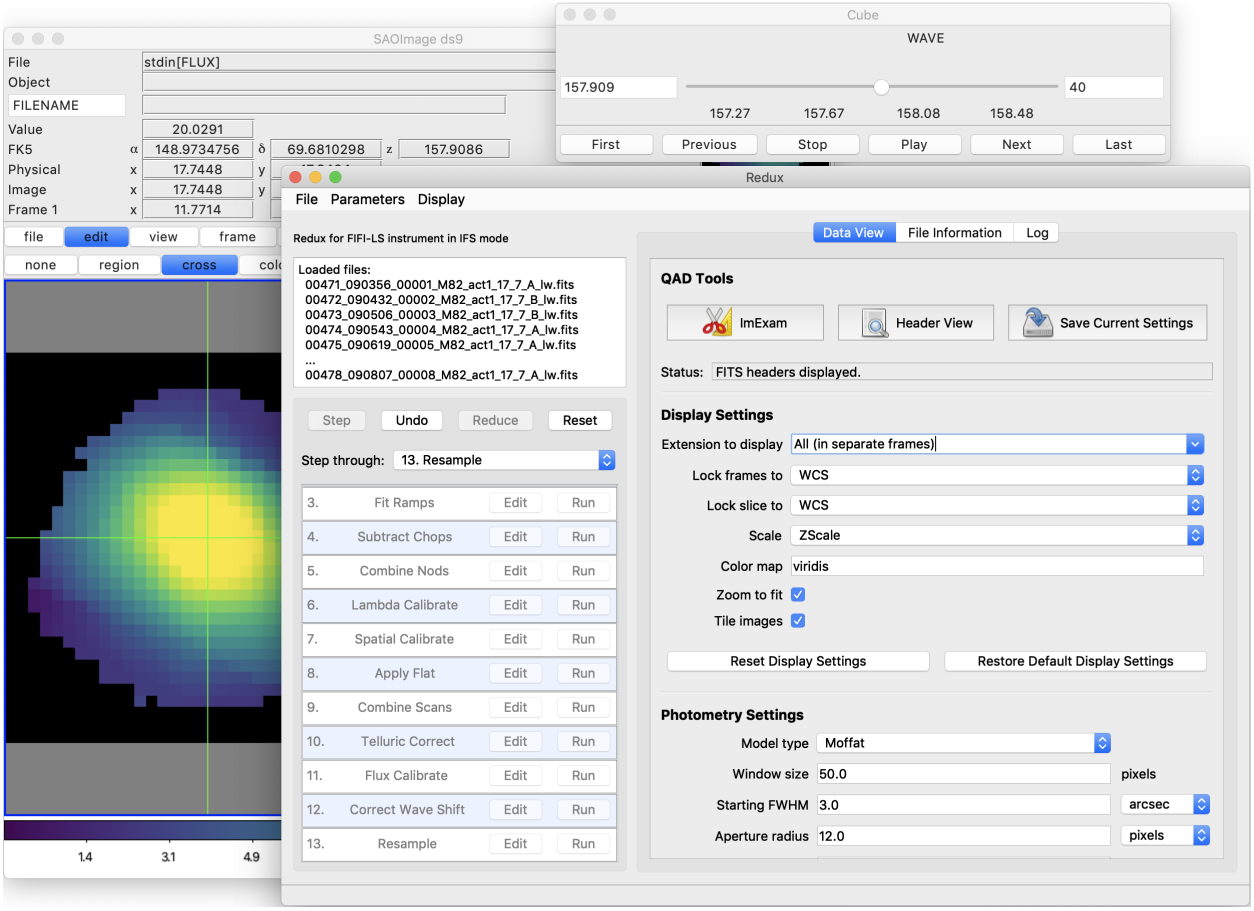

Fig. 22: Data viewer settings and tools.

- Lock cube slices for separate frames together, in image or WCS coordinates.
- Set the image scaling scheme.
- Set a default color map.
- Zoom to fit image after loading.
- Tile image frames, rather than displaying a single frame at a time.

Changing any of these options in the Data View tab will cause the currently displayed data to be reloaded, with the new options. Clicking **Reset Display Settings** will revert any edited options to the last saved values. Clicking **Restore Default Display Settings** will revert all options to their default values.

In the **QAD Tools** section of the **Data View** tab, there are several additional tools available.

Clicking the **ImExam** button (scissors icon) launches an event loop in DS9. After launching it, bring the DS9 window forward, then type 'a' over a source in the image to perform photometry at that location. Typing 'c' will clear any previous results and 'q' will quit the ImExam loop. The photometry settings (the image window considered, the model fit, the aperture sizes, etc.) may be customized in the **Photometry Settings**. After modifying these settings, they will take efffect only for new apertures (use 'c' to clear old ones first). As for the display settings, **Reset Photometry Settings** will revert to the last saved values and **Restore Default Photometry Settings** will revert to default values.

Clicking the **Header** button (magnifying glass icon) from the **QAD Tools** section opens a new window that displays headers from currently loaded FITS files in text form (Fig. 23). The extensions displayed depends on the extension setting selected (in **Extension to Display**). If a particular extension is selected, only that header will be displayed. If all extensions are selected (either for cube or multi-frame display), all extension headers will be displayed. The buttons at the bottom of the window may be used to find or filter the header text, or generate a table of header keywords. For filter or table display, a comma-separated list of keys may be entered in the text box.

Clicking the **Save Current Settings** button (disk icon) from the **QAD Tools** section saves all current display and photometry settings for the current user. This allows the user's settings to persist across new Redux reductions, and to be loaded when Redux next starts up.

12 FIFI-LS Reduction

FIFI-LS data reduction with Redux follows the data reduction flowchart given in Fig. 4. At each step, Redux attempts to determine automatically the correct action, given the input data and default parameters, but each step can be customized as needed.

Some key parameters to note are listed below.

- **Check Headers**
  - *Abort reduction for invalid headers*: By default, Redux will halt the reduction if the input header keywords do not meet requirements. Uncheck this box to attempt the reduction anyway.
- **Fit Ramps**
  - *Signal-to-noise threshold*: This value defines the signal-to-noise cut-off to flag a ramp as bad and ignore it. Set to -1 to skip the signal-to-noise cut.
  - *Combination threshold (sigma)*: This value defines the rejection threshold for the robust mean combination of the ramp slopes. Set higher to reject fewer ramps, lower to reject more.
  - *Bad pixel file*: By default, the pipeline looks up a bad pixel mask in *fifi-ls/data/badpix_files*. To override the default mask, use this parameter to select a different text file. The file must be an ASCII table with two columns: the spaxel number (1-25, numbered left to right in displayed array), and the spexel number (1-16, numbered bottom to top in displayed array). This option may be used to block a bad spaxel for a particular observation, by entering a bad pixel for every spexel index in a particular spaxel.

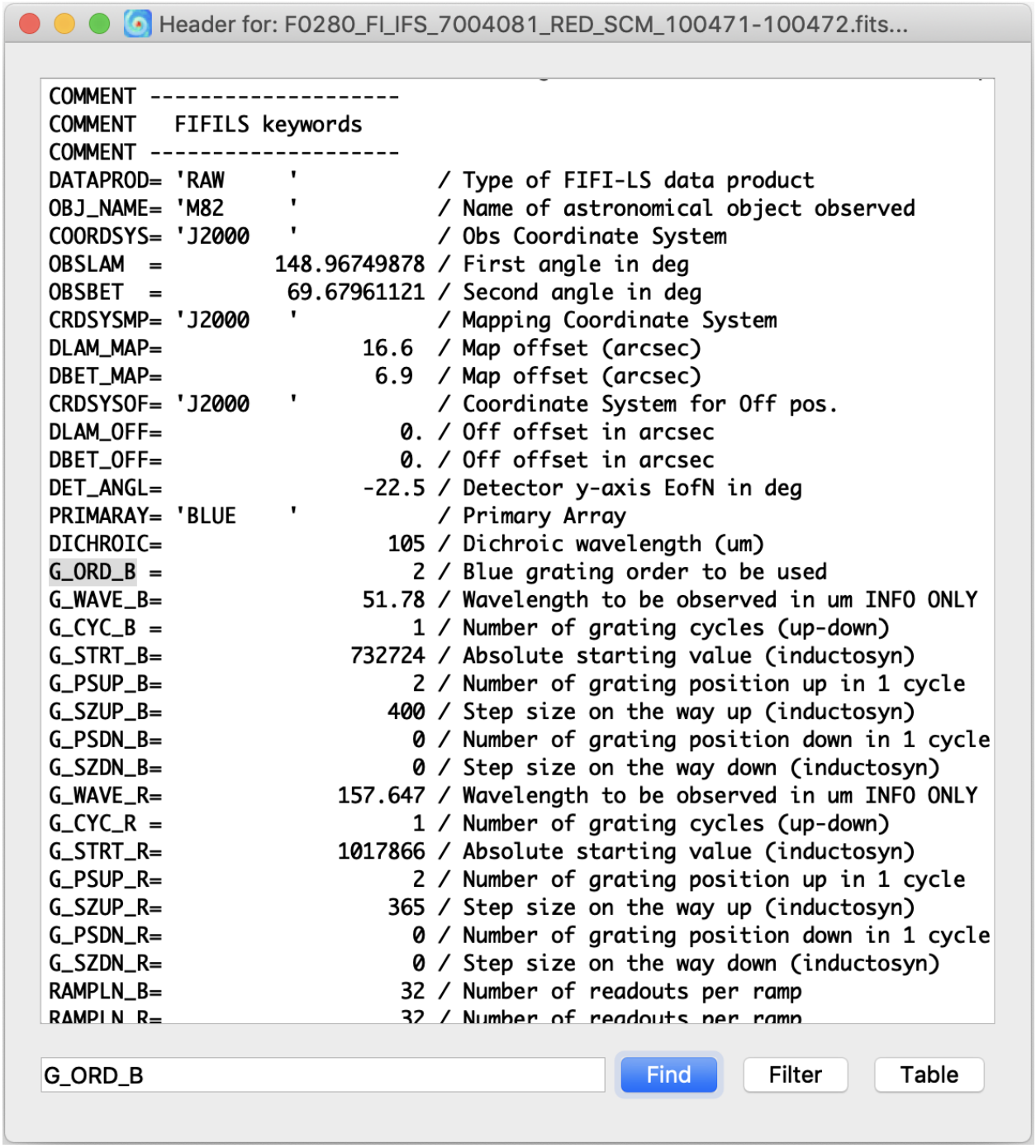

Fig. 23: QAD FITS header viewer.

  - *Remove 1st 2 ramps*: Select to remove the first two ramps. This is on by default. This option has no effect if there are fewer than three ramps per chop.

- **Combine Nods**
  - *Propagate off-beam image*: If selected, B beams will be treated as if they were A beams for all subsequent reductions. That is, the map will be produced at the B position instead of the A. All other filenames and header settings will remain the same, so use with caution. This option is mostly used for testing purposes.
- **Spatial Calibrate**
  - *Rotate by detector angle*: By default, Redux rotates the data by the detector angle to set North up and East to the left in the final map. Deselect this box to keep the final map in detector coordinates.
  - *Flip RA/Dec sign convention (+, -, or default)*: For most data, the sign convention of the DLAM_MAP and DBET_MAP header keywords, which define the dither offsets, is determined automatically (parameter value "default"). Occasionally, for particular observations, these keywords may need their signs flipped, or used as is (no flip). This is usually determined by inspection of the results of the Resample step.
- **Apply Flat**
  - *Skip flat correction*: Select this option to skip flat-fielding the data. This option is mostly used for testing purposes.
  - *Skip flat error propagation*: Deselect this option to propagate the systematic flat correction error in the flux error plane. This option is not currently recommended: the systematic error is stored in the CALERR keyword instead.
- **Combine Scans**
  - *Correct bias offset*: Select this option to subtract an overall bias offset between the individual scans.
- **Telluric Correct**
  - *Skip telluric correction*: Select to skip correcting the data for telluric absorption. This option is mostly used for testing.
  - *ATRAN directory*: Use this option to select a directory containing ATRAN FITS files. This must be set in order to use water vapor values for telluric correction.
  - *Cutoff value*: Modify to adjust the transmission fraction below which the telluric-corrected data will be set to NaN.
  - *Use WV values*: Select to use water vapor values from the header (keyword WVZ_OBS) to select the ATRAN file to apply. This option will have no effect unless the ATRAN directory is set to a location containing ATRAN files derived for different PWV values.
- **Flux Calibrate**
  - *Skip flux calibration*: Select to skip flux calibration of the data. The flux will remain in instrumental units (ADU/sec), with PROCSTAT=LEVEL_2. This option is mostly used for testing.
  - *Response file*: Use this option to select a FITS file containing an instrumental response spectrum to use in place of the default file on disk.
- **Correct Wave Shift**
  - *Skip wavelength shift correction*: Select to skip applying the correction to the wavelength calibration due to barycentric velocity. In this case, both telluric-corrected and uncorrected cubes will be resampled onto the original wavelengths. This option is mostly used for testing.
- **Resample**
  - *Skip coadd*: If selected, a separate flux cube will be made from each input file, using the interpolation algorithm. This option is useful for identifying bad input files.

- *Interpolate instead of fit*: If set, an alternate resampling algorithm will be used, rather than the local polynomial surface fits. This option may be preferable for data with small dither offsets.
- *Weight by errors*: If set, local fits will be weighted by the flux errors, as calculated by the pipeline.
- *Fit rejection threshold (sigma)*: If the fit value is more than this number times the standard deviation away from the weighted mean, the weighted mean is used instead of the fit value. This parameter is used to reject bad fit values. Set to -1 to turn off.
- *Positive outlier threshold (sigma)*: Sets the rejection threshold for the input data, in sigma. Set to -1 to turn off.
- *Negative outlier threshold (sigma)*: If non-zero, sets a separate rejection threshold in sigma for negative fluxes, to be used in a first-pass rejection. Set to -1 to turn off.
- *Spatial oversample*: This parameter controls the resolution of the output spatial grid. The value is given in terms of pixels per reference FWHM for the detector channel used. For the BLUE camera, the reference FWHM is 5.0 arcseconds; for RED, it is 10.0 arcseconds. A value of 5 resamples BLUE data at 1 arcsecond per pixel and RED data at 2 arcseconds per pixel.
- *Spatial surface fit order*: This parameter controls the order of the surface fit to the spatial data at each grid point. Higher orders give more fine-scale detail, but are more likely to be unstable. Set to zero to do a weighted mean of the nearby data.
- *Spatial fit window*: This parameter controls how much data to use in the fit at each grid point. It is given in terms of a factor times the average spatial FWHM. Higher values will lead to more input data being considered in the output solution, at the cost of longer processing time. Too-low values may result in missing data (holes) in the output map.
- *Spatial smoothing radius*: Set to the fraction of the fit window to use as the radius of the distance-weighting Gaussian. Lowering this value results in finer detail for the same input fit window. Too low values may result in noisy output data; too high values effectively negate the distance weights.
- *Spatial edge threshold*: Specifies the threshold for setting edge pixels to NaN. Set lower to block fewer pixels.
- *Spectral oversample*: This parameter controls the resolution of the output spectral grid. The value is given in terms of pixels per reference spectral FWHM at the central wavelength of the observation.
- *Spectral surface fit order*: This parameter controls the order of the surface fit to the spectral data at each grid point.
- *Spectral fit window*: This parameter controls how much data to use in the fit at each wavelength grid point. It is given in terms of a factor times the average spatial FWHM. Higher values will lead to more input data being considered in the output solution, at the cost of longer processing time. Too-low values may result in missing data (holes) in the output map.
- *Spectral smoothing radius*: Set to the fraction of the fit window to use as the radius of the distance-weighting Gaussian, in the wavelength dimension.
- *Spectral edge threshold*: Specifies the threshold for setting edge pixels to NaN, in the wavelength dimension. Set lower to block fewer pixels.

Part VII

Data quality assessment

After the pipeline has been run on a set of input data, the output products should be checked to ensure that the data has been properly reduced. Data quality and quirks can vary widely across individual observations, but the following general guideline gives some strategies for approaching quality assessment for FIFI-LS data.

- Check the output to the log file (usually called *redux_[date]_[time].log*), written to the same directory as the output files. Look for messages marked ERROR or WARNING. The log will also list every parameter used in the pipeline steps, which may help disambiguate the parameters as actually-run for the pipeline.
- Check that the expected files were written to disk: there should, at a minimum, be a scan-combined file (*SCM*), a flux-calibrated file (*CAL*), and a resampled file (*WXY*).
- Look at each plane of the reduced image in the *WXY* file. Check that the resampling seems to have completed successfully: there should not be excessive holes in the map, or bad pixels away from the edges of the image. If there are, the spatial resampling may need to be redone with modified parameters.
- Look at the spectra for a sampling of spatial pixels in the *WXY* file. Check that there are no sudden dropouts or other discontinuities in the spectrum that are not associated with poor atmospheric transmission. If there are such discontinuities, the wavelength resampling may need to be redone with modified parameters.

Part VIII

Appendix A: Sample configuration files

The below is a sample FIFI-LS Redux parameter override file in INI format. If present, the parameter value overrides the default defined by the FIFI-LS reduction object. If not present, the default value will be used. The parameters displayed here are the current default values.

```
# Redux parameters for FIFI-LS instrument in IFS mode
# Pipeline: FIFI_LS_REDUX v2_0_0
[1: checkhead]
    abort = True
[2: split_grating_and_chop]
    save = False
[3: fit_ramps]
    save = False
    parallel = True
    s2n = 30.0
    thresh = 5.0
    badpix_file = ""
    remove_first = True
[4: subtract_chops]
    save = False
[5: combine_nods]
    save = False
    offbeam = False
[6: lambda_calibrate]
    save = False
[7: spatial_calibrate]
    save = False
```

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```
    rotate = True
    flipsign = default
[8: apply_static_flat]
    save = False
    skip_flat = False
    skip_err = True
[9: combine_grating_scans]
    save = True
    bias = True
[10: telluric_correct]
    save = False
    skip_tell = False
    atran_dir = ""
    cutoff = 0.6
    use_wv = False
[11: flux_calibrate]
    save = True
    skip_cal = False
    response_file = ""
[12: correct_wave_shift]
    save = False
    skip_shift = False
[13: resample]
    save = True
    parallel = True
    skip_coadd = False
    interpolate = False
    error_weighting = True
    fitthresh = -1
    posthresh = -1
    negthresh = -1
    xy_oversample = 5.0
    xy_order = 2
    xy_window = 3.0
    xy_smoothing = 0.6666666666666666
    xy_edge_threshold = 0.7
    w_oversample = 8.0
    w_order = 2
    w_window = 0.5
    w_smoothing = 0.5
    w_edge_threshold = 0.5
```

Sample FIFI-LS configuration file, located in *fifi-ls/data/header_info/headerdef.dat*. Values marked with a Y in the *reqd?* column are keywords required to be present in input data. They must meet the type and range requirements listed for grouping and data reduction to be successful.

```
#
# This table lists keywords, allowed values, and defaults for
# all keywords to be written to output files.  Keywords
# required to be present in input files for correct data
# processing are marked with a 'Y'. A '.' in min, max, or enum
# means no requirement.  The combine column designates the
# algorithm to be used to calculate the value for the
# header of a product made from multiple input files.
#
# keyword  reqd?  default  type    combine     min    max     enum
#-----------------------------------------------------------------
AIRSPEED     N    -9999.   float   first       .      .       .
ALTI_END     Y    -9999.   float   last        0.     60000.  .
ALTI_STA     Y    -9999.   float   first       0.     60000.  .
AOR_ID       N    UNKNOWN  string  first       .      .       .
AOT_ID       N    UNKNOWN  string  first       .      .       .
ASSC_AOR     N    UNKNOWN  string  concatenate .      .       .
ASSC_MSN     N    UNKNOWN  string  concatenate .      .       .
ASSC_OBS     N    UNKNOWN  string  concatenate .      .       .
ATRNFILE     N    UNKNOWN  string  concatenate .      .       .
BDPXFILE     N    UNKNOWN  string  concatenate .      .       .
BGLEVL_A     N    -9999.   float   mean        .      .       .
BGLEVL_B     N    -9999.   float   mean        .      .       .
C_CHOPLN     Y    -9999    int     first       7      256     .
C_SCHEME     Y    UNKNOWN  string  first       .      .       2POINT
CHOPPING     Y    T        bool    first       .      .       .
CHPAMP1      N    -9999.   float   first       -1125  1125    .
CHPAMP2      N    -9999.   float   first       -1125  1125    .
CHPANGLE     N    -9999.   float   first       -360.  360.    .
CHPCRSYS     N    UNKNOWN  string  first       .      .       TARF|ERF|SIRF
CHPFREQ      Y    -9999.   float   first       0.25   25.     .
CHPPHASE     N    -9999    int     first       0      1000    .
CHPPROF      N    UNKNOWN  string  first       .      .       2-POINT|3-POINT
CHPSYM       N    UNKNOWN  string  first       .      .       .
CHPTIP       N    -9999.   float   first       -301.  301.    .
CHPTILT      N    -9999.   float   first       -301.  301.    .
CREATOR      N    UNKNOWN  string  first       .      .       .
DATAQUAL     N    UNKNOWN  string  first       .      .       NOMINAL|USABLE|
                                                               TEST|PROBLEM|FAIL
DATASRC      Y    UNKNOWN  string  first       .      .       ASTRO|CALIBRATION|
                                                               LAB|TEST|OTHER|
                                                               FIRSTPOINT
DATATYPE     N    UNKNOWN  string  first       .      .       IMAGE|SPECTRAL|
                                                               OTHER
DATE         N    UNKNOWN  string  first       .      .       .
DATE-BEG     N    UNKNOWN  string  first       .      .       .
DATE-END     N    UNKNOWN  string  last        .      .       .
DATE-OBS     Y    UNKNOWN  string  first       .      .       .
DBET_MAP     Y    -9999.   float   first       -36000 36000   .
DEPLOY       N    UNKNOWN  string  first       .      .       .
DETCHAN      Y    UNKNOWN  string  first       .      .       BLUE|RED
DETECTOR     N    UNKNOWN  string  first       .      .       .
DETSIZE      N    UNKNOWN  string  first       .      .       .
DICHROIC     Y    -9999    int     first       .      .       105|130
```

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DITHER	N	F	bool	first	.	.	.
DLAM_MAP	Y	-9999.	float	first	-36000	36000	.
DTHCRSYS	N	UNKNOWN	string	first	.	.	TARF|ERF|SIRF
DTHINDEX	N	-9999	int	default	.	.	.
DTHNPOS	N	-9999	int	first	.	.	.
DTHOFFS	N	-9999.	float	first	.	.	.
DTHPATT	N	UNKNOWN	string	first	.	.	NONE|3-POINT| 5-POINT|9-POINT| CUSTOM
DTHXOFF	N	-9999.	float	first	.	.	.
DTHYOFF	N	-9999.	float	first	.	.	.
EQUINOX	N	-9999.	float	first	.	.	.
EXPTIME	Y	-9999.	float	sum	0.02	1000	.
FBC-STAT	N	UNKNOWN	string	last	.	.	FBC_OFF|FBC_QS| FBC_DY|FBC_ON
FILENAME	Y	UNKNOWN	string	first	.	.	.
FILENUM	N	UNKNOWN	string	first	.	.	.
FILEREV	N	UNKNOWN	string	first	.	.	.
FLATFILE	N	UNKNOWN	string	concatenate	.	.	.
FLIGHTLG	N	UNKNOWN	string	first	.	.	.
FOCUS_EN	N	-9999.	float	last	-5000	5000	.
FOCUS_ST	N	-9999.	float	first	-5000	5000	.
G_CYC_B	Y	-9999	int	first	0	100	.
G_CYC_R	Y	-9999	int	first	0	100	.
G_ORD_B	Y	-9999	int	first	1	2	.
G_PSDN_B	Y	-9999	int	first	0	100	.
G_PSDN_R	Y	-9999	int	first	0	100	.
G_PSUP_B	Y	-9999	int	first	0	100	.
G_PSUP_R	Y	-9999	int	first	0	100	.
G_STRT_B	Y	-9999	int	first	0	2098176	.
G_STRT_R	Y	-9999	int	first	0	2098176	.
G_SZDN_B	Y	-9999	int	first	0	20000	.
G_SZDN_R	Y	-9999	int	first	0	20000	.
G_SZUP_B	Y	-9999	int	first	-20000	20000	.
G_SZUP_R	Y	-9999	int	first	-20000	20000	.
GRDSPEED	N	-9999.	float	first	.	.	.
HEADING	N	-9999.	float	first	.	.	.
HEADSTAT	N	UNKNOWN	string	first	.	.	ORIGINAL|UNKNOWN| CORRECTED|ERROR| MODIFIED
IMAGEID	N	-9999	int	default	0	.	.
INSTCFG	N	UNKNOWN	string	first	.	.	DUAL_CHANNEL
INSTMODE	N	UNKNOWN	string	first	.	.	SYMMETRIC_CHOP| ASYMMETRIC_CHOP| BRIGHT_OBJECT| SPECTRAL_SCAN| TOTAL_POWER
INSTRUME	Y	FIFI-LS	string	first	.	.	FIFI-LS
KWDICT	N	UNKNOWN	string	first	.	.	.
LASTREW	N	UNKNOWN	string	first	.	.	.
LAT_END	N	-9999.	float	last	.	.	.
LAT_STA	N	-9999.	float	first	.	.	.
LON_END	N	-9999.	float	last	.	.	.
LON_STA	N	-9999.	float	first	.	.	.
MAPCRSYS	N	UNKNOWN	string	first	.	.	EQUATORIAL| GALACTIC|ECLIPTIC| USER

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MAPINTX	N	-9999.	float	first	.	.	.
MAPINTY	N	-9999.	float	first	.	.	.
MAPNXPOS	N	-9999	int	first	.	.	.
MAPNYPOS	N	-9999	int	first	.	.	.
MAPPING	N	F	bool	first	.	.	.
MCCSMODE	N	UNKNOWN	string	first	.	.	.
MISSN-ID	Y	UNKNOWN	string	first	.	.	.
NEXP	N	1	int	sum	0	.	.
NODAMP	N	-9999.	float	first	.	.	.
NODANGLE	N	-9999.	float	first	-360	360	.
NODBEAM	Y	UNKNOWN	string	default	.	.	A|B
NODCRSYS	N	UNKNOWN	string	first	.	.	ERF|ECRF|GALRF| TARF|FPIRF|FFIRF| WFIRF|SIRF|USER
NODDING	Y	T	bool	first	.	.	.
NODN	N	-9999	int	first	.	.	.
NODPATT	Y	UNKNOWN	string	first	.	.	.
NODSETL	N	-9999.	float	first	.	.	.
NODSTYLE	Y	UNKNOWN	string	first	.	.	NMC|C2NC2
NODTIME	N	-9999.	float	first	.	.	.
OBJECT	Y	UNKNOWN	string	first	.	.	.
OBS_ID	Y	UNKNOWN	string	first	.	.	.
OBSBET	N	-9999.	float	first	-90.	90.	.
OBSDEC	N	-9999.	float	first	-90.	90.	.
OBSERVER	N	UNKNOWN	string	first	.	.	.
OBSLAM	N	-9999.	float	first	0.	360.	.
OBSRA	N	-9999.	float	first	0.	24.	.
OBSTYPE	Y	UNKNOWN	string	first	.	.	OBJECT| STANDARD_FLUX| STANDARD_TELLURIC| STANDARD_WAVECAL| LAMP|FLAT|DARK| BIAS|SKY|BB| GASCELL|LASER| FOCUS_LOOP
OPERATOR	N	UNKNOWN	string	first	.	.	.
ORIGIN	N	UNKNOWN	string	first	.	.	.
PIPELINE	N	UNKNOWN	string	first	.	.	.
PIPEVERS	N	UNKNOWN	string	first	.	.	.
PIXSCAL	N	-9999.	float	first	.	.	.
PLANID	N	UNKNOWN	string	first	.	.	.
PLATSCAL	Y	-9999	float	first	.	.	.
PROCSTAT	Y	UNKNOWN	string	first	.	.	.
PRODTYPE	N	UNKNOWN	string	first	.	.	.
RAMPLN_B	Y	-9999	int	first	0	256	.
RAMPLN_R	Y	-9999	int	first	0	256	.
RAWUNITS	N	ADU/s	string	first	.	.	.
RESFILE	N	UNKNOWN	string	concatenate	.	.	.
RESOLUN	N	-9999.	float	first	.	.	.
RSPNFILE	N	UNKNOWN	string	concatenate	.	.	.
SCANNING	N	F	bool	first	.	.	.
SCNDEC0	N	-9999.	float	first	-90.	90.	.
SCNDECF	N	-9999.	float	last	-90.	90.	.
SCNDIR	N	-9999.	float	last	.	.	.
SCNRA0	N	-9999.	float	first	0.	24.	.
SCNRAF	N	-9999.	float	last	0.	24.	.
SCNRATE	N	-9999.	float	last	.	.	.

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SIBS_X	N	-9999	int	default	.	.	.
SIBS_Y	N	-9999	int	default	.	.	.
SLIT	N	UNKNOWN	string	first	.	.	.
SPATFILE	N	UNKNOWN	string	concatenate	.	.	.
SPECTEL1	Y	UNKNOWN	string	first	.	.	NONE|FIF_BLUE
SPECTEL2	Y	UNKNOWN	string	first	.	.	NONE|FIF_RED
SRCTYPE	N	UNKNOWN	string	first	.	.	POINT_SOURCE| EXTENDED_SOURCE| OTHER|UNKNOWN
SUBARRNO	N	-9999	int	first	.	.	.
TELAPSE	N	-9999.	float	sum	0.	.	.
TELCONF	N	UNKNOWN	string	first	.	.	.
TELEL	N	-9999.	float	first	0.	90.	.
TELEQUI	N	UNKNOWN	string	first	.	.	.
TELESCOP	N	UNKNOWN	string	first	.	.	.
TELDEC	N	-9999.	float	first	-90.	90.	.
TELLOS	N	-9999.	float	first	-180	180	.
TELRA	N	-9999.	float	first	0.	24.	.
TELVPA	N	-9999.	float	first	0.	360.	.
TELXEL	N	-9999.	float	first	-90.	90.	.
TEMP_OUT	N	-9999.	float	first	.	.	.
TEMPPRI1	N	-9999.	float	first	-273.	.	.
TEMPPRI2	N	-9999.	float	first	-273.	.	.
TEMPPRI3	N	-9999.	float	first	-273.	.	.
TEMPSEC1	N	-9999.	float	first	.	.	.
TRACERR	N	F	bool	or	.	.	.
TRACKANG	N	-9999.	float	first	.	.	.
TRACMODE	N	UNKNOWN	string	first	.	.	OFF|CENTROID|ROF| LIMB|OFFSET| ROF+OFFSET| CENTROID+INERTIAL| ROF+INERTIAL| OFFSET+INERTIAL| ROF+OFFSET+INERTIAL
TSC-STAT	N	UNKNOWN	string	last	.	.	.
UTCEND	N	UNKNOWN	string	last	.	.	.
UTCSTART	N	UNKNOWN	string	first	.	.	.
WAVECENT	N	-9999.	float	first	0.	.	.
WAVEFILE	N	UNKNOWN	string	concatenate	.	.	.
WVSCALE	N	-9999.	float	mean	0.	.	.
WVZ_END	N	-9999.	float	last	0.	.	.
WVZ_STA	N	-9999.	float	first	0.	.	.
XPOSURE	N	-9999.	float	sum	0.	.	.
ZA_END	Y	-9999.	float	last	0.	90.	.
ZA_START	Y	-9999.	float	first	0.	90.	.