Updated optical modeling of JWST coronagraph performance contrast, stability, and strategies

Updated Optical Modeling of JWST Coronagraph Performance, Stability, and Strategies

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ABSTRACT

We update performance simulations and contrast predictions for JWST’s coronagraphs based on the latest information on the as-built telescope and instrument properties, including both static and dynamic contributions to wavefront error. By combining optical modeling of the telescope, instruments and coronagraph optics along with STScI’s rigorously-validated exposure time calculation engine, we develop updated contrast models including contributions from effects such as target acquisition residuals, stellar color differences, etc. We present assessments of the impact of wavefront error changes over time between science and PSF reference stars, using modeled wavefront drifts on various timescales based on available observatory structural/thermal/optical modeling and tested performance during the OTIS cryo test, extrapolated to on-orbit conditions. For NIRCam we explore tradeoffs between different occulting masks at a given wavelength. Between now and the start of Cycle 1 science, these and other updated simulations will enable the science community to prepare analysis tools and PSF subtraction software to hit the ground running with JWST coronagraphic observations.

Keywords: JWST, wavefront sensing, active optics, space telescope operations

1. INTRODUCTION

The James Webb Space Telescope’s NIRCam and MIRI instruments both include coronagraph masks designed to allow characterization of exoplanets, circumstellar disks, and other high-contrast scenes at near- and mid-infrared wavelengths. There are 5 coronagraphs of different types in NIRCam\textsuperscript{1,2} and 4 in MIRI\textsuperscript{3,4} collectively usable with various spectral filters spanning 1.8 – 23 μm. Each uses a particular combination of image plane occulting mask and pupil plane Lyot stop to suppress on-axis starlight, as shown in Figure 1. The achievable inner working angles vary with wavelength and type of coronagraph mask (0.18-0.8\arcsec for NIRCam, 0.3-2.2\arcsec for MIRI). The 1.8 to 23 μm wavelength range contains a wealth of spectral features that can be used to characterize the atmospheres of extrasolar planets and brown dwarfs, or the compositions of dust and ice particles comprising circumstellar protoplanetary and debris disks. For disks, JWST will span the transition from scattered light to thermal emission, providing sensitivity to different dust particle populations in terms of particle size, temperature, and radius from the star.

In comparison to terrestrial high contrast facilities using adaptive optics, such as Gemini/GPI, VLT/SPHERE, or Subaru/SCExAO, JWST’s coronagraphs will generally not match the angular resolution or inner working angle (in large part simply due to the difference in telescope diameters). But JWST will have dramatically greater raw sensitivity than any high contrast AO facility, due to its cold temperature and location far above atmospheric and terrestrial thermal emission. For example, in terms of ability to detect faint point sources sufficiently far from the star to be not speckle-dominated, JWST NIRCam will be 50× more sensitive than Gemini/GPI at 2 μm\textsuperscript{*}, or 500× more than Keck NIRC2 at 4 μm. Such order-of-magnitude leaps in performance offer the potential to open entirely new parts of parameter space to our study—assuming we can indeed effectively remove the speckle field of stellar point spread functions to achieve the necessary high contrast.

\textsuperscript{*}This comparison factors in the roughly 2× difference in off-axis coronagraphic throughput for the two instruments, \sim 16% for NIRCam versus \sim 38% for GPI.
Deposited gold neutral density (OD=3, or 10^{-0.448140474656})

There are three sombrero-squared circular masks, 5'' on a side, are aligned along the top of the

Figure 5 shows the computed pupil intensity distributions for sources occulted by the 4

Due to the complexity of the JWST PSF, the coronagraph cannot fully suppress the diffraction pattern (i.e. the occulters

Using the computed pupil images, for each occulter pattern the holes in its corresponding Lyot stop were defined by the

For P, IIRCam, F33.5M

... at 3.3 µm, is used as the primary example mode for subsequent contrast plots.
Several past works have presented simulations of contrast performance and PSF subtraction for the NIRCam and MIRI coronographs, under various assumptions about telescope wavefront stability and other relevant factors. Now that the JWST Optical Telescope Element (OTE) has been assembled, integrated, and tested, we have better insights into the expected levels of wavefront stability. We also have more mature tools for integrated modeling of observatory performance. Therefore we can revisit earlier assumptions about wavefront stability for coronographic observations in order to derive our best estimates for JWST high contrast based on our current knowledge of the observatory’s expected properties.

1.1 Lessons from High Contrast Science with Hubble

High contrast strategies for JWST should build on experience from many years of successful coronagraphy using the Hubble Space Telescope. JWST and Hubble differ in many regards, most obviously that JWST is an active segmented telescope versus a passive monolith. Activecommanding of JWST’s mirrors will be critical for achieving alignment after launch and deployment—but subsequent corrections will be infrequent (separated by weeks to months) given the thermally benign conditions at L2. JWST’s passive optical stability is expected to be comparable to that of Hubble, as we describe in more detail below. Thus it seems likely that strategies effective on Hubble will also prove effective on JWST. In particular:

- **Even with diffraction-limited coronagraphy in space, more contrast gain comes from PSF subtraction than from coronagraph suppression.** Typically the coronagraphs in ACS, NICMOS, and STIS suppress the stellar PSF halo speckle noise by a factor of a few; subtraction of a matched PSF star enables suppression by factors of a hundred or more. Obtaining matched PSF calibrators is a crucial ingredient to reach high contrast. This directly motivates the JWST standard science policy to require all coronagraphic observations to be paired with at least one PSF calibration.

- **Modern PSF subtraction algorithms (KLIP, LOCI, SOSIE, S3, NMF, etc) make use of large reference libraries to generate optimal PSFs.** An extensive and sophisticated library of algorithms is now available, including forward modeling methods for calibrating algorithm biases. These least squares or principal component analysis methods generate synthetic PSF calibrations matched to each science exposure in terms of its time-variable speckle field, coronagraph internal alignments, stellar color, etc. For HST, PCA-based subtractions have yielded order-of-magnitude improvements in contrast for NICMOS and STIS coronagraphy. These algorithms are all now available for use on JWST. This directly motivates the policy that all PSF reference calibrator observations will have no proprietary time, to allow astronomers to reduce their data using the richest possible communal PSF library. Any simulations trying to model achieved contrast on a dynamic time-variable telescope ought to factor in the expected use of such algorithms during data reductions, not just simple classical PSF subtraction.

- **Even non-optimal coronagraphs can achieve high performance, with careful attention to PSF calibration.** Due to optical packaging constraints, the ACS coronagraph’s focal plane mask was located in a highly aberrated beam prior to the corrective optics for the HST primary’s spherical aberration. This limited the inner working angle, but superb contrast was still achieved. The STIS “bent finger” BAR5 occulter was damaged before launch, and went unused for many years—but recently it has become an effective and popular observing mode, and with careful PSF subtraction achieves contrasts comparable to GPI at the smallest inner working angle of any coronagraph ever on Hubble. These results are in large part a consequence of the above points: if the majority of the contrast gain comes from PSF subtraction, there is more ability to tolerate less-than-ideal modes and still achieve high contrast, so long as those mode’s PSFs can still be calibrated and subtracted. These examples encourage us to maintain operational flexibility for JWST’s coronagraphs and modes. For instance, in some cases we can gain in efficiency by observing in NIRCam observations using filters paired with “non-optimal” occulting masks, in particular by pursuing parallel operations of the long and short wave channels. Alternatively, we can pursue gains in inner working angle by aggressively using the smallest possible occulting masks; depending on the particular science target, the tradeoff between better inner working angle and slightly reduced contrast can be beneficial or indeed required.
1.2 Simulation Methods

We performed simulations using WebbPSF\textsuperscript{25, 26}† version 0.7 to model coronagraphic observations for a variety of scenarios as described below. WebbPSF includes 10 different independent statistical realizations of the OTE wavefront error; these are not representative of any sort of time series, but rather are completely independent realizations of the optical error budgets for launch, deployment, and commissioning which we can take as starting points for coronagraphic simulations. We can use these 10 cases to estimate uncertainties in our simulation results. For each case of interest, we iterated over the 10 independent statistical realizations, generated simulated coronagraphic PSFs for the science target, for a reference star, and an unocculted PSF as a calibration for the off-axis PSF. The 10 cases are combined to yield an average contrast curve and an uncertainty range in that contrast. Overall photometric counts were normalized using calls to the Pandiea exposure time calculator engine\textsuperscript{‡}.

To derive contrast curves, we followed a similar data reduction process as will be needed on real observations. Each target and PSF reference pair was aligned to subpixel precision using a Fourier cross-correlation, scaled as necessary to account for different stellar brightnesses, and subtracted to yield speckle residuals. The software functions for these tasks were adapted from those in the PanCAKE package\textsuperscript{§}. We then applied a normalized copy of the off-axis coronagraphic PSF as a matched filter for source detections, and computed the contrast as the standard deviation in each annulus of the matched-filtered residuals as a function of radius from the star. To account for reduced companion throughput near the occulter, we correct the inner portion of each contrast curve by dividing by the transmission of the occulting spot, a smooth band-limited function in the case of NIRCam. However we skip the correction for small number statistics at the smallest radii; this is not a large correction for the ≥ 3\(\lambda/D\) coronagraph masks in NIRCam. We report all contrasts as 5σ values.

To keep the number of scenarios simulated to tractable level, we selected the NIRCam MASK335R round mask and F335M filter as our reference case. The MASK335R occulter is the middle size of NIRCam’s 3 round masks, and is expected to be a popular workhorse mask for exoplanet searches and disk characterizations. The F335R filter (3.3 micron medium band) matched to the design wavelength of that spot is in the NIRCam long channel, in the mid-IR regime where JWST’s improvement over ground facilities is most dramatic, but is still relatively short wavelength so as to be more sensitive to drifts than longer filters. We believe this mode to be representative of typical contrast performance and dependence on physical effects; future work can extend such simulations to a broader range of filters and wavelengths as needed.

Many of our simulations focus on isolating the effect on contrast of some particular physical factor. We can divide those into two general categories, static and dynamic. Static factors include all those which affect contrast even in the ideal scenario of a perfectly stable telescope, for instance any spectral mismatch between the science target and PSF calibrator, or fundamental limits such as photon noise and detector readout noise. For most JWST modes, target acquisition residuals can be a significant factor. Dynamic factors include changes in wavefront between science and calibrator stars, or changes in the line-of-sight jitter convolution kernel.

To clearly show which physical effect limits performance in different regimes, we typically simulate each effect one at a time (e.g. we produce separate contrast curves for target acquisition residuals, wavefront drifts, and photon noise, even though in reality any given observation will necessarily have all those effects combined together.). In cases where some contrast is depicted as below the photon noise floor, that should be read as meaning that the photon noise floor will dominate and set the overall achieved contrast. Of course, that floor level is itself dependent on target brightness, integration time, detector properties, and so on in the usual fashion.

2. FACTORS AFFECTING CONTRAST ON A STATIC TELESCOPE

Figure 2 depicts predicted contrast limits for NIRCam F335M for the case of a static telescope (no time-variable wavefront error). The top two black lines show the raw contrast (i.e. prior to any PSF subtraction) for the cases of regular imaging and coronagraphy using the MASK335R round occulter. The coronagraph suppresses the stellar PSF effectively, resulting in a gain of about 2 orders of magnitude in contrast. But even so, the raw

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1\textsuperscript{See} https://webbpsf.readthedocs.io
2\textsuperscript{https://jwst.etc.stsci.edu and https://pypi.org/project/pandeia.engine/}
3\textsuperscript{Pandeia Coronagraphy Advanced Kit for Extractions; github.com/spacetelescope/pandeia-coronagraphy}
contrast remains many orders of magnitude above the fundamental limits set by photon and detector read noise (as shown in gold for a 3600 s observation of a star with $K$ magnitude 5; this scales with exposure time and stellar brightness in the expected manner). Typically, stellar PSF photon noise dominates in the inner few arcseconds, then background noise will dominate further out (that background consisting of detector noise, zodiacal light, and observatory thermal emission, with their relative proportions depending on wavelength). PSF subtraction is then needed to improve beyond the raw contrast. But what factors limit the effectiveness of PSF subtraction for JWST?

2.1 Target Acquisition residuals

In many cases a significant limiting factor is target acquisition residuals, in particular the different offsets of the target and PSF calibrator relative to the coronagraph spot. Unlike ground-based AO coronagraphs such as GPI and SPHERE, JWST does not include any closed-loop capability for sensing and controlling alignment directly during coronagraphic integrations. (The FGS will sense and correct the observatory’s pointing in closed loop, but based on a separate guide star rather than the coronagraphic target). While details of the target acquisition differ for MIRI and NIRCam, both rely on centroid measurements through an ND filter of the star offset slightly from the occulting spot, after which a spacecraft small angle maneuver is commanded to align the star and occulter. The predicted pointing residuals have $\sigma = 5$ mas per axis for the relevant sizes of moves. The resulting offsets between science observation and PSF star pointings (Figure 3, pointings shown in gold and blue) will lead to residual differences in the speckle patterns that limit contrast (Figure 2, blue line).

Prior works by our team have demonstrated that these differences can be mitigated effectively by the “small grid dither” strategy: observing the PSF calibrator at a small set of pointings intentionally offset around the mask with enough spacing to encompass the science observation pointing. PSF subtraction using this reference library is much more effective at removing the speckle halo than a single classical subtraction.27,28 Predicated contrast gains can be more than an order of magnitude, depending on mode. For our F335M example, the use of the NIRCam “9 point circle” small grid for the PSF star as shown in Figure 3 reduced the effect of pointing residuals to a completely negligible level below the noise floor (green line in 2). Even with the extra cost in observing time for the dithered calibrator star, small grid dithers are a strongly recommended observing strategy for JWST.
2.2 Stellar Color Differences between Target and PSF stars

In many cases the need to color-match PSF stars and science targets will be less strict for JWST observations than for HST coronagraphy. In part this is due simply to the use of narrower spectral filters, particularly for the MIRI FQPMs, especially in comparison to the very broad unfiltered bandpass of HST STIS. In part it is astrophysical in origin; at infrared wavelengths stellar spectra over a wide range of effective temperatures follow intrinsically similar Rayleigh-Jeans slopes. However observers should be mindful of temperatures where molecular features become present in the atmospheres of cool stars, in particular the CO bands; for instance in F444W there is a substantial change in spectrum between K0V and K2V.

For our F335M+MASK335R example we computed the contrast limits set for a G0V target with a PSF calibrator that differs by 5 subtypes (i.e. a G5V or F5V calibrator for our G0V target). The limit on contrast by the color mismatch was $< 3 \times 10^{-7}$ at small radii, and much less at wide radii, entirely negligible compared to photon and background noise for our fiducial case. The narrow and medium band filters are very robust against color differences. A more extensive set of such simulations by J. Leisenring demonstrated that even for wide band filters like F444W, differences of a few subtypes often have very small effects, with the significant exception of the emergence of CO features in some cases as noted above. Observers, especially those using medium or narrow filters, will often have considerable flexibility in choice of PSF calibrator stars.

3. CORONAGRAPHIC CONTRAST ON A DYNAMIC TELESCOPE

To understand the impact of wavefront error variations on coronagraphic contrast, we must consider both the spatial and temporal scales on which the wavefront varies. Different spatial frequencies will “leak through” a given coronagraph into the speckle field by different amounts, as shown in Figure 4. Smooth low spatial frequencies are more strongly rejected than higher-order variations or abrupt discontinuities between adjacent segments. On the other hand, 4 segments are blocked entirely by the NIRCam Lyot stops (see Fig 1), so NIRCam has zero sensitivity to any changes of those segments. MIRI on the other hand is sensitive to motions of all segments. Its greater robustness due to its longer operating wavelengths is countered by the intrinsically greater susceptibility to wavefront variations of the FQPM coronagraph architecture. In any of these modes, the temporal frequencies of variations—in comparison to typical timescales of observation sequences—will set to what extent PSF subtraction strategies can mitigate the speckles.

JWST’s optical stability is expected to be comparable to Hubble, with variations over time measured in tens of nanometers rms. (Hubble’s well-known focus “breathing” is about 35 nm rms wavefront error.) The relevant spatial scales of variation are a few cycles across the aperture (segments are expected to move with respect to one another, with little to no deformation of the segment surfaces themselves). The relevant timescales of variations are anywhere from minutes (duration of typical single integrations) to weeks or months (elapsed time between multiple coronagraphic observations in one or more observing programs).
Figure 4: Impact on contrast of two different spatial modes of wavefront variation. The left panels show hypothetical wavefront drifts that might occur between the science target and PSF calibrator; the right panels show the resulting contrast limits after classical PSF subtraction. In this idealized case we assume perfect target acquisitions and neglect all other factors affecting contrast. The same amount of wavefront drift (i.e. identical values for r.m.s. differential wavefront error) will in general have dramatically different impacts on contrast depending on its spatial frequencies.

3.1 Modeling wavefront instabilities from observatory thermal response to slews

The primary expected driver of changes in the JWST OTE’s optical state is thermal drifts following changes in observatory pitch angle with respect to the sun. The observatory design is required to have wavefront changes no larger than 55 nm rms on timescales of weeks after a maximum change in attitude. Prior studies have shown that active wavefront control, including potentially predictive control, can substantially mitigate such drifts; conversely, smart scheduling can minimize how often large thermally-adverse changes in spacecraft attitude occur.29 The JWST wavefront control operations strategy will strive to keep the telescope wavefront as nearly constant as practical. It should thus be possible to make use of observations that are widely separated in time (weeks to months) as part of a PSF reference library, as is also the case for Hubble.

Figure 5 shows the predicted OTE optical response to a “limiting case” maximum thermal change, a single slew from the inner to outer edges of the field of regard, based on integrated modeling efforts by the JWST project team across Goddard, Northrop Grumman, and Ball. The predicted WFE drift is about 40 nm rms within the first week, and 55 nm rms on very long timescales—in the absence of any optical control and after the maximum possible change in sun pitch angle. In practice, we would sense and correct for this drift within the first week. More realistic observation schedules mostly feature smaller slews between observations, though near-maximum slews do occur from time to time, in particular around thruster burns for orbit and momentum management.

The lower panels in Figure 5 show the effect of such drifts on the achieved contrast in example NIRCam and MIRI coronagraphic observations, for a hypothetical target star and exposure depth. For both cases, even after a worst-case slew, the levels of wavefront drift of timescales less than a day do not substantially reduce the predicted contrast compared to other limiting factors. Even for the unrealistic and pessimal case of a maximum slew between the target and PSF calibrator observations, as long as they were observed back-to-back within a few kiloseconds of one another, the resulting contrast should not be substantially degraded by the wavefront drifts predicted by the integrated modeling.
Figure 5: Model-predicted wavefront drift of the JWST OTE in response to changes in observatory illumination, for the limiting-case maximum slew, and the potential impact on contrast. Results shown here are from the spring 2017 integrated modeling cycle. Top panel: After a slew from the “hot” to "cold" sides of the field of regard, the OTE structure slowly adjusts to the new thermal equilibrium. This results in approximately 10 nm rms ΔWFE on timescales of 1 day, and 55 nm rms after ≥ 14 days. Bottom two panels: Potential degradation of contrast for various amounts of WFE between science target and SPF calibrator, for representative NIRCam and MIRI modes. Given the slow thermal response, for back-to-back science and calibrator observations separated by on the order of 10 ksec or less, the wavefront drift has negligible impact. The resulting contrast limit in such a case is not by ΔWFE, but by TA residuals, and background, photon, and detector noise.
3.2 OTE Stability and OTIS Testing Results

A key goal of the OTIS cryo vacuum test was to verify to what extent the OTE’s thermal response matches model predictions. Overall the OTE’s structural response to thermal perturbations was much as expected, especially in terms of the response on long timescales to slow thermal perturbations. However a few anomalous behaviors on shorter timescales were observed and subsequently investigated thoroughly until well understood.7,8 Details are available in JWST project reports from the “PFR-190” study effort. To briefly summarize, the two major unexpected phenomena were:

- Fast (time constant \( t_C \sim 2 \) minutes) oscillations of OTE wavefront correlated with the activation of electronics heaters in the ISIM Electronics Compartment (IEC), eventually diagnosed as a side effect of non-flight-like overly-stiff mechanical supports used for the ground test environment. Careful subsequent tests with the mechanical offloading changed to a more flight-like configuration showed that the oscillations were no longer present, or at least were reduced below the measurement threshold of \( \lesssim 5 \) nm rms.

- Medium-timescale \( (t_C \sim 2 – 6 \) hours) drifts in response to changes in test chamber thermal state, in particular the opening and closing of the COCOA interferometer shutter.30 Investigations after the OTIS test diagnosed this as due to insufficient slack in portions of the OTE “frill” stray light baffle and the insulation closeouts around the primary mirror segment assemblies’ edges, and these portions of the OTE were reworked to achieve the correct clearances. However since the rework could not be tested in a second OTIS cryo test, there remains some uncertainty about the eventual on-orbit behavior. Models predict the post-rework OTE frill and closeouts will still be sensitive enough to thermal state to result in changes up to \( \sim 16 \) nm rms in response to maximum changes in spacecraft sun pitch angle.

The time scale of the “frill drift” term is particularly problematic since it is roughly comparable to the expected durations for many typical coronagraph observations, an hour or a few hours. It is too fast to allow observing both a science target and calibrator together on timescales much shorter than the drift. Yet it is too slow to wait after a slew for the drift to fully equilibrate, and too slow calibrate out by averaging over many drift timescales. In contrast the “IEC-like” fast oscillations could be averaged over provided that at least a few tens of minutes of observation time per filter are desired, which will often be the case.

As well as the relevant timescales of variations, the characteristic spatial patterns of distortion for the above effects were characterized using COCOA interferometer measurements. This information enables us to propagate such disturbances through coronagraph simulations. During the PFR-190 investigation, such simulations for several hypothetical levels of wavefront error helped clarify the potential impacts on science if the instabilities were not mitigated. As noted above, the frill and some closeouts on the OTE were reworked in late 2017 and early 2018. The IEC-driven oscillation was conclusively shown to be due to ground support mounts that will not be present in flight—but we can still consider modeling it further as a proxy for “unknown unknowns” that might arise in flight to cause rapid wavefront error variations.

3.3 Modeling Multiple Simultaneous Wavefront Variations in a Flight-Like Scenario

To assess the potential contrast performance in a plausible semi-realistic scenario in which multiple physical effects occur simultaneously, we built a toy model for OTE wavefront history based on all of the above. This model includes three distinct contributions to OTE wavefront error with spatial patterns, timescales, and amplitudes given in Table 1: a slow component representing the OTE backplane’s structural response to thermal slewas, a medium-speed term representing the predicted response of the OTE frill and PMSA closeouts post-rework, and a fast component based on the IEC oscillation representing some unknown factor causing small, fast, random variations. We developed a wavefront model in WebbPSF for each of those implemented as a set of rigid-body motions of the primary mirror segments. The three models could then be scaled independently and summed together with the base wavefront map representing the long-term time average static OTE WFE as seen by NIRCam.

At each time step, the amplitudes of the slow “OTE backplane” and medium “OTE frill” terms are computed based on an exponential relaxation towards an equilibrium level defined by the observatory attitude, with time dependencies given in Table 1.
### WFE Spatial Pattern

<table>
<thead>
<tr>
<th>Assumed Mechanism and Motivation</th>
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<tr>
<td>Thermal distortion of OTE structure in response to slews in pitch angle relative to the sun. Response as predicted by observatory integrated modeling.</td>
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<tr>
<td>Faster thermal distortion from OTE frill and close-outs placing tension on OTE structure. Preliminary estimated in-flight performance after frill rework to increase slack.</td>
</tr>
<tr>
<td>Even faster pseudo-random or cyclic drifts. Same spatial pattern as observed cycling at OTIS, now known to be due to non-flight-like GSE hardware mounts for IEC. Proxy for small random “unknown unknowns”.</td>
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</tbody>
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<table>
<thead>
<tr>
<th>Amplitude and Time Scales</th>
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<tbody>
<tr>
<td>t_C ~ 7 days</td>
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<tr>
<td>A ~ 50 nm rms</td>
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<tr>
<td>(for worst-case 50 deg pitch changes)</td>
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<tr>
<td>t_C ~ 2 hours</td>
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<tr>
<td>A ~ 16 nm rms</td>
</tr>
<tr>
<td>(for worst-case 50 deg pitch changes; preliminary values based on modeling as of 2018 May)</td>
</tr>
<tr>
<td>t_C ~ 5 minutes (Random drift)</td>
</tr>
<tr>
<td>A ~ 2 nm rms</td>
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</table>

**Table 1:** The three independent components of wavefront error included in our toy model of OTE temporal variation, used in generating the simulations shown in Figure 6. The top row is based on OTE integrated modeling predictions, while the middle and bottom rows are extrapolations in-flight adapted from OTIS cryo test results.

constants $t_{C,\text{slow}} = 7$ days and $t_{C,\text{med}} = 2$ hours respectively. In other words, after each slew the wavefront error smoothly increases or decreases based on the direction and amplitude of the change in sun pitch angle. The fast “IEC-like” term drifts based on a random walk smoothed by a convolution kernel to have a characteristic timescale of 5 minutes. At each time step corresponding to a coronagraph observation, either a science observation or PSF reference, we perform a WebbPSF simulation of NIRCam MASK335R+F335M coronagraphy and save the output FITS file for use in PSF subtractions.

We applied this model to a hypothetical observing scenario with an observatory attitude profile as shown in Figure 6, upper left. This pointing history was intentionally chosen to be a difficult case, having a near-maximal change in pitch ($45^\circ$) at time $t = 0$ just prior to the start of the coronagraphic science observation. That slew takes 1800 s to complete, followed by FGS guide star acquisition and coronagraphic target acquisition; the coronagraphic science observation starts at $t = 1$ hour after the slew began. At $t = 2$ hours the observatory slews 1 degree to the PSF calibrator star, performs target acquisition, and observes the PSF star from $t = 2.2 - 2.8$ hours in a 9-point small grid dither pattern. The rest of the observing period is filled out with various slews chosen more or less arbitrarily to represent other science activities. The resulting time series WFE model is shown in Figure 6, lower left, with separate lines indicating the 3 different components and the total delta WFE. For simplicity we show each term relative to a zero point defined by the WFE state during the science observation.

The right panel of Figure 6 shows the resulting contrast. If we use only a single PSF calibrator observed immediately after our science observation, the contrast is significantly impacted, limited to around 2e-5 at 1 arcsec as shown in the red line. Examination of the WFE time series shows this is primarily due to the “frill” term, as expected since its characteristic timescale is comparable to the duration of an observation visit, and thus comparable to the time elapsed between the science target and PSF calibrator. The total WFE drift during our time series is dominated by the frill term, with amplitude around $16$ nm rms; while the backplane term potentially has higher amplitudes up to $55$ nm rms, it drifts so slowly that it does not exceed $5$ nm rms on the

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*Note this is in no sense a precise thermal model of observatory response; rather it’s a simplified 1D semi-analytical model with plausible first-order behavior for each WFE term.*
Hypothetical in-flight time series: observatory attitude and ΔWFE

Figure 6: Coronagraphic simulations using a toy model for multiple simultaneous wavefront variations demonstrate that KLIP subtraction using a library of reference stars can effectively mitigate the wavefront changes to achieve high contrast. **Left top:** Hypothetical observatory attitude profile before and after a coronagraphic observation; the slew to the target starts at \( t = 0 \) and the science exposure begins at \( t = 1 \). **Left bottom:** Wavefront error amplitudes for the 3 terms shown in Table 1 for that attitude profile. The science target and 3 PSF calibrators are observed, with each PSF star getting a 9-point small grid dither. **Right:** The resulting contrasts achieved for KLIP subtractions using 1, 2, or all 3 of the reference PSFs. In this case, using all 3 PSFs enables reaching contrasts near the fundamental noise floor despite the presence of significant time-variable WFE.

The situation changes if we make use of multiple PSF stars observed with a range of different wavefront states. Let us suppose that the other observations in our hypothetical schedule also include two other PSF star measurements, as also shown in Figure 6, lower left. In this case we show one happening before the science observation and the other much later, but that particular timing is arbitrary and not essential; what matters is that the ensemble library of PSF observations contains a sufficient range of WFE states. Our resulting PSF library contains 27 individual PSFs (3 different calibrator stars times 9 small grid dither positions each) from 27 distinct telescope WFE states. (The 9 exposures on each PSF star are close in time and thus have WFE states that are strongly correlated, but not identical). We then apply the KLIP algorithm to perform principle component PSF subtraction for our science observation. Combining 2 PSF stars into the reference library improves the achieved contrast by an order of magnitude; combining all 3 improves it another 2 to 5 times, though with diminishing returns at some radii.

In this simplified model, the use of 3 PSF stars from a wide range of WFE states provided sufficient diversity to achieve a final subtracted contrast near the fundamental noise floor, even in the presence of time-variable wavefront error that would otherwise limit the contrast to 30 – 100× higher levels. This is an encouraging result, but not a surprising one: after all, reference library PSF subtraction has been highly successful for Hubble observations, which face roughly similar amounts of wavefront variation. In practice we may expect to need a larger number of PSFs in our reference library to capture all the variations; the timing of the PSF star observations in this example were chosen to ensure good sampling of all 3 WFE components with just 3 PSF observations. That said, if we understand the timescales of variations sufficiently well, observers could...
potentially intentionally arrange the scheduling of PSF observations to be scheduled in such a manner. The Thermal Slew activity during observatory commissioning will be our first opportunity to measure the thermal response timescales after the OTE is fully aligned.

This remains a simplified model; it will be a significant task for JWST observers in Cycle 1 to assess how similar the observatory’s in-flight behavior is to this model, on what timescales and with what amplitudes the wavefront varies, and how best to assemble PSF libraries representative of that diversity. Here we have assumed WFE variation with 3 distinct components, but what dimensionality will the true problem have? The OTE has well over a hundred controllable degrees of freedom, but wavefront drifts will very likely be dominated by a handful of correlated modes. Collaborative efforts of Cycle 1 coronagraph observers will help identify best practices for PSF star observations. It may be possible to use ancillary information to support such studies, such as the periodic wavefront sensing measurements or other engineering telemetry, but exactly how best to do so is not well understood yet. Assuming the observatory wavefront sensing & control operations succeed in keeping the OTE stable on the longest timescales (weeks to years), it should be possible to gradually assemble a large reference library of PSFs over many cycles, as has been done for HST. If so, it may be the case that even early Cycle 1 data can be later reanalyzed to reach deeper levels of contrast once more comprehensive PSF libraries are in hand.

4. TRADEOFFS BETWEEN NIRCAM CORONAGRAPHY MASKS

As noted above, Hubble observations have demonstrated the scientific effectiveness of some “suboptimal” coronagraph designs, such as the narrow and bent BAR5 occulter in STIS. Wedge occulters are a particularly interesting case since they offer an ability to trade between inner working angle and contrast through positioning the target at different widths. A Hubble example is use of the WedgeA1.0 and WedgeA0.6 positions on the STIS coronagraph mask.

In the case of JWST, NIRCam’s two occulting wedges are a natural candidate for this trade. Each filter has an associated nominal pointing corresponding to \(4\lambda_{\text{max}}/D\) based on the maximum wavelength in the bandpass. Observations with the target positioned at the narrow edge of the mask instead can improve the inner working angle by a factor of \(2 - 3\). The amount of starlight that leaks through the coronagraph increases by a similar factor. Depending on the efficacy of PSF subtraction, the impact to final contrast may be even less than this (e.g. an excellent subtraction reaching near the photon noise limit might only have a \(\sqrt{3}\) reduction in contrast). Depending on science case, this tradeoff can be well worth it, enabling observations of some targets that are otherwise unobservable. Figure 7 demonstrates this with simulated observations of the planet 51 Eri b at \(r = 0.49''\).

Due to efforts by our team and colleagues at STScI, the use of the narrow end of either NIRCam bar occulter is now an available but unsupported mode. In Cycle 1, shared-risk observations by the NIRCam and Telescope GTO teams will test and assess contrast in this mode. Assuming positive results this could become offered as a supported mode in subsequent cycles. This development plan is directly based on the successful commissioning of the HST STIS coronagraph’s BAR5 mask.

NIRCam’s three round masks do not offer as much flexibility as the bar occulters, but there are still multiple combinations worth considering, particularly trading between the round masks optimized for 3.3 and 4.3 microns. Any LW filter that can be used with one can also be used with the other. In general, using the larger occulter will provide slightly better contrast, but at a cost of larger inner working angle (0.81” versus 0.63” for 50% transmission); the difference in achieved contrast post PSF subtraction may be relatively small, in which case the better inner working angle is preferred. Also, there is a significant cost in overhead time to switch masks since the lengthy target acquisition process must be repeated for each mask, but there is minimal overhead to switch filters while remaining on the same mask. Programs using several filters will thus be more time-efficient if all observations are done with the same occulting mask. Of the two, we recommend the MASK335R mask with its better inner working angle. Furthermore, this strategy can be extended even further once planned software enhancements are completed to allow parallel readout of the SW and LW channels during coronagraphy. MASK335R is positioned so as to allow useful readout of SW observation using a filter around 2 microns; MASK430R is not useful in this mode given its projected position falls in the gap between two of the SW
detectors. Given the benefits of MASK335R over MASK430R, and the value of assembling a large shared PSF reference library, we encourage users of the round masks to strongly consider the use of MASK335R for any LW channel coronagraphy regardless of wavelength. That said, there are indeed science cases for which MASK430R is the better choice.

This same strategy is also applicable to entirely non-coronagraphic modes, such as direct imaging in filters that may not have coronagraphs available, or using one of JWST’s integral field spectrographs in NIRSpec or MIRI. The contrasts achieved in such modes even with careful PSF subtraction will not equal the contrasts achieved with the coronagraphs, but even “moderate“ contrasts may offer compelling science capabilities. In particular, given the power of medium resolution spectroscopy for atmospheric characterization of planets and brown dwarfs, applying PSF subtractions methods with the NIRSpec IFU appears very attractive for characterization of substellar companions in not-too-challenging parts of parameter space for contrast and separation. Such observations are planned for Cycle 1 by both GTO and ERS teams.

5. CONCLUSIONS

Key factors that may limit JWST coronagraph performance include target acquisition residuals, stellar spectral differences, fundamental photon & background noise, and perhaps most challenging, wavefront variations on multiple timescales. Observation planning can benefit from simulations that clearly delineate the effects of these terms, allowing observers to understand which limiting factors are most stringent for their particular observations.
We have presented such simulations in particular for one example coronagraph mode on NIRCam; future work can apply these simulation frameworks to additional modes, or to particular science observations planned for Cycle 1. We intend to release these simulation tools in subsequent releases of WebbPSF and the PanCAKE coronagraph extension to Pandeia.

Using models for wavefront variation based on integrated modeling and OTIS cryovac testing of the OTE flight hardware, we assessed the potential effects of wavefront error variations on JWST coronagraphic contrast. Using only classical PSF subtraction, such variations can reduce the achievable contrast by potentially a factor of 10 or more. However, principle component analysis PSF subtraction methods, such as the KLIP algorithm, with sufficiently large reference libraries should work well to achieve high contrast even in the presence of dynamic WFE variations just as is the case for Hubble, and for high contrast AO instruments. Careful PSF subtraction using reference libraries should also open capabilities for relatively good contrasts in non-optimal modes as well: smaller inner working angles with narrow occulters, direct imaging with PSF subtraction, and IFU spectroscopy with PSF subtraction.

Understanding the diversity and timescales of WFE variations, establishing best practices for PSF observations, and building shared reference libraries in all the modes of interest will take collaborative community efforts after launch. Those efforts to achieve deep coronagraphic contrasts will let us take full advantage of JWST’s unprecedented raw sensitivity, orders of magnitude beyond what can be achieved from the ground, to open a tremendous discovery space for coronagraphic characterization of planets, brown dwarfs, and circumstellar disks.

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