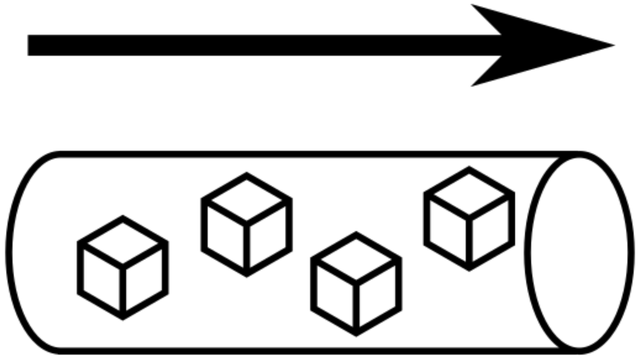
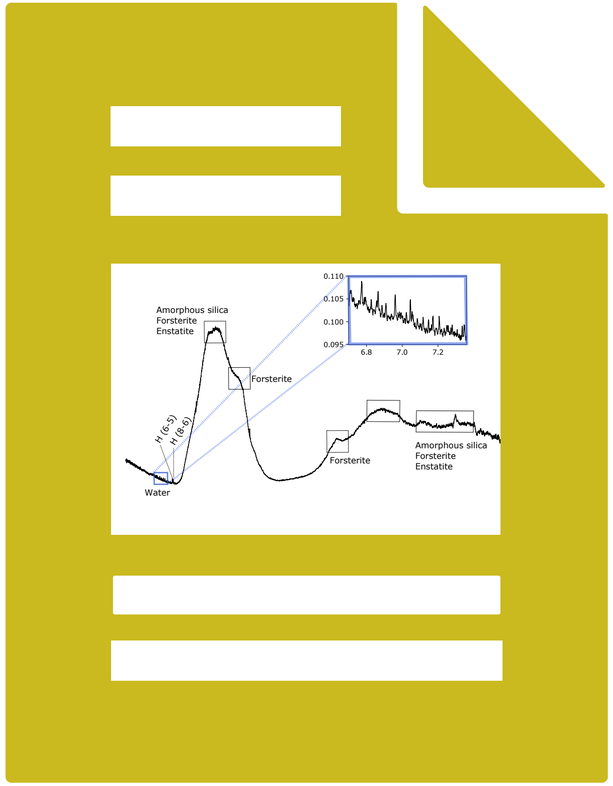
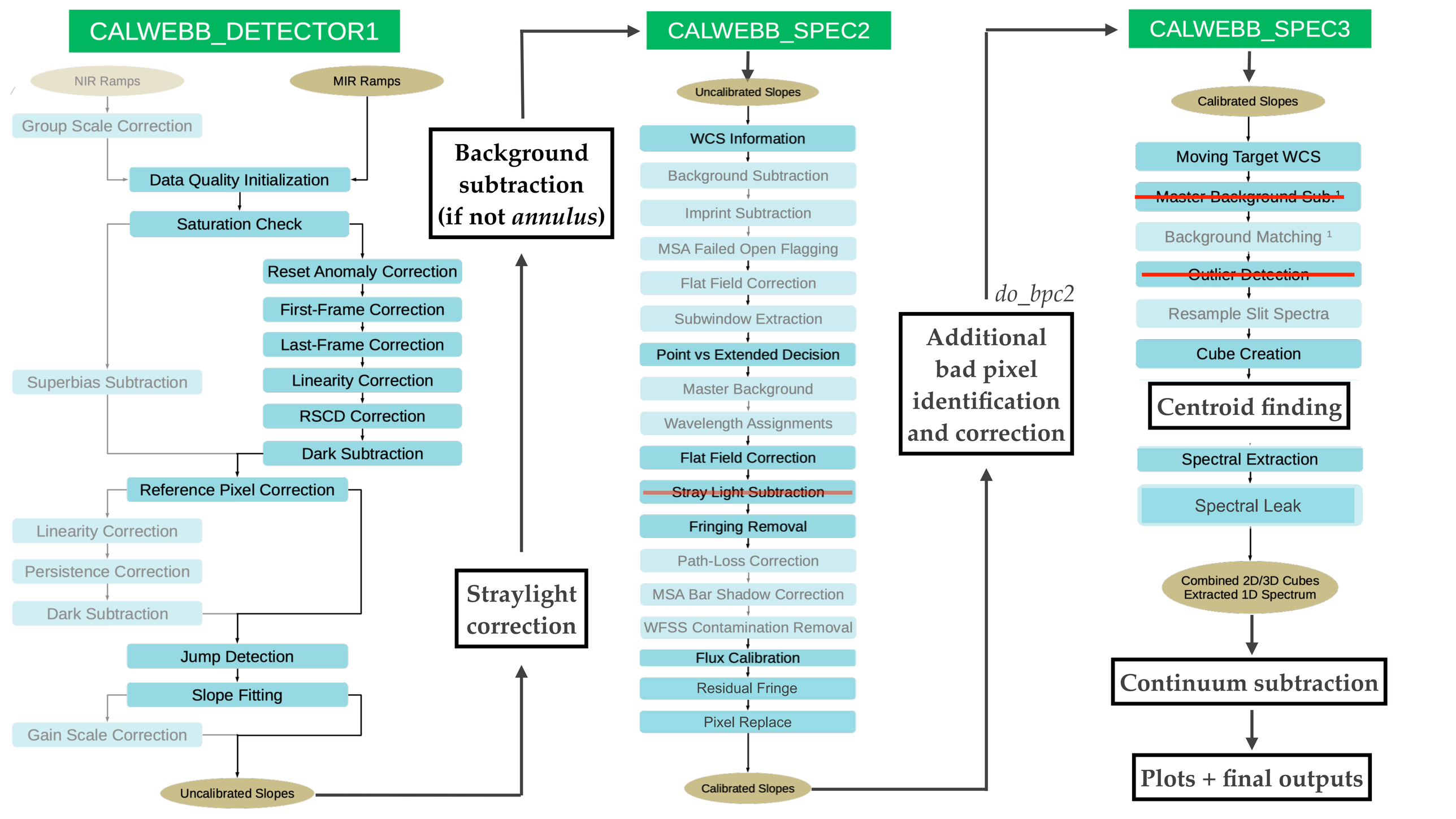
MINDS: Notebook update

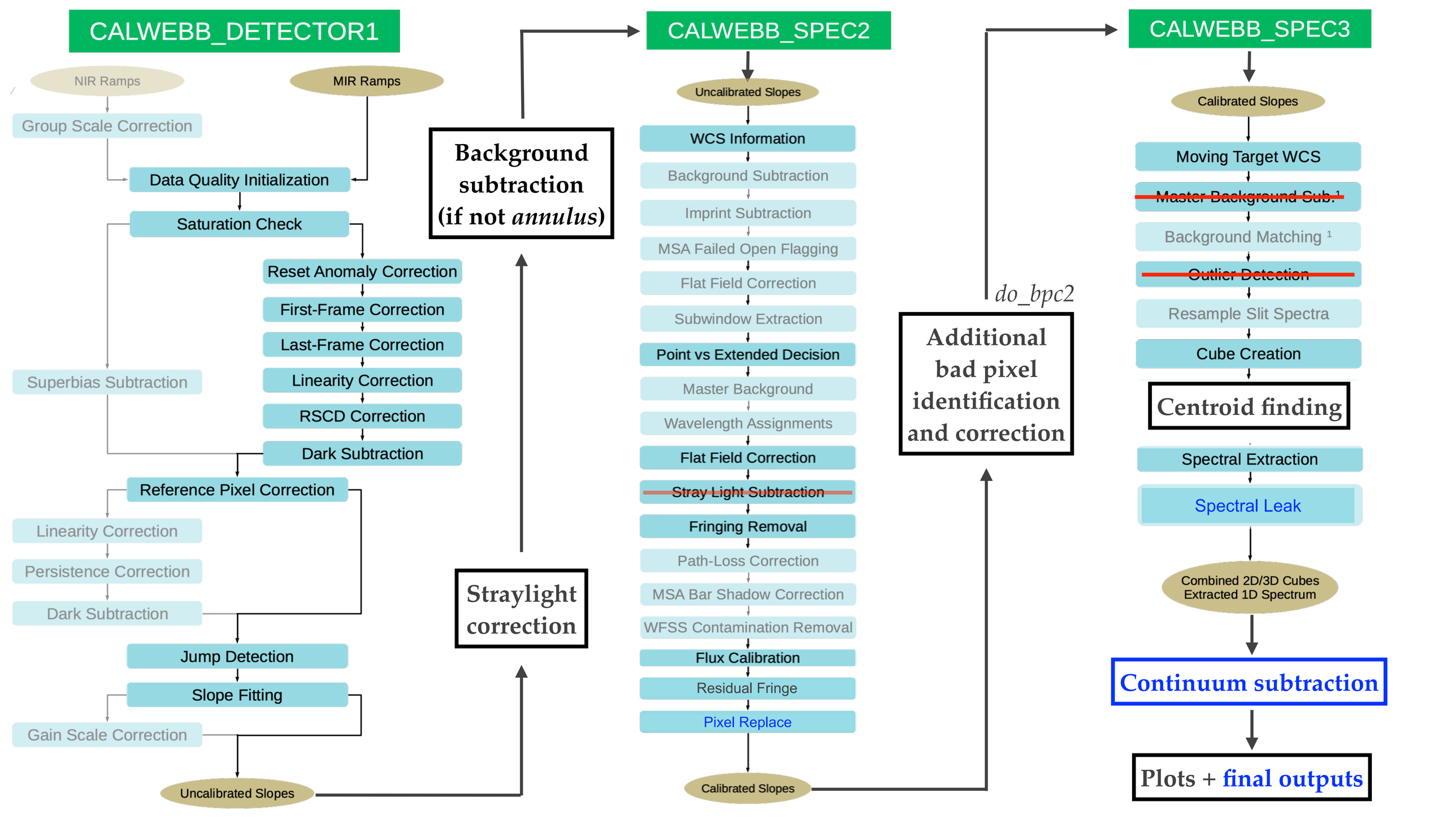


Notebook v8



MINDS meeting (14/02/2024)


CALWEBB_DETECTOR1
NIR Ramps
MIR Ramps
Group Scale Correction
Data Quality Initialization
Saturation Check
Reset Anomaly Correction
First-Frame Correction
Last-Frame Correction
Linearity Correction
RSCD Correction
Dark Subtraction
Superbias Subtraction
Reference Pixel Correction
Linearity Correction
Persistence Correction
Dark Subtraction
Jump Detection
Slope Fitting
Gain Scale Correction
Uncalibrated Slopes
Background subtraction (if not annulus)
Straylight correction
CALWEBB_SPEC2
Uncalibrated Slopes
WCS Information
Background Subtraction
Imprint Subtraction
MSA Failed Open Flagging
Flat Field Correction
Subwindow Extraction
Point vs Extended Decision
Master Background
Wavelength Assignments
Flat Field Correction
Stray Light Subtraction
Fringing Removal
Path-Loss Correction
MSA Bar Shadow Correction
WFSS Contamination Removal
Flux Calibration
Residual Fringe
Pixel Replace
Calibrated Slopes
do_bpc2
Additional bad pixel identification and correction
CALWEBB_SPEC3
Calibrated Slopes
Moving Target WCS
Master Background Sub.[1]
Background Matching [1]
Outlier Detection
Resample Slit Spectra
Cube Creation
Centroid finding
Spectral Extraction
Spectral Leak
Combined 2D/3D Cubes
Extracted 1D Spectrum
Continuum subtraction
Plots + final outputs

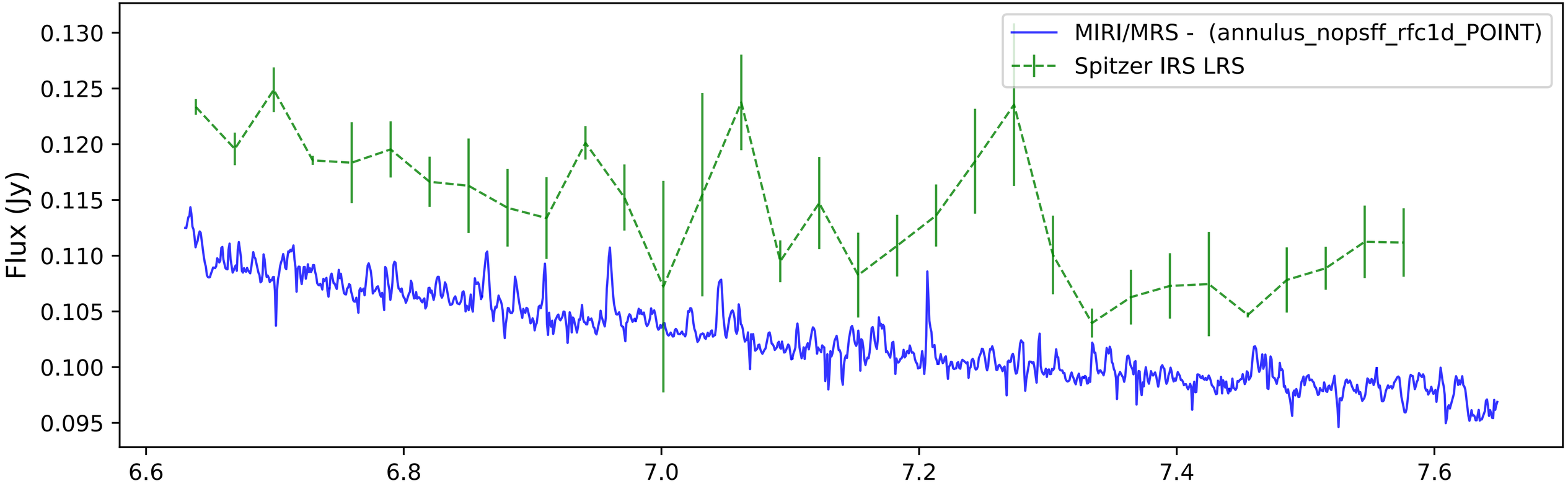

CALWEBB_DETECTOR1
NIR Ramps
MIR Ramps
Group Scale Correction
Data Quality Initialization
Saturation Check
Reset Anomaly Correction
First-Frame Correction
Last-Frame Correction
Linearity Correction
RSCD Correction
Dark Subtraction
Superbias Subtraction
Reference Pixel Correction
Linearity Correction
Persistence Correction
Dark Subtraction
Jump Detection
Slope Fitting
Gain Scale Correction
Uncalibrated Slopes
Background subtraction (if not annulus)
Straylight correction
CALWEBB_SPEC2
Uncalibrated Slopes
WCS Information
Background Subtraction
Imprint Subtraction
MSA Failed Open Flagging
Flat Field Correction
Subwindow Extraction
Point vs Extended Decision
Master Background
Wavelength Assignments
Flat Field Correction
Stray Light Subtraction
Fringing Removal
Path-Loss Correction
MSA Bar Shadow Correction
WFSS Contamination Removal
Flux Calibration
Residual Fringe
Pixel Replace
Calibrated Slopes
do_bpc2
Additional bad pixel identification and correction
CALWEBB_SPEC3
Calibrated Slopes
Moving Target WCS
Master Background Sub.[1]
Background Matching [1]
Outlier Detection
Resample Slit Spectra
Cube Creation
Centroid finding
Spectral Extraction
Spectral Leak
Combined 2D/3D Cubes
Extracted 1D Spectrum
Continuum subtraction
Plots + final outputs

TL;DR

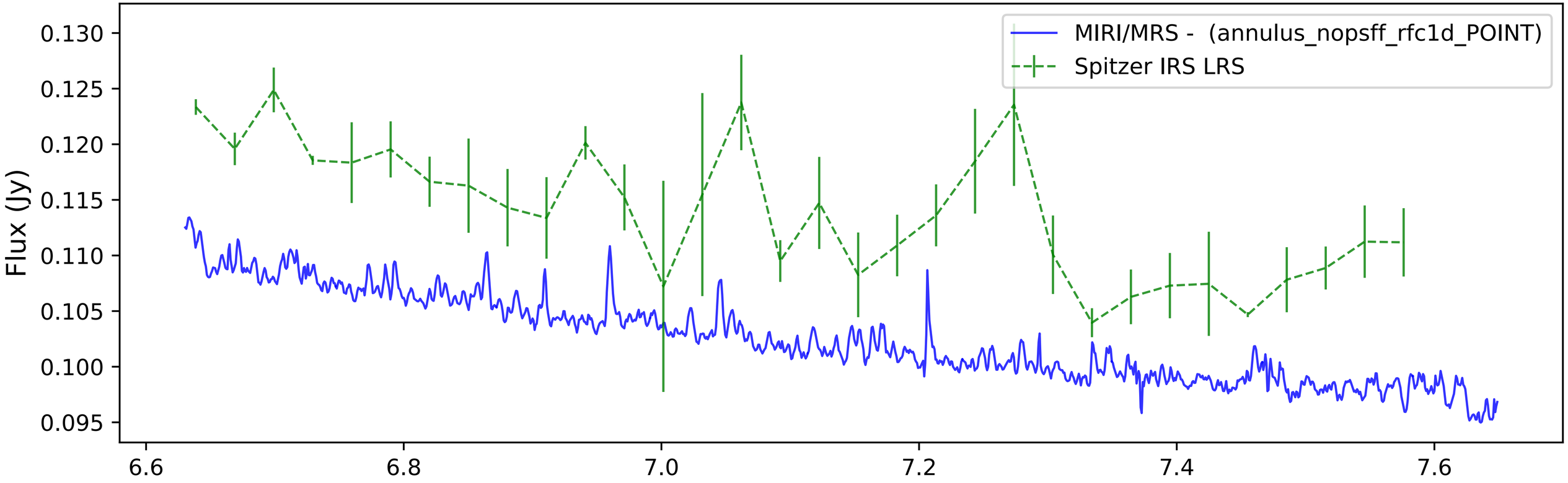
Changes in MINDS notebook v8

- **`pixel_replace`** step now used by default => cleaner spectra (but do_bpc2 still recommended)
- **Spectral leak fix** now included by default (affects spectrum at ~12.2 μm)
- Broken multiprocessing… now fixed
- Outputs now also include a **continuum estimate** and a **continuum-subtracted spectrum** (thanks Milou!)
- `psff` option not recommended for now (lack of time correction for photometric calibration)
- **All previously shared material are still mostly relevant (see end of this presentation)**

Before (v007)

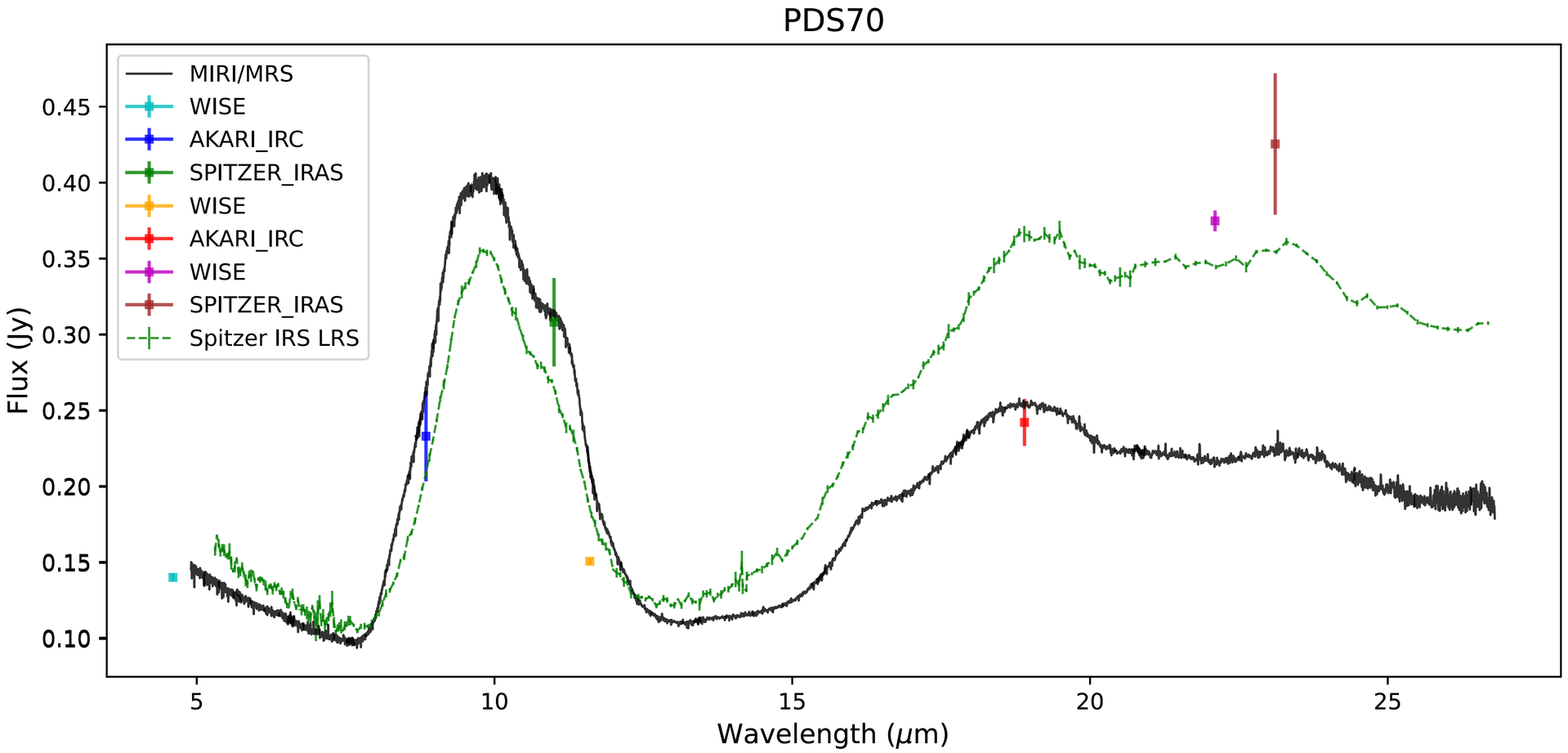

MIRI/MRS - (annulus_nopsff_rfc1d_POINT)
Spitzer IRS LRS
Flux (Jy)
0.130
0.125
0.120
0.115
0.110
0.105
0.100
0.095
6.6
6.8
7.0
7.2
7.4
7.6

Effect of pixel_replace



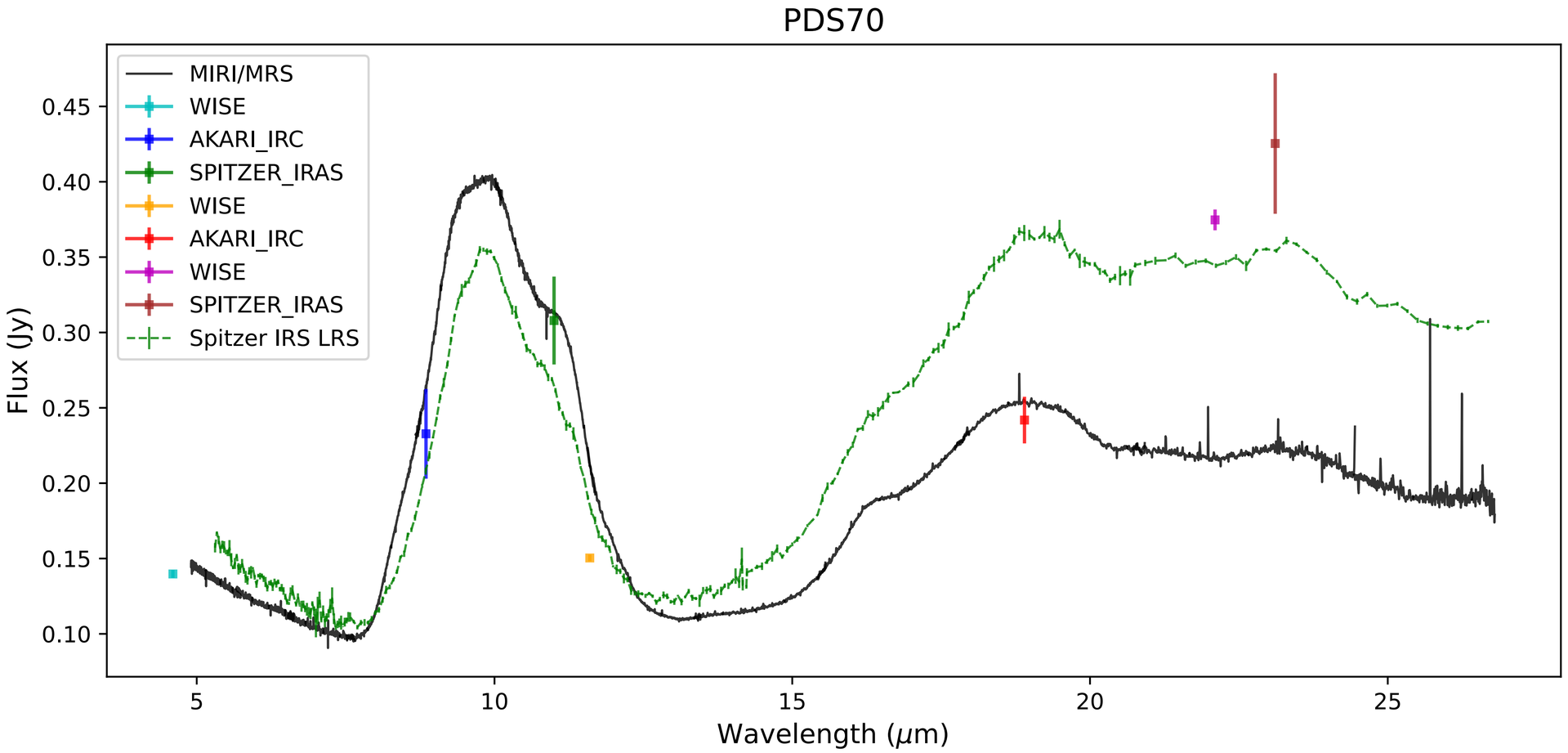
do_bpc2 / pixel_replace / outlier_detection ?

do_bpc2 only (v007)



do_bpc2 / pixel_replace / outlier_detection ?

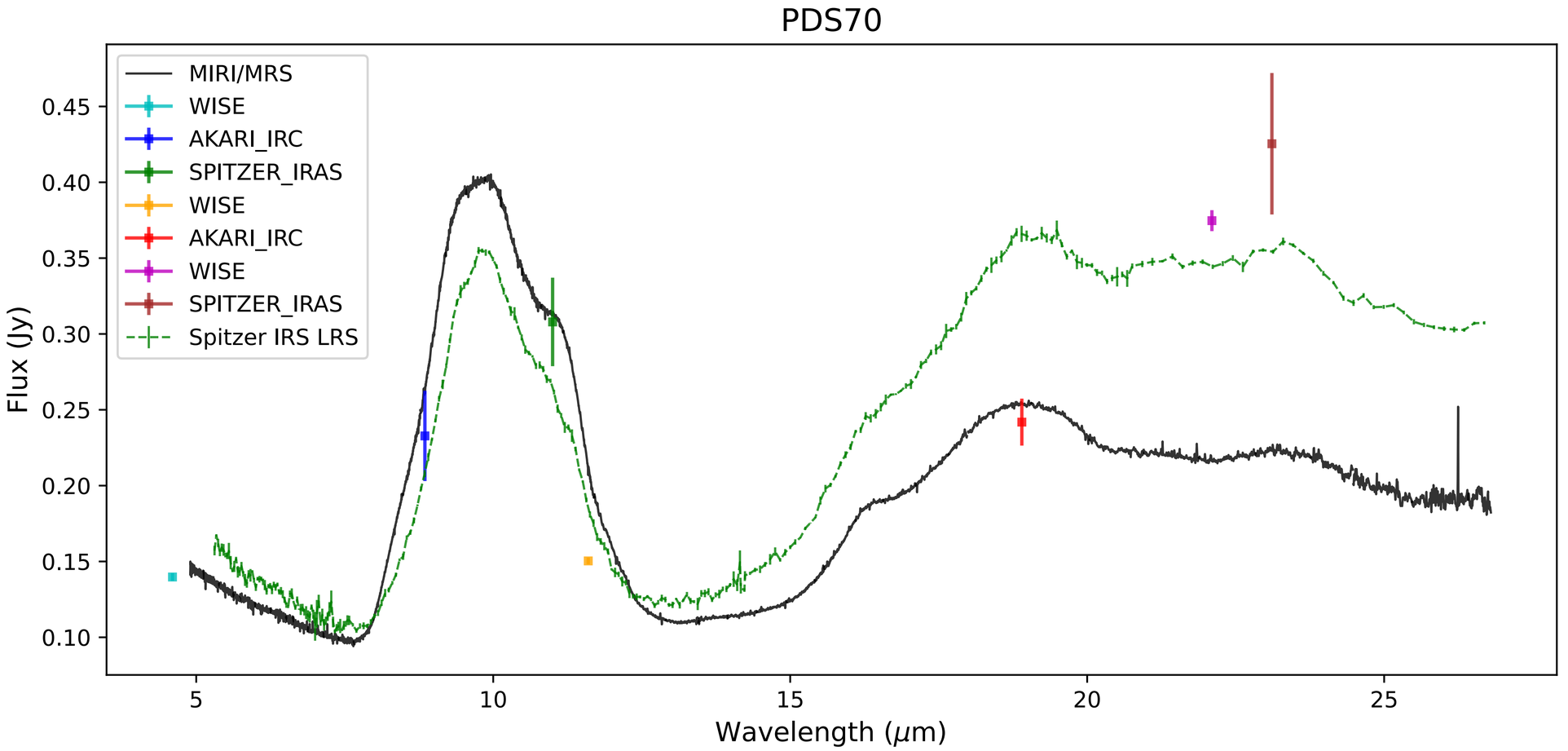
pixel_replace only



- Lower noise level overall
- But some large outliers

do_bpc2 / pixel_replace / outlier_detection ?

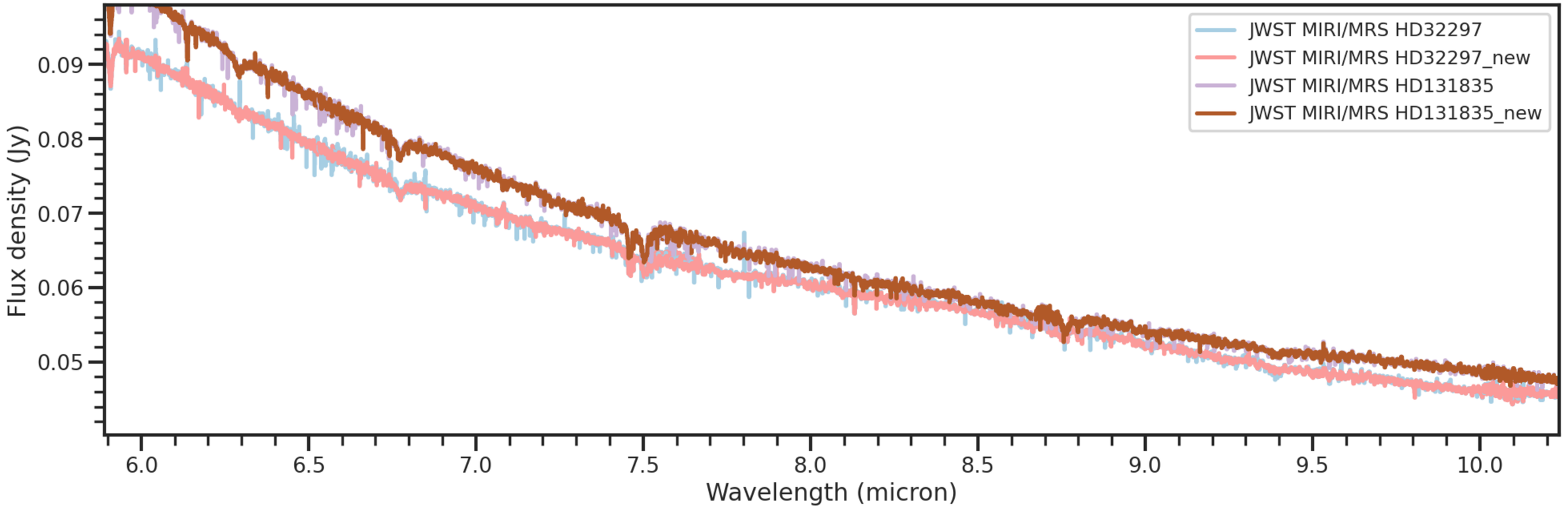
pixel_replace + outlier detection step



- Lower noise level overall
- Outlier detection step captures most of them

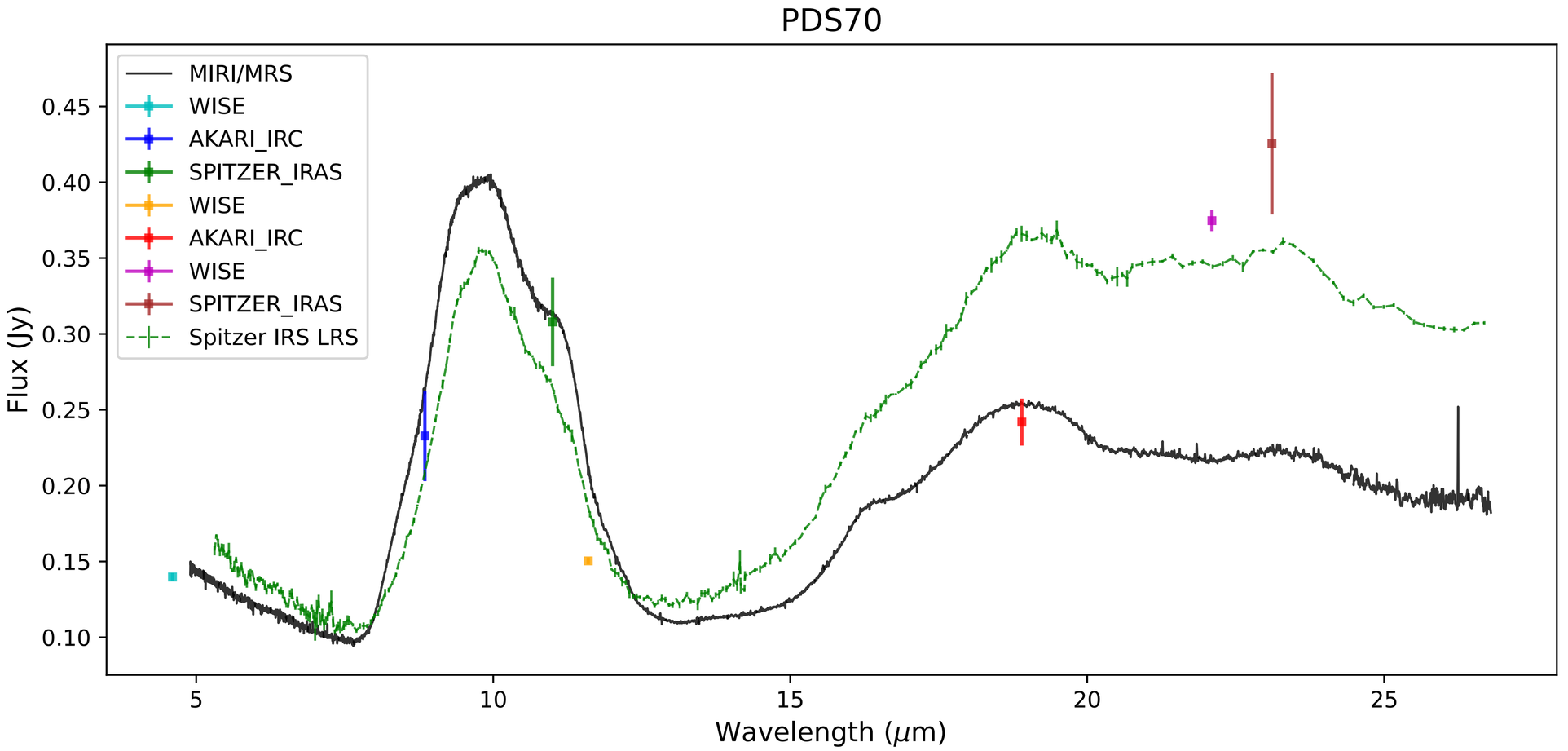
do_bpc2 / pixel_replace / outlier_detection ?

pixel_replace + outlier detection step



do_bpc2 / pixel_replace / outlier_detection ?

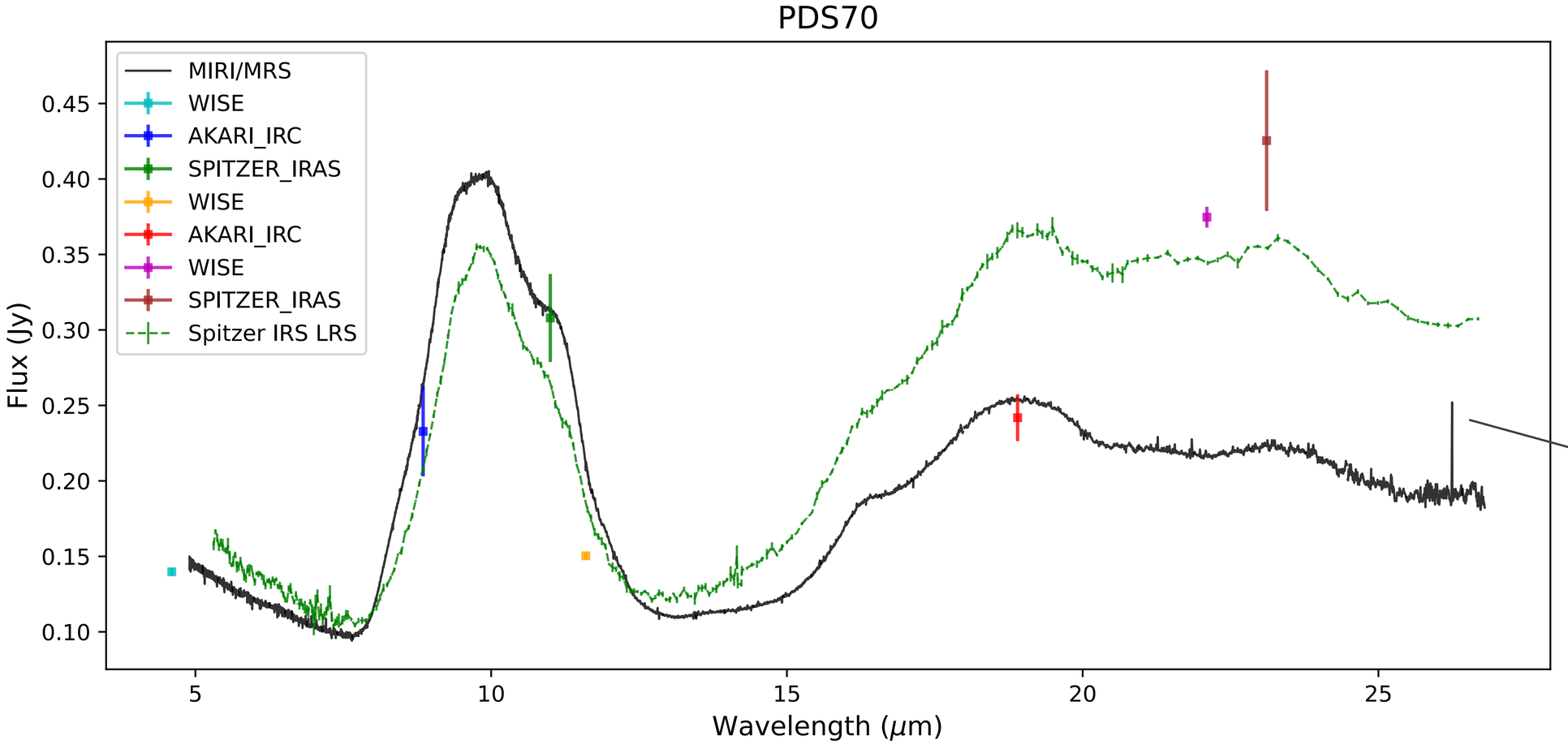
pixel_replace + outlier detection step



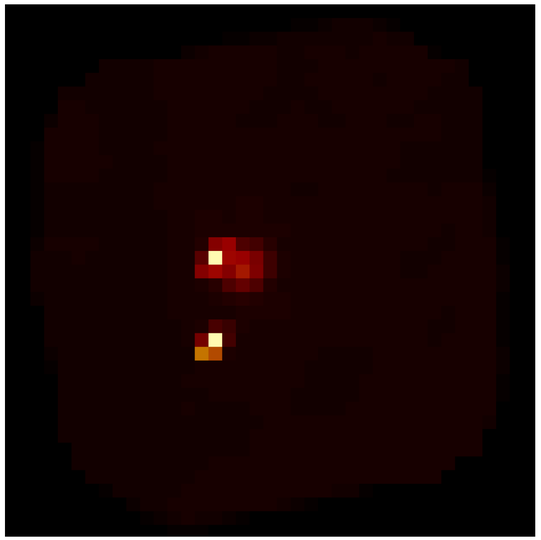
- Lower noise level overall
- Outlier detection step captures most of them

do_bpc2 / pixel_replace / outlier_detection ?

pixel_replace + outlier detection step

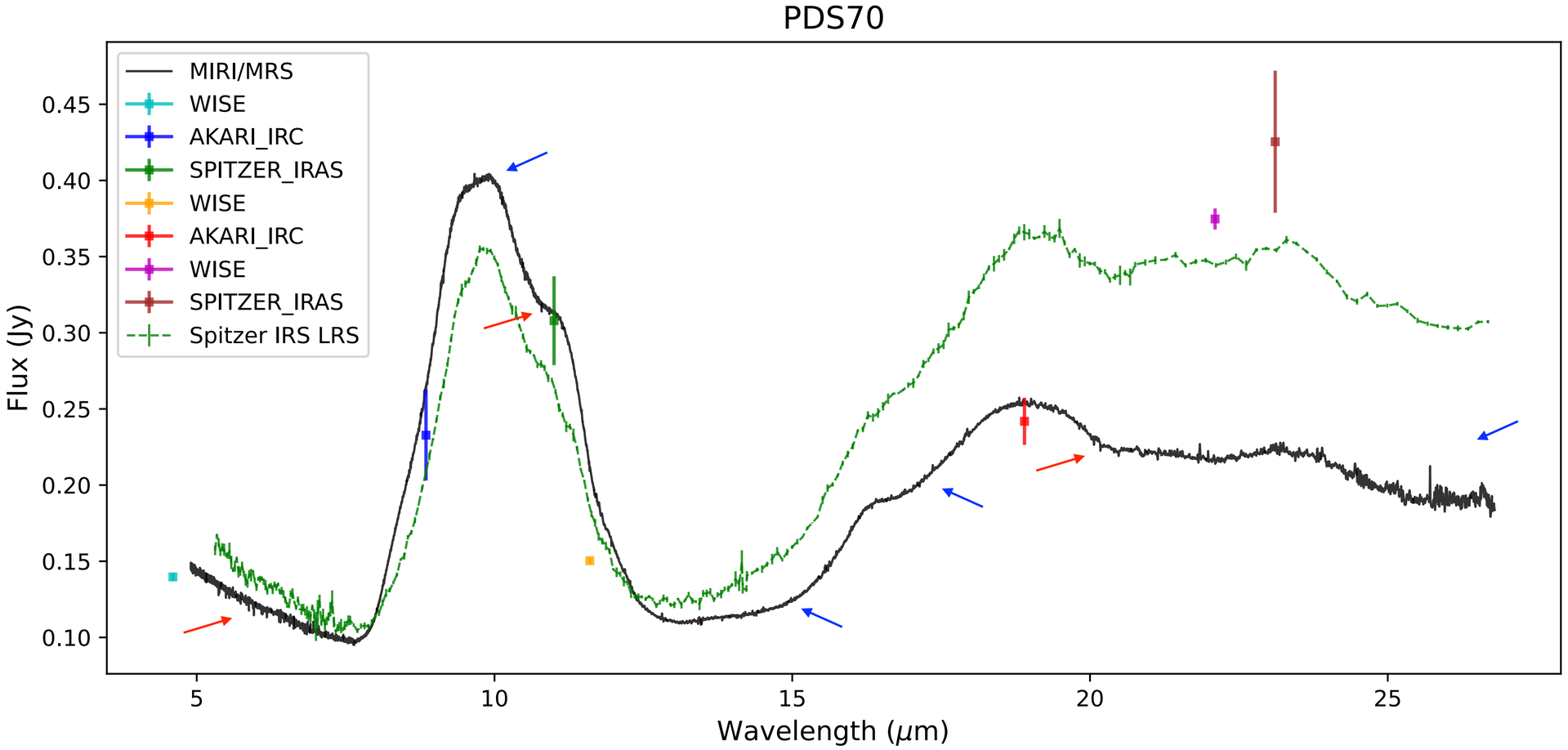


- Lower noise level overall
- Outlier detection step captures most of them
- Residual spikes are not real lines



do_bpc2 / pixel_replace / outlier_detection ?

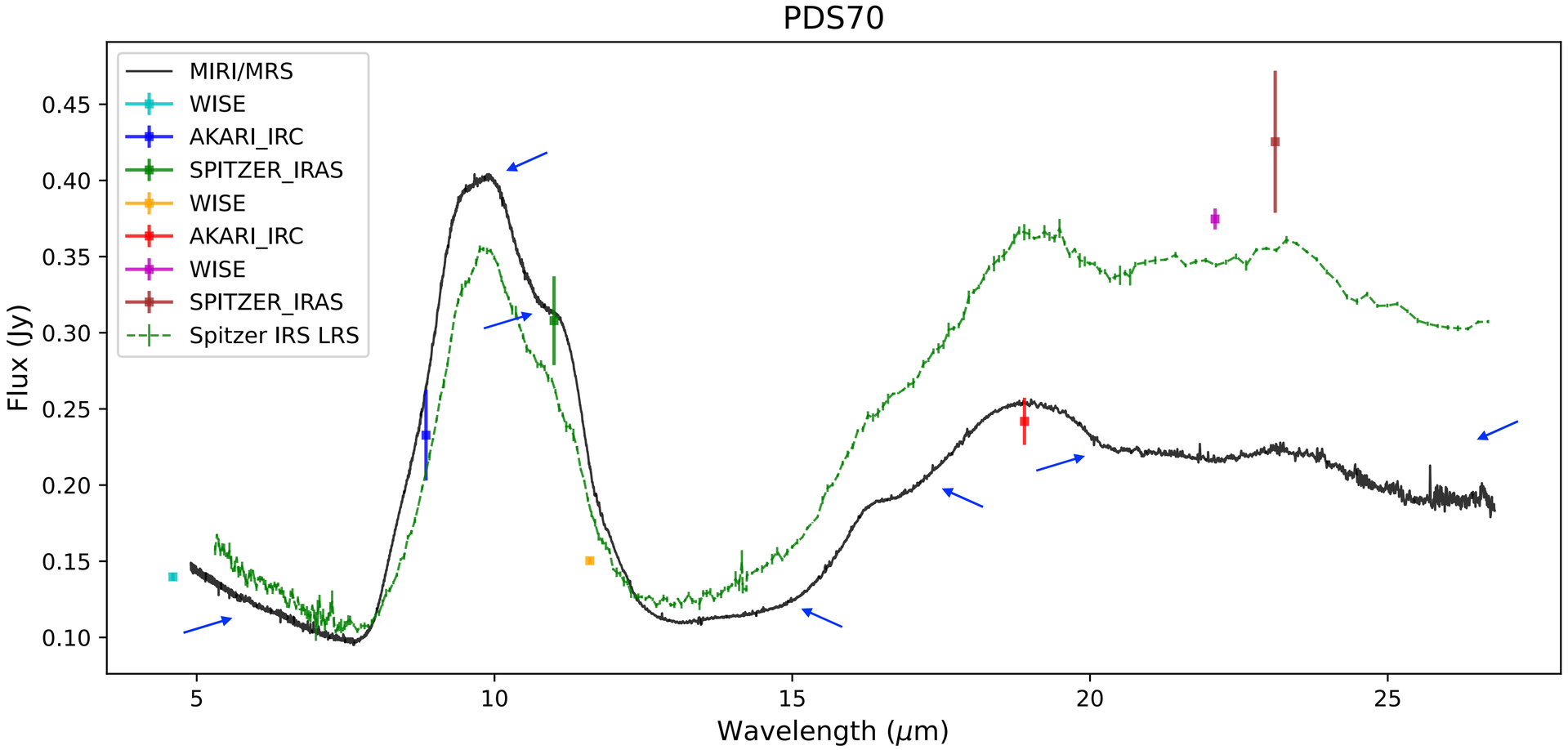
do_bpc2 + pixel_replace + outlier detection step



- Lower noise level overall
- Outlier detection step captures most of them
- do_bpc2 helps to get rid of more residual spikes

do_bpc2 / pixel_replace / outlier_detection ?

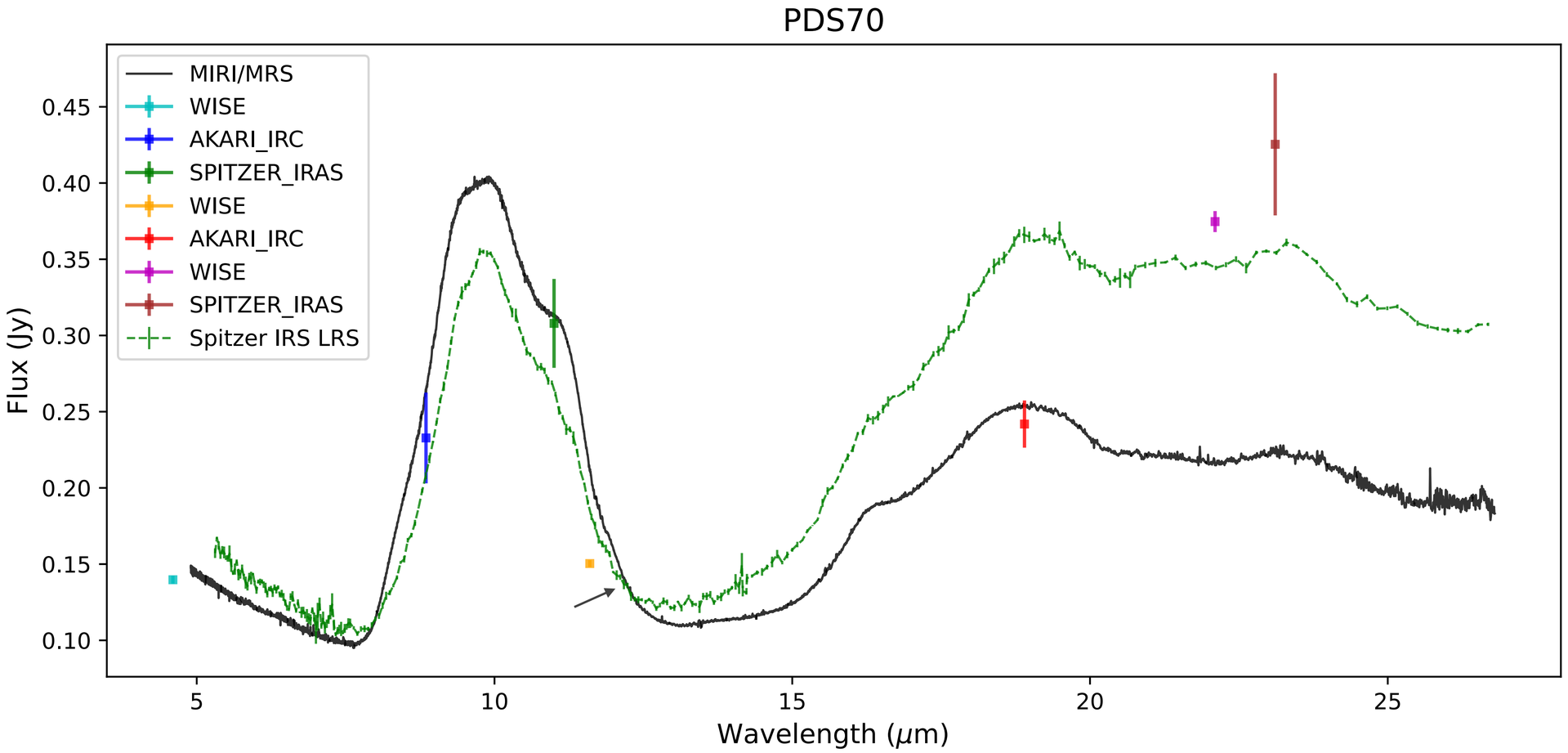
do_bpc2 + pixel_replace **=> best compromise?**



- Lower noise level overall
- do_bpc2 + pixel_replace get rid of even **more** residual spikes than including outlier detection
- The latter seems to introduce some spikes (or not correct some outliers)

Spectral leak fix at 12.2 µm

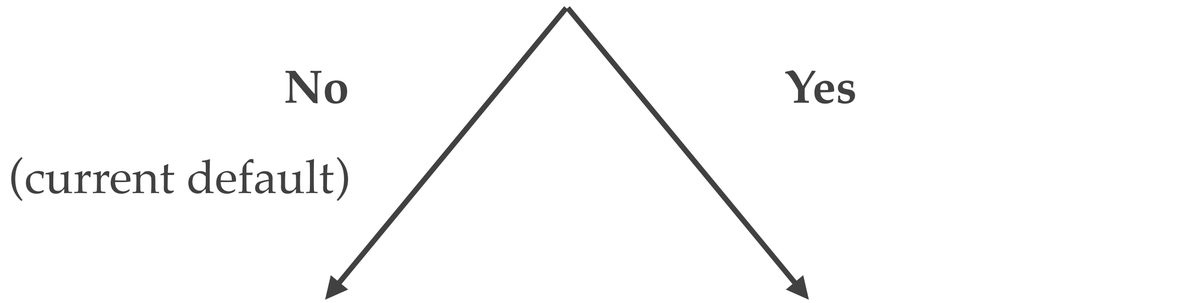
do_bpc2 + pixel_replace + spectral leak fix **=> defined as default combo**



- Lower noise level overall
- do_bpc2 + pixel_replace get rid of even **more** residual spikes than including outlier detection
- The latter seems to introduce some spikes (or not correct some outliers)
- **No more excess at 12.2 µm**

Open question

- Continuum subtraction code involves interpolating over ~11.5μm region. Does the new spectral leak correction removes this need?



Default: Continue to mask the region before continuum estimation.

New reference files and jwst pipeline update

New CRDS reference files affecting MIRI-MRS

- [2024-01-23] jwst_1185.pmap: new **bad pixel** reference file**s** => recommendation: reduce again
- [2023-12-22] jwst_1179.pmap: new **specwcs** reference files for channels 3C, 4A, 4B, and 4C
  - Corrections of up to a few tens of km/s
  - Cutoff moved from 27.9 μm to 28.7 μm
- [2023-11-29] jwst_1150.pmap: inclusion of **point-source specific** correction factors for:
  - Spectral leak
  - Across slice throughput
  - Wavelength correction tables

New reference files and jwst pipeline update

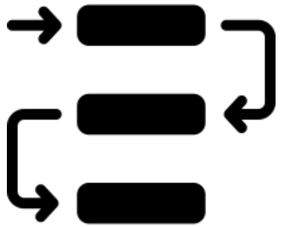
jwst pipeline updates
(latest version: v1.13.4)

Major Improvements:

- Build 10.0 (2023-12)
  - `pixel_replace` step (bad pixel correction) => better quality spectra
  - extract1D step can now accept an aperture size argument
- Build 9.3 (2023-08)
  - Outlier detection step (partly?) fixed… but see below.

Remaining caveats of the official pipeline

- Residual fringing
  => Additional dedicated correction on spectrum may be desirable depending on the source.
- Outlier detection step (based on tests with PDS 70)
  => still not as good as dedicated bad pixel correction done in MINDS notebook (recommended even if slower)
- Automatic centroid finding not always reliable (priv. comm. Milou/Leiden):
  => requires dedicated centroiding in MINDS notebook
- Spectral leak? (Unclear message on website. Seems to work on PDS 70 — to be tested on more sources)



Installation and dependencies

```
conda create -n minds_env python=3.9 jupyter
```
← Create new conda environment with Python3.9 and Jupyter

```
pip install vip_hci
```
← Additional routines than JWST pipeline

```
pip install opencv-python
```
← Required by JWST pipeline `Detector1` class

```
pip install jwst
```
← Install JWST pipeline

```
pip install spectres pybaselines
```
← New dependencies required for continuum subtraction

```
pip install -U "ray[default]"
```
← Optional dependency for better multiprocessing

Helping material

User guidelines and troubleshooting tips:

https://docs.google.com/document/d/1h2b8VK39rslipiWncgdXua6tHOxWjApay_LX5EmB05k/edit?usp=sharing

1. How to download the data and where to place them?

- Download uncalibrated data (suffix: *uncal.fits) using https://github.com/spacetelescope/jwst_mast_query. This involves generating a MAST token (https://auth.mast.stsci.edu/token) and setting the MAST_API_TOKEN environment variable as described here. Then adapt a config file with your favorite text editor in order to set what you want to download (example config file here), and run the download with:

  jwst_download.py -v –config jwst_query.cfg

- Create a subfolder named *stage0* in the folder you want to use as working directory during the reduction with the MINDS notebook (or adapt the parameter *input_dir* in cell [2] of the notebook accordingly).
- In the *stage0* subfolder, **only** place *uncal.fits from your science target.
- If you have dedicated background observations, place the associated *uncal.fits files in a different subfolder and adapt the corresponding parameter in the MINDS notebook accordingly.

2. How to use the notebook (TLDR version)?

- Set the parameters in cell [2]. A few parameters are data-specific (see Sec. 3), leave the others as default as a first try (these mostly correspond to jwst pipeline defaults).
- Run all cells (leave them as is).
- Check your results in the *final_outputs* folder (details in Sec. 4).
- Try with other parameters if not satisfied and/or for safety checks – check out Secs. 5 and 6 for good practices and troubleshooting help, respectively.

3. How to set free parameters in the MINDS notebook?

- The data reduction parameters that you're the most likely to adapt are in cell [2].
- Parameters in cell [4] were once free parameters that have now been extensively tested. You probably won't need to change them – except if recommended otherwise by experienced notebook users.

• • •

Helping material

User guidelines and troubleshooting tips:

https://docs.google.com/document/d/1h2b8VK39rslipiWncgdXua6tHOxWjApay_LX5EmB05k/edit?usp=sharing

What to include in your publication?

https://www.overleaf.com/project/638eff3f9adba6d72a97167d

2. OBSERVATIONS

Example template sentences (adapt values in *italics*):

- The disk of *PDS 70* was observed on *August 1, 2022* with the Mid-InfraRed Instrument (MIRI; Rieke et al. 2015; Wright et al. 2015) of JWST as part of Guaranteed Time Observation (GTO) program 1282 (PI: Th. Henning).
- The Medium Resolution Spectroscopy (MRS; Wells et al. 2015) mode was used, which involves four Integral Field Units (IFUs): channel 1 (4.9−7.65 μm), channel 2 (7.51−11.71 μm),

• • •

3. DATA REDUCTION WITH SHARED NOTEBOOK

- Hybrid pipeline relying on the standard JWST pipeline (Bushouse et al. 2023, note: *quote version used and adapt reference accordingly*) using CRDS context (*quote relevant jwst_nnnn.pmap* file), and complemented with routines from the VIP package (Gomez Gonzalez et al. 2017; Christiaens et al. 2023) to compensate for known issues in the standard JWST pipeline.
- The pipeline is structured around three main stages that are the same as in the JWST pipeline, namely Detector1, Spec2 and Spec3.
- After the first stage (Detector1), stray light is corrected, and a background estimate subtracted (*note: only if* `bkg_method=ddither` or `bkg_method=sdither`).
- If `bkg_method=ddither`: To remove the background, we carried out a direct pair-wise dither subtraction. (optional: This method is more suited to fainter sources where the resulting PSF overlap is minimal and reduce noise level in the spectrum, but can lead to a minor flux discrepancy with prior Spitzer measurements due to self-subtraction.)
- If `bkg_method=sdither`: To estimate and remove the background, we leveraged the four-point dither pattern to obtain a first guess on the background map, then refined it using a median-filter which both smoothed the background estimate and removed residual star signals from it.
- If `psff=True`: We then employ point-source optimized reference flat-field and photometry calibration files in Spec2, following the methods presented in Gasman et al. (2022). These present the advantage of not requiring the additional residual fringe step included in the standard pipeline, hence can better preserve the shape of molecular

1. How to download the data and where to place them?

- Download uncalibrated data (suffix: *uncal.fits) using https://github.com/spacetelescope/jwst_mast_query. This involves generating a MAST token (https://auth.mast.stsci.edu/token) and setting the MAST_API_TOKEN environment variable as described here. Then adapt a config file with your favorite text editor in order to set what you want to download (example config file here), and run the download with:

  jwst_download.py -v –config jwst_query.cfg

- Create a subfolder named *stage0* in the folder you want to use as working directory during the reduction with the MINDS notebook (or adapt the parameter *input_dir* in cell [2] of the notebook accordingly).
- In the *stage0* subfolder, **only** place *uncal.fits from your science target.
- If you have dedicated background observations, place the associated *uncal.fits files in a different subfolder and adapt the corresponding parameter in the MINDS notebook accordingly.

2. How to use the notebook (TLDR version)?

- Set the parameters in cell [2]. A few parameters are data-specific (see Sec. 3), leave the others as default as a first try (these mostly correspond to jwst pipeline defaults).
- Run all cells (leave them as is).
- Check your results in the *final_outputs* folder (details in Sec. 4).
- Try with other parameters if not satisfied and/or for safety checks – check out Secs. 5 and 6 for good practices and troubleshooting help, respectively.

3. How to set free parameters in the MINDS notebook?

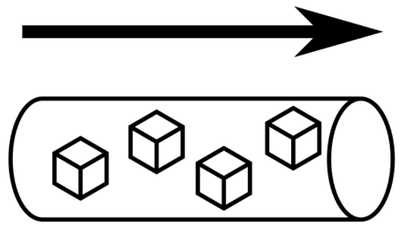
- The data reduction parameters that you're the most likely to adapt are in cell [2].
- Parameters in cell [4] were once free parameters that have now been extensively tested. You probably won't need to change them – except if recommended otherwise by experienced notebook users.

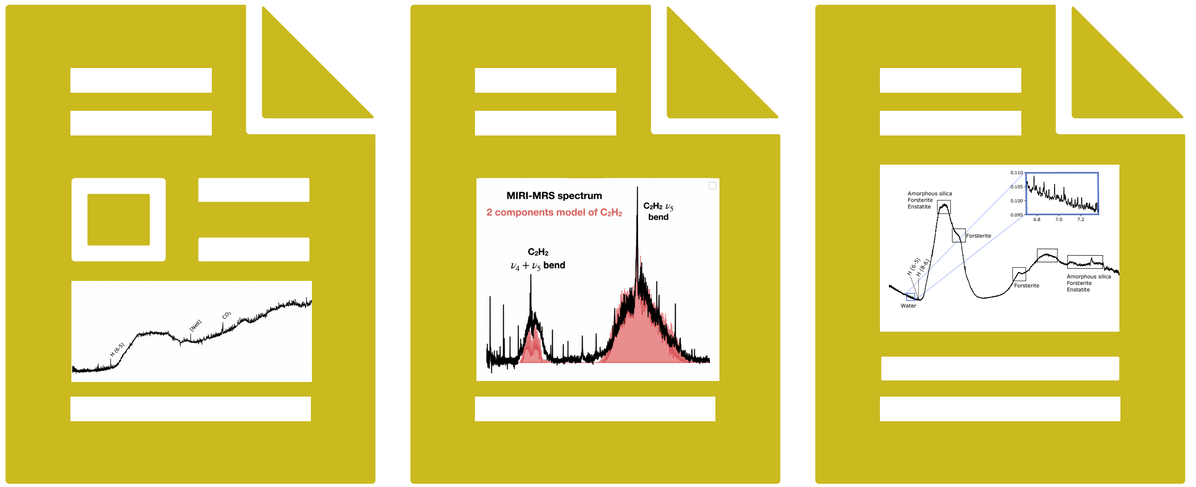
• • •

Summary and next steps

- MINDS notebook v008 ready for use with latest jwst pipeline and CRDS files (+helping material)
- Open question: NIRSPEC data reduction.
- Notebook for analysis of resolved emission ready for use (lead: Matthias) => incorporate in next MINDS notebook version.
- Enhanced (detector based) point-source spectrum extraction is investigated by Danny.

MIRI MIDINFRARED DISK SURVEY





...