TECHNICAL REPORT

SPACE TELESCOPE SCIENCE INSTITUTE
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Title: NIRSpec Subarrays for Planetary Transits and other Bright Targets	Doc #: JWST-STScI-001601, SM-12 Date: October 27, 2008 Rev: -
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1.0 Introduction

“Planetary Systems and the Origins of Life” is one of the four headline science cases for JWST. The JWST Science Working Group and the Exoplanets Working Group have defined a 1.6” aperture for NIRSpec, motivated by the scientific potential of obtaining near-infrared spectra of exoplanets. This report assesses the implications of this scientific driver and its consequent hardware change on NIRSpec operational modes.

One of the most promising techniques for studying exoplanets is to obtain a very high-S/N spectrum of the host star while the planet is in transit to measure spectral features from molecules (water, ozone) in the planet’s atmosphere in absorption against the parent star. Taking the catalog of known exoplanet systems as a representative parent sample from which JWST could draw these high-priority targets, we find that >85% of planet-hosting stars are too bright to be observed without saturating the NIRSpec detectors as their readout modes are currently configured. We present a scientific and technical case for implementing small “subarrays” on the detector behind the 1.6” arcsec square aperture that is being considered for planetary transit observations. The proposed subarrays will extend the bright limit of NIRSpec by 4 mag to cover ~90% of known planetary systems and all known transiting systems. To simplify the planning, scheduling, and calibration of planetary transit data we plan to define a special-purpose “bright target” observing template that may obtain dedicated calibration observations contemporaneously with the science observations. We also describe the impact of subarrays on data calibration and the tradeoffs between scientific capability and complexity of available observing templates.

2.0 NIRSpec Readout Modes

The NIRSpec detectors have a full-well capacity of approximately 60000 electrons. Thus signal to noise ratios greater than ~250 require the addition of separate readouts. S/N ratios of 10^3 - 10^6 are required to detect the extremely weak absorption of a transiting planet atmosphere against the parent star. For NIRSpec to obtain useful spectra of

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[1] Thanks for advice from Tracy Beck, Mike Regan, Jeff Valenti, Kailash Sahu, and Ron Gilliland

transiting planets, it must be able to support S/N ratios of ≥ 10000 at $R \geq 1000$. Because of the possibility of failed open shutters and a limited contrast ratio of the Microshutter Array (MSA), NIRSpec's fixed slits are the best way to obtain these high S/N data.

The NIRSpec science team and STScI have defined default subarrays of size $n_x = 2048$ and $n_y = 64$ for each of the fixed slits. These subarrays span the full range of the detector segments in the dispersion (x) direction, taking in zero-bias reference pixels on each edge of each segment. The default subarray heights are tuned to span twice the full height of the 3.5" fixed slits, taking in unilluminated pixels above and below the aperture.

The time required to readout a subarray, and therefore the minimum time between reads or resets, is given by:

$$t_f = 10 * (n_x + 5) * (n_y + 1) \ \mu s \tag{1}$$

where $n_x \leq 2048$, $n_y \leq 2048$ and each must be a power of 2. The number of pixels in the subarray is constrained to be $n_x * n_y \geq 1024$. Thus, the minimum subarray size is $n_x = 128$, $n_y = 8$. This subarray has a readout time of $t_f = 0.012$ s.

3.0 The Need for Small Subarrays

The key fact about subarrays is that they reduce the minimum time between readouts or resets, and so enable observation of brighter stars without saturating the full well depth of the detectors. The technical case for NIRSpec subarrays applied to exoplanet transits is made in a 2007 note by Peter Jakobsen, which this note follows closely.

Figure 1 shows a simple calculation of S/N ratio for a range of subarray sizes using the relations between source magnitude, subarray size, and spectral resolution as derived by Jakobsen. The calculations in Figure 1 assume a source observed for a total of 1 hour exposure time at R = 1000 at 2.5 μm. NIRSpec throughput is relatively flat for this calculation, so the results are not sensitive to the assumed wavelength. The overplotted histogram shows the AB magnitude distribution (in arbitrarily scaled bin heights) of the current public database of extrasolar planet host stars (downloaded from exoplanets.eu, on January 6, 2009), converted from the published V-band magnitudes using the V-K vs. T_{eff} relation from Worthey & Lee (2006). This database is taken here as representative of the parent population from which JWST investigators might draw targets. The existing sample has a large fraction of planets discovered by the radial velocity technique, which favors bright stars that give high S/N; ground-based searches will likely continue to fall preferentially at AB < 8. The majority of candidates to be discovered by Corot and Kepler will be fainter than AB = 9 (Gillon et al. 2005), and so should be readily observable by any subarray set tuned to enable observations of the brighter sources used here.

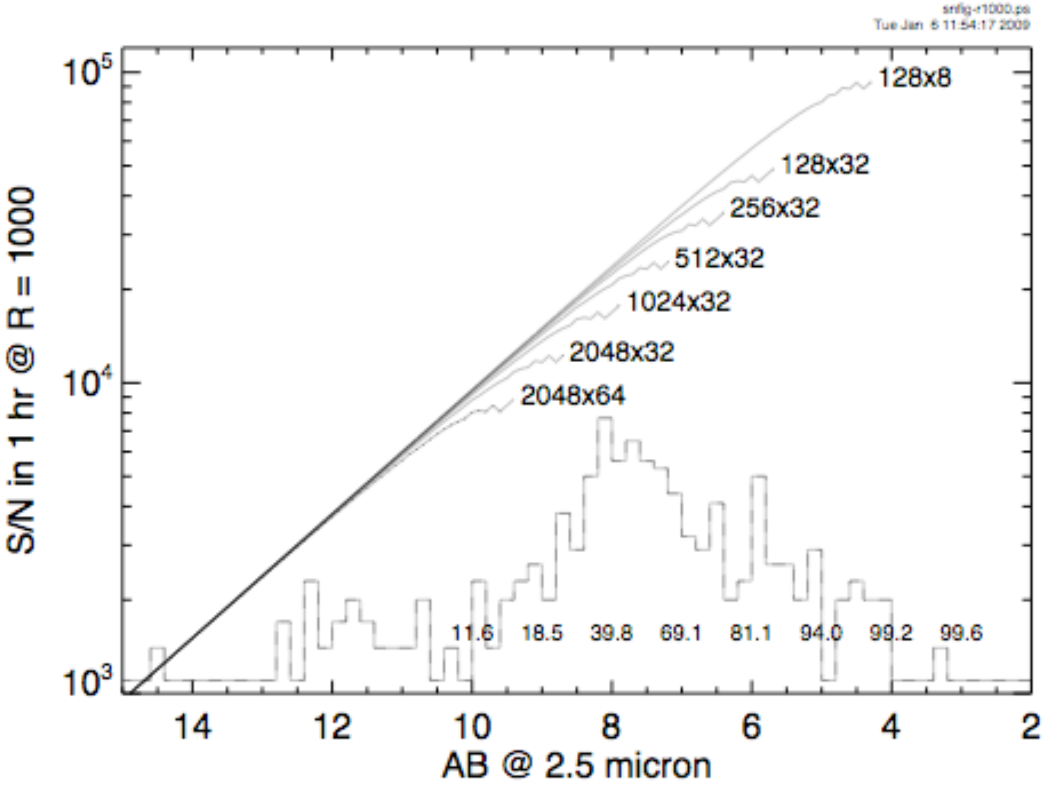

Figure 1: The S/N ratio obtained for a total 1 hr integration for bright transit sources, as a function of AB magnitude at 2.5 micron. The solid curves show the expected S/N ratio for subarrays of various sizes. The histogram shows the magnitude distribution of the 190 known extrasolar planets (exoplanets.org), together with the percentage of the sample fainter than the indicated magnitude (e.g., 88.9% of the exoplanet sample has AB > 6).

These curves assume that at least two reads will occur between resets, and that the first read following each reset will establish the zeropoint for the exposure. The point where the curve in Figure 1 stops for each subarray represents the brightest magnitude that does not saturate the detector for that subarray in the minimum readout time, e.g. AB = 9.5 for 2048 x 64. At this point, the detector full well is saturated in the fastest readout cadence (reset-read-read, reset-read-read, etc.). This figure raises several important points:

1) For R = 1000 and 1 hr total integration time the default 2048 x 64 subarray can access only ~15% of the exoplanet sample that is fainter than AB = 9.5.
2) If a given source does not saturate in a given subarray, then the S/N obtained is not much improved for smaller subarrays: at AB = 10 the difference between the default 2048 x 64 subarray and the smallest possible, 128 x 8, is only 18% in delivered signal to noise for a 1 hr integration.
3) Following (2), the main effect of using smaller subarrays is that brighter targets can be observed without saturation: the smallest subarray can go 5 magnitudes fainter than the default subarray, and access 97% of the exoplanet sample.

4) Subarrays with $n_x < 2048$ generally do not obtain data for the full wavelength coverage of the selected grating. To allow the user to focus on absorption features of interest, there should be some flexibility in the placement of the subarray center in addition to a choice of subarray size.

5) This figure shows S/N ratio per resolution element. Note that even higher S/N ratios, $> 10^5$ can be achieved for targets where only photometry is desired by summing over all the available resolution elements in a spectrum (Brown et al. 2001; Charbonneau et al. 2002). This technique can be used to measure changes in the integrated light of a transiting system with high precision but complete loss of spectral information. The curves in Figure 1 still show the brightest stars that can be observed with this technique, but the achievable S/N ratios are approximately $\sqrt{(n_x/2)}$ higher, e.g. 3.6×10^5 for AB ~ 6 and $n_x = 128$ for R = 1000.

Each NIRSpec grating has a "hard limit" beyond which it cannot go – this is the brightest source that can be observed with the smallest subarray. These "hard limits" are AB = 3, 4, and 8 for the R = 2700, 1000, and 100 modes, respectively.

We therefore arrive at the following conclusions concerning the scientific motivations and impact of subarrays:

1) Subarrays smaller than the default must be implemented to enable high S/N observations for planetary transits around stars brighter than AB ~ 9, which includes ~85% of all planetary systems known to date.

2) Choosing the smallest subarray to implement is effectively choosing the brightest target that will be observable. The smallest "legal" NIRSpec subarray (128x8) can access 97% of the exoplanet sample. With this subarray the R = 2700 mode gets all but one star because it disperses the light onto more pixels and so can go about 1 mag brighter than R = 1000.

3) Apart from any practical hindrances to the implementation or calibration of small subarrays, we would choose to implement a range of subarrays down to the smallest possible to enable observations up to the hard limits of NIRSpec, with substantial freedom for the user to choose the combination of n_x and n_y that maximizes S/N for the target and wavelength range of interest.

4.0 Tradeoffs with Practical Considerations: Proposal Planning, Implementation, Operation and Calibration Issues

If we assigned no weight to operational complications or calibration difficulties we would allow to the user to freely select n_x, n_y, and the x (wavelength) position of the subarray to fine-tune their S/N and wavelength coverage. However, this approach needlessly complicates the observing templates, on-board scripts, and calibration pipeline. Within the constraints that n_x and n_y must be powers of 2 and must multiply to > 1024, there are still 26 legal combinations; if we require further that $n_x > n_y$, there are still 22 legal combinations. We therefore want to define a smaller set of subarrays that optimally balances scientific capability with operational simplicity and calibration accuracy. There are three categories of practical consideration to account for:

Operational: Each subarray must be implemented separately in the on-board commanding scripts. Each subarray must therefore be tested during script development, and likely also during instrument thermal vacuum testing and during on-orbit commissioning. It is very likely that 22 possible subarray combinations will consume in development and testing time far more than they pay back to the user in flexibility and increased S/N. This is especially true since far away from the saturation point all subarrays obtain essentially the same S/N – the user should then choose the largest wavelength coverage with little effect on S/N.

Proposal planning: The PPS must include selectable elements, such as pull down lists, for each of the subarrays we chose to enable. Too many choices will be confusing to the user and will be difficult and time-consuming for instrument scientists to support. We therefore want to minimize this complexity.

Calibration: In addition to unique development, implementation, and planning tasks, each subarray will require unique calibration steps and reference files. For instance, each subarray will require its own dark frame. We wish to minimize complexity in the data calibration by restricting the user to a small set of subarrays.

Subarrays complicate data calibration for another important reason: depending on their size and location on the detector, they may lack the light-insensitive reference pixels that provide zero-slope measurements of detector bias drifts. Subarrays smaller than n_x = 1024 will almost certainly miss the edges of the detector segments, and so will not contain reference pixels. In the absence of reference pixels, information about bias drifts during the exposure is lost because the zero-bias reference pixels are not read out. Thus, if we choose to allow subarrays too small to contain reference pixels, we must have another means of measuring the "background" under the stellar spectrum, which for our purposes consists of pixel-to-pixel random noise and non-linear bias variations.

For subarrays without reference pixels, the only option for estimating variations in detector "background" is to use unilluminated pixels "above" and "below" the source spectrum. For the 1.6" aperture, a subarray with n_y = 32 will provide 16 pixels to sample the light from the source, and 8 pixels above and below the aperture to provide estimates of the time-varying detector background under the source[2]. For most subarrays this detector area will exceed the number of reference pixels available from the default fixed slit subarray. This default subarray has n_x = 2048 and n_y = 64, and 2 * 64 * 4 = 512 reference pixels (4 per row at end edge of the segment). By contrast, a 128x32 subarray will have 2 * 8 * n_x = 2048 pixels being read out along with the spectrum. This should provide a lower-noise estimate of the detector background underneath the spectrum than the 512 reference pixels covered by the default subarray. Subarrays with $n_y \leq 16$ will not include unilluminated pixels behind the 1.6" aperture and so will lack reference pixels *and* any other pixels that could be used to derive a background correction. For this reason, we recommend against any subarrays with $n_y < 32$, even though they could extend the bright-target range by ~1.5 mag. This is one of the important tradeoffs of enabling small subarrays, and we prefer in this case to obtain data that is more readily

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[2] Depending on the exact placement of the 1.6" aperture, it is possible that not all these 8 rows above and below will be unilluminated – some rows may receive light from the sky seen through the other fixed slits. The calibration treatment of these row is TBD.

calibrated in exchange for giving those few bright stars with AB < 4.5. Only 5 of the 190 stars shown in Figure 1 are brighter than this, and none of these are known to be transiting systems.

There is another calibration issue raised by subarrays that lack reference pixels. Without reference pixels, only the background regions on either side of the aperture can be used to estimate the detector background under the spectrum. This can be thought of as a well-matched time varying background. However, Mike Regan has pointed out that subtracting a well-matched background must be done before the slopes are determined, that is we should not subtract a time-averaged background from a time-averaged source spectrum. This apparently requires a change to the order in which slope determination and background subtraction are executed in the pipeline as it is currently conceived.

After considering small subarrays in light of operational, planning, implementation, and calibration issue, we find that:

1) Small subarrays should be limited in their range of available sizes and positions to minimize the number of separate choices that must be implemented and tested.
2) Subarrays that do not extend to the edge of the detector segments will not include reference pixels for the monitoring of bias drifts during the integration. For this reason, we advocate a minimum $n_y = 32$ to include two “background” regions above and below the source spectrum.
3) Allowing for “background” estimates to come from regions adjoining the source spectrum instead of reference pixels requires that the subtraction of a time varying-background occur before the slopes are determined during pipeline calibration. This may require a change to the calibration algorithm or a special case for these subarrays, and the cost of doing this should be weighted in when deciding how to implement these small subarrays.

5.0 Recommendations

Subarray Size: In summary, we propose that small subarrays should be adopted, and that the minimal useful set has $n_y = 32$, and $n_x = 128$, 256, 512, 1024, and 2048. The user can then select their optimal combination of wavelength coverage and S/N for each target.

Subarray Positioning: In considering the positioning of the subarrays in the detector x (wavelength) coordinate, we must account for the fact that a wide range of spectral diagnostics will be of interest to planetary transit investigators, and any predefined set of positions may lead to certain features being truncated at the end of a subarray. This situation calls for flexibility in the placement of subarrays in wavelength that should be left up to the user. The NIRSpec ASICs already possess the capability to place the corners of a subarray freely in 1-pixel steps on the detector using the ROWCORNER and COLCORNER parameters. We recommend that ROWCORNER (y) be fixed appropriately for the 1.6” aperture but that COLCORNER should be configurable at proposal planning time to allow the observer to focus on their features of interest. The permitted values of COLCORNER will be fixed separately for each subarray and grating combination to span the illuminated detector space and no further. For instance, the R = 100 spectrum occupies only ~325 pixels in the spectral dimension, so can be covered by a

n_x = 128 subarray with a center that moves over the 325-128 = 297 central pixels of the illuminated spectrum. These details still need to be worked out once the wavelength to pixel mappings are known, but will depend somewhat on where the 1.6” aperture is placed and how many pixels in the dispersion direction are occupied by the spectrum for each grating.

APT should be programmed to take in a central wavelength along with a choice of subarray and return to the user the wavelength range that will be covered, calculated behind the scenes from the mapping between detector coordinates and wavelength for each grating.

We also note that subarrays should be read out with the NRSRAPID readout pattern, which does not average over four frames like the default mode. This readout pattern is optimal for obtaining the contemporaneous background estimates from the flanking pixels, which replace the missing reference pixels for detector background corrections, and for obtaining the minimum frame time.

We have not found a scientific case for scanning across the detector in wavelength during a transit. In fact, for stability and calibration accuracy it is more desirable to choose a subarray size and placement and stick with it through a transit.

Observing Templates: We expect that the number of observers who want to point JWST at 6th mag stars will be small. We plan to define a separate “bright object” observing template that will be based on a standard fixed-slit template but which will also allow access to these small subarrays. Users will be informed early in the proposal planning process that use of this special template is recommended if their target is brighter than some magnitude (say, AB = 10) and mandatory above some brighter cutoff (say, AB = 8). This special template will hide many complications of small subarrays from the average user.

Calibration: Small subarrays that move on the detector present some calibration challenges that we must account for in their definition and use. Though we expect that readout of an arbitrarily sized and placed subarray will not affect the individual responses of the pixels with respect to their properties in full-frame readout, there is a possibility that the electrical and/or thermal behavior of the detector will vary slightly from subarray to subarray. For planetary transit observations that seek S/N > 10000 and push the instrument to its limits, calibration accuracy and stability are highly desired. We therefore recommend that the bright object template include automatic wavecals (except perhaps for the smallest subarrays), dark frames, and flat fields before and after each bright target observation (e.g. at the beginning and end of a visit devoted to a transit). The exact layout of this special observing template and its calibration data will be specified further in the upcoming NIRSpec science observing template study.

Table 1: In addition to the default 2048x64 subarray, we propose that NIRSpec adopt five additional subarrays with these properties.

Subarray n_x x n_y	Frame Time (s)	AB @ Saturation R = 1000, 2700
2048x64 (default)	1.33	9.4, 8.3
2048x32	0.677	8.7, 7.6
1024x32	0.340	7.9, 6.8
512x32	0.171	7.2, 6.1
256x32	0.086	6.4, 5.3
128x32	0.044	5.7, 4.6

6.0 Data Volume Considerations

The raw volume of data produced by NIRSpec and the other JWST Science Instruments should not exceed ~250 Gbit / day (derived from the capacity of the on-board data recorder and the availability of Deep Space Network contacts). Exoplanet transit observations may generate data volumes that press this limit, because the source is a bright star and the detectors are read out with very high cadence. Though this consideration does not directly affect the choice of subarrays, we consider it here to inform data volume studies of this potentially limiting case.

We start with the assumption that the NIRSpec detectors generate 2 bytes per pixel of readout. We assume a bright target is being observed with subarrays behind one of the fixed slits at the maximum possible frame rate, given by Equation (1) above. The daily data rate is then:

$$R = (16 \text{ bits/pixel}) * n_x * n_y * (86400 \text{ s} / t_f) / 1024\text{\^{}}2 \quad \text{Gbit / day} \qquad (2)$$

or

$$R = 138.24 * n_x * n_y / (n_x + 5) / (n_y + 1) \quad \text{Gbit / day} \qquad (3)$$

The data volume R is a factor of two higher if two identically sized subarrays are read out on each detector segment. Therefore, if our smallest proposed subarray (128x32) is read out on one segment at the fastest possible frame time ($t_f = 0.044$ s) for 24 hours without pause, the daily data volume is 129 Gbit / day, or 258 Gbit/day for both SCA segments. The dependence of the data volume on the subarray size nearly cancels because the subarray size appears in both the pixel count (numerator) and frame rate (denominator) of Equations (2) and (3), so for the larger default 2048x64 subarrays the daily volumes are 136 and 272 Gbit / day for 1 and 2 SCA segments, respectively. These data rates assume 100% usage of NIRSpec reading out at its fastest possible frame rate. Since the dependence on subarray size nearly cancels out of the data volume equation, it is much more important to know how much of a typical observing day will require exposures obtained at this extreme rate, or alternatively how likely it is that such a frame rate will be sustained for a full observing day. The typical planetary transit lasts 1-3 hr, and if the observer requests an equivalent duration of “baseline” observations of the unobscured host star then the data volume from this observation alone generates only 1/8 – 1/2 as much data as the full-day case. Transits of earthlike planets 1 AU from their parent stars can take 10 hr (30 hr including baselines), and so for very bright stars might tax the data rate limits if compression is not efficient.

In the extreme case in which both SCA segments are being read out in full-frame mode by all four amplifiers, then t_f is a factor of 4 smaller than given by Equation (1) and t_f = 10.6 s. Thus four times as many full-frame reads are being executed per day than given by Equation (3). The resulting data volume is very high: 508 Gbit/day for one 1 SCA segment and 1016 Gbit / day for both SCA segments. However, the full frame will only be read out for IFU or MSA spectroscopy modes. The MSA is inappropriate for planetary transit observations, and it is difficult to imagine a scientific use case in which the MSA and full-frame readouts will be sustained at the maximum possible frame rate for more than a few hours, if that. With full frame readouts on both SCA segments it is still possible to read out 2000 times per day before generating 250 Gbit of data. The average integration time is then 43 s even if no time is included for MSA reconfigurations, mechanism movements, calibration exposures, or observatory motions. When these practical considerations are included 2000 full-frame readouts per day seems to be a very generous limit.

7.0 Key Findings

We find that:

1) As currently configured, the default subarrays in the NIRSpec observing templates permit access to only the faintest 10 – 20 % of the known population of extrasolar planets, and achieve only S/N ~ 8000 per resolution element per hour. Detector subarrays are necessary to improve JWST’s capability for this important scientific problem.
2) The full range of subarray sizes must be restricted in the observing templates to a set that captures the scientific goals without excessive complexity in the NIRSpec proposal planning, operations, and calibration systems. We propose that a minimal set of n_x = 128, 256, 512, 1024, and 2048, all with n_y = 32. This set can be further customized for each grating choice to pare back the actual set to the minimal one.
3) Small subarrays that do not contain reference pixels should instead contain pixels above and below the aperture, so n_y = 32. A well-matched background may require a change to the ordering of pipeline calibration steps. This issue requires further study and may require a special case of the pipeline to implement.
4) Users should be free to place their subarray in the detector x coordinate (dispersion direction) to cover any illuminated part of the detector for a given grating (in either 1 or possibly 8 pixel intervals). This flexibility is needed to allow the user to cover one or more interesting spectral features.

8.0 References

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