Improving JWST Data Products Workshop

TSO Pipeline Discussion | Thursday, November 16, 2023

Attendees: Néstor Espinoza, David Grant, Everett Schlawin, Taylor Bell, Drake Deming, Sarah Kendrew, Loïc Albert

Useful links:

- Calwebb Detector1 steps: https://jwst-pipeline.readthedocs.io/en/latest/jwst/pipeline/calwebb_detector1.html
- Calwebb Spec2 steps: https://jwst-pipeline.readthedocs.io/en/latest/jwst/pipeline/calwebb_spec2.html
- Calwebb Image2 steps: https://jwst-pipeline.readthedocs.io/en/latest/jwst/pipeline/calwebb_image2.html
- Calwebb TSO3 steps: https://jwst-pipeline.readthedocs.io/en/latest/jwst/pipeline/calwebb_tso3.html
- JWST Known Issues of data products link: https://jwst-docs.stsci.edu/jwst-calibration-pipeline-caveats/known-issues-with-jwst-data-products
- TSO Pipeline Caveats: https://jwst-docs.stsci.edu/jwst-calibration-pipeline-caveats/jwst-time-series-observations-pipeline-caveats

Discussion talking points:

Loïc: Is the objective of this discussion to build community or help only exoplanet stuff? Different objectives.

Néstor: We want to build community; objective is to get as close to possible products from raw to science-ready — ie, what the experts do “typically”, but for everyone.

Drake: What’s the difference between a TSO mode and just doing a lot of integrations on your “own”.

Sarah: There are limitations; e.g., 10,000 seconds limit on APT. You are also allowed to not dither in TSOs.

Nestor: Also runs the “TSO pipeline”, so products on MAST pass data through that.

1. Which **algorithmic steps** are the ones that should be left as is or worked upon — **which ones should be included**? (e.g., jump detection, spectral extraction)

   Drake: Wavelengths are not in the FITS file — so have to write a little script, takes

the wavelengths out of the calints file, and write this. Fundamental stuff like this should always be in a FITS file.

Sarah: There are reasons for this, as the wavelength is assigned in the assign_wcs step — but FITS format doesn't allow for this.

Nestor: Perhaps have a library that does this (e.g., PASTASOSS).

Drake: Also for proposals, starting and ending wavelengths are very useful.

Sarah: Bigger request from the community to have this technical data readily available (e.g., throughputs, wavelength solutions, etc.). People are running simulations, etc. You can do some of this for MIRI LRS.

[Useful to have a one-stop-shop for intermediate products — including DQ flags]

Drake: JWST Documentation is pretty good!

[Saturation & Linearity]

Everett: Thorn on this — if all spatial positions for a wavelength are marked as saturated

Taylor: Found important to mask entire column for saturated pixels — sufficient non-linear that linearity step was not doing a good job. So (a) flag entire column and (b) have ability mask previous groups. In general issues with partially saturated pixels.

Loïc: It would be nice to have the freedom to have a parameter to the saturation step to perhaps all columns with the previous group that have a saturated central pixel.

Taylor: Would be useful to perhaps be able to have a flag that can lower the saturation limit (or raise it) to a given percentage (e.g., 90%).

Loïc: With charge migration this might vary with different pixels.

Néstor: This also depends on the neighbors.

Loïc: For a given column/wavelength, however, I would force to use the same group number.

David: Perhaps set the number of groups on where saturation happens fixed for the

entire exposure to avoid using different number of groups throughout it due to perhaps varying sources.

Taylor: For MIRI, the discussion is a bit different. Given last frame and first frame effects. By default perhaps the first and last should be removed for TSOs. Moderately confident — but not absolutely confident.

David: Perhaps a parameter that can flag various first frames and last frames interactively (e.g., want to flag the first X frames and last Y frames — mark as saturated or something else).

David: Work on activate RCSD step for MIRI. This should have perhaps different thresholds —- perhaps some percentage of the number of groups — if you have many groups you can remove more frames.

[Refpix]

Everett: When you don't have reference pixels, critical to use sky pixels.

Nestor: Want to be careful with backgrounds, however, when using sky pixels.

Everett: Pre-amp offsets are the most important, and a simple strip of sky should be enough for this.

[Jump]

Drake: Probably needs improvement.

Taylor: Wonder if it's worth using the step, given one can remove at the lightcurve level.

Drake: Finding discontinuity in data on which other fields have solved.

David: Sometimes the linearity correction improvement gives rise to better detection.

[Ramp Fitting]

Taylor: People developing different algorithms for ramp fitting. All experimental. Some people like Michel Guillon applied an optimal algorithm suggest that substantially reduces noise.

David: Concern is that optimal weighting is done by last minus first — and this is

where you are biased by non-linearity.

Nestor: Perhaps doing experiments on the last item would be useful.

Worried about biases on fitting ramps to something that is not a ramp.

Loïc: A general user wouldn't probably care much about this, but useful to test this for actual exoplanet science.

[Spec2/Image2]

Taylor: Measuring centroids/traces as a function of time.

Taylor & Nestor: experiments show that extracting spectra on a fixed trace throughout the TSO is better than changing the trace as a function of time and extracting spectra at slightly different positions.

David: Tracking trace in the different directions is important (e.g., wavelength and perpendicular to wavelength). Usage might be different depending on the resolution or large movements.

Loïc: Ettiene Artigau has developed a good tool to get the X/Y and shape of second moment of those is very sensitive to detect, e.g., tilt events — it comes from knowledge of radial-velocity information. It's called SOSSISSE. Will ask to Etienne if he can share. This takes gradients of the frame from a model (which can come from your median frame) and compares that against each integration/time-stamp.

[Rectification]

Taylor: If you are using fractional pixels, it's a though problem — but if you do integer pixel rectification, then not a big deal. Useful for extraction.

Loïc: Performance-wise not cleaver to rectify, but perhaps for the community might be useful to "jump easier" or "lower the bar" to play with the data.

David: This might make the data more opaque to what is really going on.

Nestor: e.g., SOSS would be though.

2. Similarly; which **reference files** are the most impactful in those steps? (e.g., superbias step is impactful as it changes offset and gives rise to dilutions in transit depths)

Loïc: Superbias has some 1/f residuals.

Nestor: Same for darks.

Taylor: Gain files updates are unclear (e.g., MIRI).

3. For JWST TSO science, are Level 3 products sufficient to perform (e.g., exoplanet) science? If not, what would be the ideal?

Everett: x1d ints needs unpacking and a bit of a pain (Loïc). Perhaps changing format to xarray or something else would be better (that is easier to read and interact with).

Taylor: DS9 doesn't allow you to read those fits files easily for visualization. If you want to stay with fits files — make it DS9 readable!

Taylor: To zeroth-order — but if you add covariates, even more so (e.g., positions, etc.). You need to turn off the photom step in Stage2 though. Perhaps even better with optimal extraction.

David: Hard to understand e.g., the extraction trace (a simple plot) would be good.

Taylor: Diagnostic figures throughout the pipeline would be very useful.

Loïc: Masking capabilities (e.g., Order 0's) – this could be done in principle by the pipeline itself. Manual interactive masking even.

Loïc: Huge discussion on how we should replace a bad pixel. Unclear.

4. Comparison of products from different pipelines (including STScI's) for TSOs on a standard dataset might be a useful exercise, both as a standard metric to keep track of (changing) product qualities, but also to identify benefits and caveats of different algorithms — as well as the impact of each step. **What does this crowd think of e.g., a data challenge exercise and/or a running repository of data products for a standard dataset from all pipelines out there** (e.g., like an "always living" Kaggle "competition")?

Drake: Regarding a data challenge; would be beneficial to do something like this. Spitzer did the same with very good — "profitable" — results.

Nestor: In addition, having a sort of repository to store status of datasets as different pipeline versions change would be beneficial. We're building something like this within STScI, but thinking on extending this.

Taylor: Maintaining such a repository would be a low level of effort; however, getting started is what would take most of the time. This challenge was something that got started with ERS and GTO teams but has faded off.

Nestor: Propose that you bring these ideas back to your institutions and discuss. Feeling in the room is that this is a good idea; so we could create a Data Challenge Workshop — one week, days blocked on actually doing work and showing progress at the end as we move. This could be the week — "the excuse" — on which everyone blocks meetings etc. to get this done.