SOSS Simulator Guide

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ABSTRACT

The Single Object Slitless Spectroscopy (SOSS) mode will primarily be used for transit or secondary eclipse spectroscopy of exoplanets. In that mode, NIRISS stares continuously at a bright star and its cross-dispersed grism produces traces that span 850-2800 nm in order 1 and 600-1400 nm in order 2. A cylindrical weak lens on the entrance surface of the grism introduces a defocus (only along the spatial axis) to spread each monochromatic light onto about 22 pixels to enable observations of stars as bright as J=8.1 (in the standard 256x2048 subarray readout mode for a CDS integration) or J=7.0 in the bright 96x2048 subarray mode. The 1-D simulator bypasses generating 2-D images and simply uses a model stellar atmosphere as well as a model planet transmission which, coupled to our knowledge of the instrument's throughput, allows to calculate the number of photons gathered during an observation. The user selects a BT-Settl stellar atmosphere models (from 3200 K to 6000 K in steps of 100 K), a planet model (hot Jupiters, mini Neptunes, Jupiters of various temperatures, Earthlike planets, GJ1214b planets), important planet and star physical parameters such as temperature, radius and density and the transit configuration. The 1-D simulator then computes photon counts, observing efficiency and signal-to-noise ratios for the observation.

Here is a <u>link to the SOSS Simulator</u>. Or if the link does not work for you: http://maestria.astro.umontreal.ca/niriss/simu1D/simu1D.php

Subject headings: Transit, Spectroscopy, JWST, NIRISS, SOSS, Simulator

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1. Simulator Goals

- To help the NIRISS Science Team members evaluate potential targets for our GTO program.
- To keep things simple and see what photon noise can yield and use this as a baseline for more involving 2-D simulations.
- To fold in our best knowledge of what the Observatory+NIRISS throughput can produce.

2. Input Parameters - Star and Planet Atmosphere Models

2.1. Stellar Atmosphere Models

We use BT-Settl models of solar metallicity, $\log(g) = 4.5$, rounded to the nearest 100 K. Models span the temperature range of $T_{eff} = 400$ K to $T_{eff} = 5500$ K, in steps of 100 K. In addition, there are models for $T_{eff} = 5800$ K and $T_{eff} = 6000$ K. Should your target have a higher temperature, use the 6000 K model. That will not make a big difference because the SOSS samples the Rayleigh-Jeans side of the Planck curve and the spectrum is scaled to the correct J-band magnitude anyway.

2.2. Planet Atmosphere Models

Have various sources: Fortney, Eliza Miller-Ricci Kempton, Sara Seager, Lisa Kaltenegger. Will sort these. Have mini-Neptunes, Hot and warm Jupiters, Venus and Earth-like, water worlds, with and without clouds.

More to be written here...

3. Input Parameters - Scaling the Atmosphere

Scaling the planet atmosphere model is needed in case the system you want to simulate is not exactly the planet which the model atmosphere was computed for (i.e. most of the cases). For instance, one may want to model a GJ1214b-like with half the mass of the actual GJ1214b or with a slightly lower temperature. Here is the logic when checking the box to scale the model. First, the concept of scale height is needed. The scale height is the increase in altitude for which the atmospheric pressure decreases by a factor of e (Wikipedia). It is given by $H = kT/\mu g$, where ρ is the planet density, R is the planet radius (either solid radius or radius where the atmosphere is opaque at all wavelengths) and T is the planet atmosphere temperature. It is the scale height that can be scaled (to make it more puffy or denser) before being applied to a specific simulation.

Planet atmosphere models usually come in the form of wavelength-dependent planet radius as a function of wavelength (for the Fortney, Morley, Seager models). For those models, the atmosphere scale height can be retrieved by subtracting the solid planet radius or the radius of the most transparent wavelength from the wavelength-dependent radius of the model, i.e. $H_{model} = R(\lambda)_{model} - R_{solid,model}$. Then, if one requests to use that model for a planet that has a different temperature, density or radius, we can scale H_{model} such that $R(\lambda)_{simu} = R_{solid,simu} + H_{model} \times X_{H}$, where X_{H} , the scaling factor, is:

$$X_{H} = \frac{(T_{\rm simu}/T_{\rm model})}{(R_{\rm simu}/R_{\rm model}) \times (\rho_{\rm simu}/\rho_{\rm model})}$$

This is why the input form requires those 3 parameters.

Some exoplanet atmosphere models (MRK) come as transit depth vs wavelength. For those, the scale height can be traced back by using the appropriate star radius and planet radius used to generate the models.

Scaling a model may be good to first order but is a method that should be used with caution. For instance, changing the temperature may affect the chemistry and change the species abundances. So try to use a model that resembles (T, surface gravity) the system that you want to simulate.

3.1. Scaling the Planetary Atmosphere Model

The planetary transit depth relative to the star flux, $\frac{\Delta F}{F}$, corresponds to the ratio of the surface area of the planet relative to that of the star:

$$\left(\frac{\Delta F}{F}\right) = \left(\frac{\pi R_p^2(\lambda)}{\pi R_\star^2}\right) = \left(\frac{R_{\text{solid}} + H(\lambda)}{R_\star}\right)^2 \approx \left(\frac{R_{\text{solid}}^2}{R_\star^2}\right) + \left(\frac{2R_{\text{solid}}H(\lambda)}{R_\star^2}\right) = C + \delta I \qquad (1)$$

Note that the transit depth is composed of a constant (the solid radius or radius at which the atmosphere is considered opaque) and of a wavelength-dependent term, which we treat as the planet atmosphere scale height. The scale height, H, is given by:

$$\mathbf{H} = \frac{\mathbf{kT}}{\mu \mathbf{g}} \tag{2}$$

where the surface gravity, g, can be substituted for:

$$g = \frac{GM_p}{R_p^2} = \frac{4\pi}{3} G\rho R_p \tag{3}$$

The scale height then becomes:

$$H = \frac{kT}{\mu(\frac{4\pi}{3}G\rho R_{\rm p})} = \left(\frac{3k}{4\pi\mu G}\right) \left(\frac{T}{\rho R_{\rm p}}\right) \propto \left(\frac{T}{\rho R_{\rm p}}\right)$$
(4)

Now, most planet atmosphere models come in the form of a wavelength-dependent radius, $R_p^m(\lambda)$, or in the form of a wavelength-dependent transit depth, $D^m(\lambda) = \frac{\Delta F}{F}$, where the m upperscript stands for *Model*. The question is how to scale a model to apply it to a simulation for a planet with different physical parameters (T, ρ , R_p). We simply multiply the model scale height, H_{model} , by the ratio of the equilibrium temperatures, densities and radii. The scaling factor, X, is:

$$X = \frac{H_{simu}}{H_{model}} = \left(\frac{T_{simu}}{\rho_{simu}R_{p,simu}}\right) / \left(\frac{T_{model}}{\rho_{model}R_{p,model}}\right) = \left(\frac{T_{simu}}{T_{model}}\right) \left(\frac{\rho_{model}}{\rho_{simu}}\right) \left(\frac{R_{p,model}}{R_{p,simu}}\right)$$
(5)

And to apply that scaling factor, we use this:

$$R_{p,simu}(\lambda) = R_{solid,simu} + X \cdot H_{model} = R_{solid,simu} + X \cdot (R_{p,model}(\lambda) - R_{solid,model})$$
(6)

4. Input Parameters - System Physical Parameters

The star radius (along with the planet radius) is used to compute the transit depth. The star effective temperature is rounded to the nearest 100 K and the closest BT-Settl model is used. We convolve the raw model to the NIRISS optics resolution (about 1.6 pixels fwhm). A very important parameter is the J-band magnitude of the target. It is used to scale the model flux to the appropriate level and determines how many photons are detected. The planet temperature and density are used only if the *scaling the model scale height* box is checked.

5. Input Parameters - Observing Configuration

5.1. Out to In Factor

The Out-to-In Factor is defined in Figure 1. The time spent establishing the lightcurve baseline when out of transit can be the limiting factor if it is less than the time spent in the transit. For strong atmospheric features like hot Jupiters, it is probably fine to use an Out-to-In Ration of ≈ 1 or less. For systems requiring multiple visits, it is probably wise to have this factor be greater than 1 and use as many visits as possible. There is a compromise between adding visits or increasing that ratio, in which overheads play an important role.

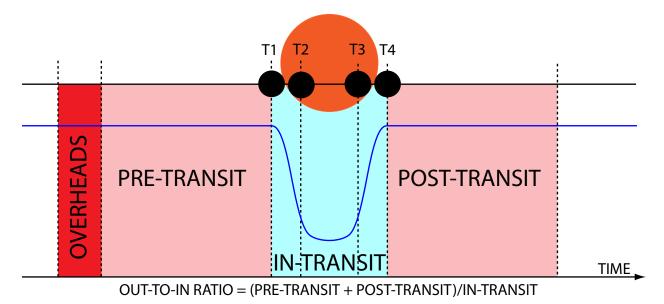


Fig. 1.— Sketch of a transit light curve. The transit duration adopted is from T1 to T4. The Out-to-In Ratio is the total time elapsed out-of-transit divided by the time during transit. The overheads are **not** included in this simulator but they consist in 30 minutes for the slew and, if the observation needs to be scheduled with a better than 24h precision, an additional 1 hour penalty for the visit.

5.2. Transit Duration

We use the T_{14} convention for the transit duration (see Figure 1).

5.3. Number of Transits

We assume that the instrument and telescope are so perfect that no systematic offset exists between visits and that light curves can simply be stacked to improve the signal-tonoise ratio as the square root of the number of transits.

6. Input Parameters - Instrument Setup

6.1. Pixel Binning

By default, the pixel binning in both orders is set to 2, the Nyquist-limited sampling that produces the highest resolving power. Regardless of the chosen binning, images will be saved in always exactly the same, full resolution of 256 by 2048, 96 by 2048 or 2048 by 2048. Pixel binning is applied downstream during the analysis to increase the signal-to-noise ratio at the expense of degrading the resolving power. Assuming a well behaved gaussian noise, binning increases the SNR as the square root of the binning. e.g. binning of 8 doubles the SNR from the default while decreasing the resolving power by 4. Keep in mind that the trace dispersion in order 2 is naturally twice that in order 1 such that one can probably bin the order 2 by a larger factor than order 1. To see the effect, try running the simulator with the order 2 pixel binning set to twice that of order 1 and inspect the Resolving Power plot to see the effect. It should produce an almost continuous line from the blue to the red.

6.2. Noise Floor

This parameters defaults to 30 ppm to mimick what is currently best achieved with WFC3 onboard the Hubble Space Telescope. The noise floor represents the systematic noise of unkown origin (probably detector-related) that limits the quality of differential spectrocopy. That would be the level below which one can not achieve better accuracy when increasing the integration time. Without this parameters, one would expect to reach the photon-noise limit (photon noise = square root of the number of photons, e.g. if $n=10^{12}$ photons, then $\Delta n=10^6$ photons and the accuracy is 1 ppm. The noise floor is added in quadrature to the other sources of noise.

6.3. Sub-Array Size

The take home message is this: use the STANDARD mode (256×2048) if your target is J=8.1 or fainter. If not, read on.

The Sub-Array is the size of the detector region that will be read out and saved onboard the telelescope. The reason why there are 3 possible sub-arrays (96×2048 - BRIGHT, 256×2048 - STANDARD and 2048×2048 - FULL-FRAME) is to effectively play with the exposure time and enable in the BRIGHT mode the observation of brighter stars without saturating. Near-IR detectors do not have shutters and the minimum integration time is set by how fast the detector is read. Witha 10 microsecond per pixel speed, the BRIGHT sub-array integrates photons for a minimum of 1.97 seconds and the STANDARD sub-array for 5.24 seconds. They both use a single amplifier to do so. The FULL-FRAME mode uses 4 amplifiers and can readout the full detector in ≈ 10.5 seconds. In short, the BRIGHT sub-array can observe a J=7.1 star without saturating while the STANDARD sub-array can observe a J=8.1 star without saturating (both for a conventional reset-read-read strategy).

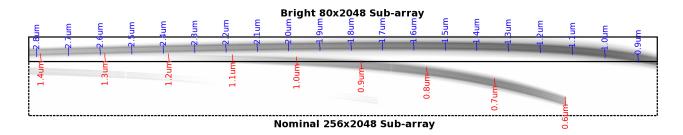


Fig. 2.— The BRIGHT (plain line) and STANDARD (dash line) sub-array readouts offered with the SOSS. The default STANDARD sub-array size captures all of the wavelength coverage from 0.6 to 1.4 microns in order 2 and 0.85 to 2.8 microns in order 1. The BRIGHT mode reads out only the order 1 trace or wavelengths from 1.05 to 2.8 microns, leaving out order 2 almost entirely. Not shown but available is a FULL-FRAME readout of all detector pixels for which an advantage could be to offer reference traces from other astrophysical sources in the field (that has not been demonstrated yet) but has the potential disadvantage of producing cross-talk from other amplifiers onto the one with our science target. The BRIGHT and STANDARD sub-array are read out using only one amplifier so don't have this potentiel issue.

6.4. Number of Read Frames per Ramp (a.k.a. NGROUP in an Integration)

This is the number of times the detector is readout up the ramp before ending the integration and resetting the well. The number of reads in the simulator is also referred to as NGROUP in the JWST jargon (which for your confusion uses N_{read} in a different meaning, be warned!). Figure 3 illustrates the sampling up-the-ramp. For the simulator, you should set the number of reads to the highest possible number without saturating. You can tell if the target saturates by looking for yellow data points in the Spectrum Realization figure. The highest the number of reads, the more efficient is the observation. Refer to Figures 4,5,6 to estimate the number of reads that should be used for a given star magnitude.

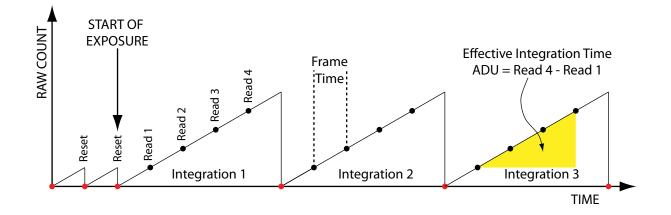


Fig. 3.— Up the ramp sampling example for NGROUP=4 (Number of reads = 4). For the SOSS, a visit will produce a single exposure containing a very large number of integrations, each consisting in a reset followed by a number of non-destructive reads. The frame time is set by the size of the sub-array and the integration time is $(N-1)\times T_{\text{frame}}$. The sky efficiency is therefore (N-1)/(N+1), where N is the number of reads, also known as N_{group}.

7. Instrument Specific Considerations

7.1. Throughput

A key input in making simulations is the instrument throughput. Figure 7 presents our estimate of the Observatory+NIRISS+GR700XD+Detector throughput.

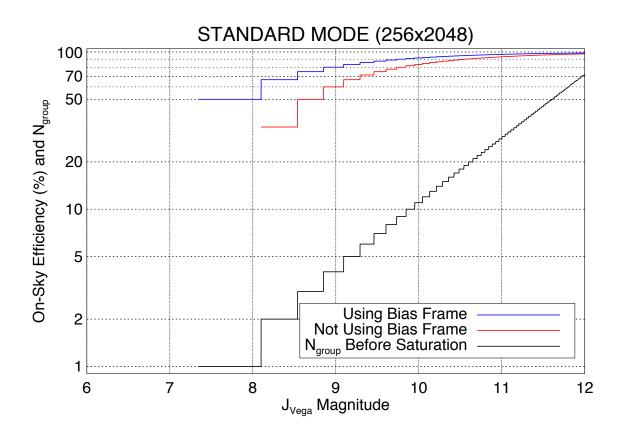


Fig. 4.— On-sky efficiency and number of reads (N_{group}) as a function of J-band magnitude. The **red line** represents the on-sky efficiency in the conventional method of subtracting read 1 from the last read to calculate the flux, or Correlated Double Sampling. That method requires at least two reads up-the-ramp and produces the cleanest noise properties. The **blue line** corresponds to the on-sky efficiency when subtracting an independently acquired bias frame from the last read to calculate the flux. That method also refereed to as superbias subtraction suffers from higher uncertainty coming from kTC noise (50+ electrons RMS) not subtracted by using an uncorrelated bias frame. Notice that the red line starts at N_{group} = 1 and pushes the saturation limiting magnitude down by 0.75 magnitudes which is why we invoke that method to enable observing brighter stars. In the simulator, we adopt the conventional (red line) method for calculating efficiency and integration time, except for the case where the number of reads is 1. Also, notice that the left end of the blue and red curves correspond to the saturation limiting magnitude in J-band. The **black line** represents the number of reads allowed before saturation.

7.2. Saturation

In order to compute saturation, we assume:

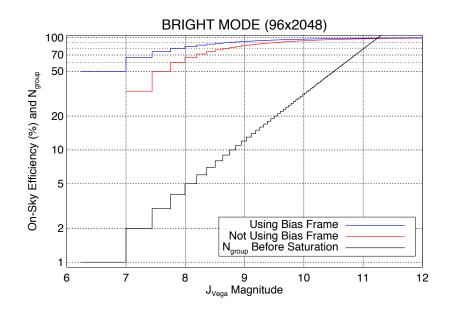


Fig. 5.— On-sky efficiency and number of reads (N_{group}) as a function of J-band magnitude for the BRIGHT MODE.

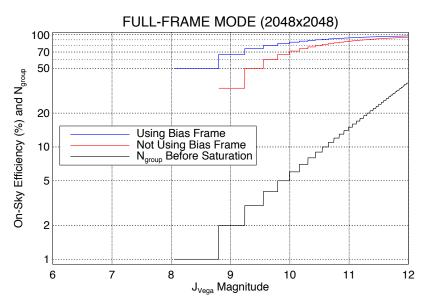


Fig. 6.— On-sky efficiency and number of reads (N_{group}) as a function of J-band magnitude for the FULL-FRAME MODE.

- 1. The effective collecting area of the telescope is 25.3 m^2 .
- 2. The detector full-well depth at saturation is 75000 electrons (with a 1:1 electron:photon yield).

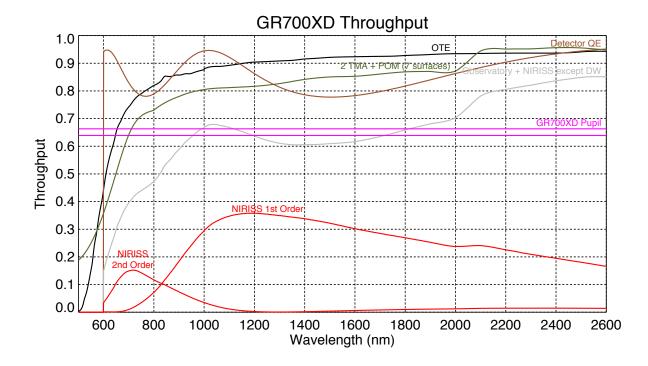


Fig. 7.— Estimated throughput of the GR700XD and other optical components of NIRISS and JWST. The red line is the curve used in the simulator and it includes the detector QE.

- 3. The spectral trace is that presented in Figure 8 with the peak pixel receiving about 7% of the total monochromatic light.
- 4. For saturation purposes, the clock starts ticking as the start of the reset and ends as the last frame starts being read. In other words, $T_{sat} = T_{frame} \times N_{group}$ where N_{group} is another designation for the number of reads and T_{frame} is the time to go through the process of reading or resetting the detector once.

7.3. Spectroscopic dispersion

We use a constant dipsersion of 0.964 nm/pixel in order 1 and 0.479 nm/pixel in order 2.

7.4. Integration Time and Efficiency

As depicted in Figure 3, the start of an integration proceeds seamlessly immediately after the end of the previous integration without overheads, beside the frame time lost to reset. Two conventions can be adopted regarding the observing efficiency (the fraction of time the detector sees photons).

The conventional approach in obtaining usable images is to subtract read 1 from the last read (CDS method). This means that the effective time during which photons are integrated is $T_{int} = T_{frame} \times (N_{group} - 1)$ while the wall clock time is $T_{clock} = T_{frame} \times (N_{group} + 1)$ for an efficiency $T_{int}/T_{clock} = (N_{group} - 1)/(N_{group} + 1) = 1/3$ at the minimum $N_{group} = 2$. We adopt that convention in our simulator when N_{group} is 2 or greater.

Rather than doing CDS image subtraction, another approach is to fit a ramp of $N_{group} + 1$ images where the additional image can be thought of as the image immediately after the detector is reset. We call that image the bias (or superbias) and it is not actually available for each integration. It is rather obtained as a calibration from a high-quality dark series. Using the superbias increases the integration time by one frame time thus the efficiency $T_{int}/T_{clock} = (N_{group})/(N_{group} + 1) = 1/2$ for the case of $N_{group} = 1$. The problem with using the superbias is that a substantial amount of noise (the kTC noise, ≈ 50 electrons rms) appears in the fitting for that image (in comparison, the conventional CDS subtraction naturally cancels that component). When observing bright targets with the SOSS, this additional noise component is small compared with the gain of increasing the effective integration time. But it is not currently known if using the superbias introduces other systematic problems. We therefore adopt this convention for $N_{group} = 1$ only.

8. Signal and Noise Calculations

First, the model star spectrum is read, convolved to the optics resolution (about 1.6 pixels fwhm) and scaled according to the J-band magnitude. Secondly, the model planet atmosphere (radius as a function of wavelength, $R(\lambda)_{planet}$) is read.

Then, the number of photons per spectral bin integrated in (S_{in}) and out (S_{out}) of transit are:

$$S_{out} = F_{\lambda, star} \cdot \frac{\lambda}{hc} \cdot T \cdot A \cdot \epsilon \cdot t_{out} \cdot d \cdot bin \cdot N_{transit}$$
(7)

$$S_{in} = F_{\lambda, star} \cdot \left(1 - \left(\frac{R(\lambda)_{planet}}{R_{star}} \right)^2 \right) \cdot \frac{\lambda}{hc} \cdot T \cdot A \cdot \epsilon \cdot t_{in} \cdot d \cdot bin \cdot N_{transit}$$
(8)

where:

 $F_{\lambda,star}$ is the star model atmosphere flux in Watt/m²/µm $\frac{\lambda}{hc}$ is to convert to photons T is the wavelength-dependent instrument throughput A is the JWST effective collecting area, 25.3 m² ϵ is the integration efficiency: N_{group} ≥ 2 : (N_{group} - 1)/(N_{group} + 1), N_{group} = 1: 50% t_{in} is the integration time during transit t_{out} is the integration time out of transit d is the spectral dispersion in µm per pixel bin is the pixel binning, 2 for Nyquist N_{transit} is the number of transits observed $R(\lambda)_{planet}$ is the wavelength-dependent planet radius R_{star} is the stellar radius

The noise associated with these integrated number of photons is the photon noise:

$$N_{out} = \sqrt{S_{out}} \tag{9}$$

$$N_{\rm in} = \sqrt{S_{\rm in}} \tag{10}$$

The relative intensity, I, during transit compared to the out-of-transit baseline is:

$$I = \frac{F_{in}}{F_{out}} = \frac{F_{\lambda,star} (1 - (\frac{R(\lambda)_{planet}}{R_{star}})^2)}{F_{\lambda,star}} = \frac{S_{in}/t_{in}}{S_{out}/t_{out}}$$
(11)

and the associated uncertainty on the relative intensity, ΔI , is:

$$\frac{\Delta I}{I} = \sqrt{\left(\frac{\Delta F_{in}}{F_{in}}\right)^2 + \left(\frac{\Delta F_{out}}{F_{out}}\right)^2 + \left(\frac{N_{floor,ppm}}{10^6}\right)^2}$$
(12)

where $N_{\text{floor},\text{ppm}}$ is the systematic noise floor expressed in ppm. One could debate whether to add that systematic noise in quadrature with other gaussian noises or to impose it as soon as other noise sources reach that limit. The former way is more conservative and we use it.

The transit depth, D, is simply:

$$D = \left(\frac{R(\lambda)_{\text{planet}}}{R_{\text{star}}}\right)^2 = 1 - I$$
(13)

Therefore the uncertainty on the transit depth is the same as the uncertainty on the relative intensity:

$$\Delta \mathbf{D} = \Delta \mathbf{I} \tag{14}$$

8.1. Readout Noise

The readout noise contributes little to the total noise budget for typical cases where bright stars are observed, except at the ends of each spectral trace orders. Each spectral bin (one detector row) contains roughly 30 pixels, each having a readout noise of ≈ 17 electrons. The readout noise per image per row is therefore $\Delta = \sqrt{30} \times 17 \approx 100$ electrons. That is to be compared with the photon noise. For a well tuned observation, the last read of a ramp should have the brightest pixel be close to saturation (70000 electrons) and, knowing from the trace profile (Fig 8) that that brightest pixel integrates about 7% of the light, in that same 30 pixel row, there are about one million photo-electrons, so a noise of 1000 electrons. So the readout noise is typically 10 times smaller than the photon noise.

We use a readout noise (on a CDS subtracted pair of images) of 17 electrons per pixel. That applies for cases where $N_{group} \geq 2$. In the case of $N_{group} = 1$, the kTC noise of the superbias is used instead, i.e. 45 electrons per pixel.

9. Simulator Outputs

9.1. Parameters Actually Used

Checking the Parameters Actually Used (simu1D_parameters.txt) is a safe way to make sure the correct parameters were used as input. A former bug that reverted values in the form to their default after running the simulation is now fixed.

9.2. ASCII Output

The simulator produces 4 ascii files: the results in order 1 (simu1D_results_order1.txt) and order 2 (simu1D_results_order2.txt), a log of the output (out.txt) and a log of the errors (err.txt). The output log will finish with "The simulation ended successfully" if that is indeed the case. Otherwise, errors will be logged in the err.txt file.

The two result outputs files contain 13 columns. Here is what each column means:

- lambda_o1: Wavelength of the binned sample in nanometers.
- targetsignal_in_o1: Number of photons detected in order 1 during the transit (T_{14}) .
- totalnoise_in_o1: Uncertainty on the number of photons in order 1 during transit based on photon noise sqrt(signal) and readout noise.

- targetsignal_out_o1: Number of photons detected in order 1 out of transit (T_{14}) .
- totalnoise_out_o1: Uncertainty on the number of photons in order 1 out of transit based on photon noise sqrt(signal) and readout noise.
- snr1_in: Number of photons divided by the uncertainty in order 1 during transit.
- snr1_out: Number of photons divided by the uncertainty in order 1 out of transit.
- depth_signal_o1: Transit depth signal relative to the total star measured signal.
- depth_noise_o1: Transit depth noise relative to the total star measured signal.
- **fakedepth_o1**: One realization of the transit depth signal relative to the total star measured signal.
- **resolving_power_o1**: lambda over delta-lambda where the binned sample is considered.
- **satflag_o1**: Set to 1 if any of the native pixel is saturated.

9.3. Output Figures

A python module generates 5 figures. The Photon Count plots the number of actually integrated photons *per spectral bin*, both in and out of transit, over the total number of transits, taking into account the efficiency. It can quickly give an idea of the theoritical signal-to-noise ratio achievable (square root of that plot is the photon noise). In fact, the next figure plots exactly that, the signal-to-noise ratio achieved per spectral bin, stacking all the transits. In the noise calculations, the photon noise and noise floor are included. The third figure is the noise alone, expressed in ppm (so the inverse of SNR times 1 million). The Resolving Power plot is NIRISS specific and depends only on the pixel binning adopted, not on any other input parameter. Finally, the Spectrum Realization plot presents one realization of the spectrum, based on the signal and noise of each spectral element. The yaxis zero point is assumed to be the solid planet radius or the radius of the most transparent wavelength in the atmosphere. What is important is not the DC level but the amplitude between extreme regions of the spectrum. Yellow data points represent wavelengths where at least 1 pixel of the trace saturated. It is usually fine to have a few data points saturate when observing a bright star and using small number of reads, if it allows to add one read and improve observing efficiency.

10. Wish List

- Having a generic TESS earth or super-earth.
- Improve the numeric noise at the 1 ppm level
- Generate model plots.
- Have 2 saturation thresholds, one for valley, one for peaks of the PSF.
- Move the web page to jwst.astro.umontreal.ca
- Allow stellar spectra hotter than 6000 K.
- Allow non-transiting observations.
- Reinstate an algorithm that determines the optimal sub-array size and Ngroup.
- Extend the wavelength coverage of the output files to 500 nm and beyond 2800 nm.
- Output the saturation time.
- Use David's table for input.
- Split the input table in its natural constituents (astrophys, instrument, etc)

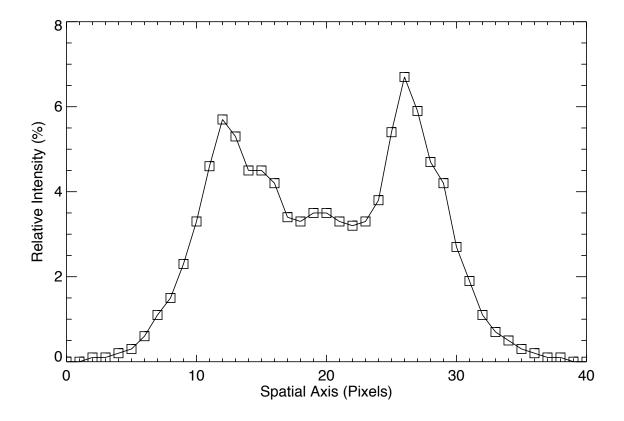


Fig. 8.— Trace profile across the spatial axis adopted for the simulator. The peak pixel receives roughly 7% of the monochromatic flux and the overall profile is about 22 pixels wide.