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SIMULATED INSTRUMENTAL CONSTRAINTS
ON SUB-STELLAR ATMOSPHERIC
RETRIEVALS FOR THE JAMES WEBB SPACE
TELESCOPE'S MID-INFRARED
INSTRUMENT.

Evert Nasedkin

*Simulated Instrumental Constraints on Sub-Stellar Atmospheric Retrievals for the
James Webb Space Telescope's Mid-Infrared Instrument.*

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TITLEBACK

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ABSTRACT

Following its launch in 2021, the James Webb Telescope will provide the best infrared observations of exoplanets and brown dwarfs to date. In particular, the Mid-Infrared Instrument (MIRI), will allow for medium resolution spectroscopy across a wide wavelength band, from $4.9\text{-}28.8\mu\text{m}$. This will allow us to derive atmospheric properties of objects at lower temperatures than currently possible. MIRI's medium resolution spectrometer (MRS) is an integrated field unit that will perform these observations, providing both spatial and spectral information about targets. Understanding the instrumental effects is critical to analyzing data from MIRI. With that in mind, the MIRISIM instrumental simulator was developed to provide observational simulations of the various sub instruments of MIRI.

This thesis improves the implementation of a thin-film fringing model for point sources to MIRISIM, considering how the fringing effect from the detector layers varies with position. Fringing is a periodic, wavelength dependent effect, and thus has a strong impact on any spectroscopic observations. A comparison to the existing model was made, demonstrating the necessity of considering this effect when analyzing data. We will improve the fringing removal by identifying the point source location from the constructed data cube, and select the correct fringe flat for removal.

Understanding the instrumental effects is key to quantifying the ability of MIRI to derive atmospheric properties. Existing literature has considered the NIRCAM instrument and the MIRI Low-Resolution Spectrometer, but to date no retrieval studies have been performed using MIRISIM, or for the MIRI MRS, though it is critical to extend wavelength coverage to improve the results of an atmospheric retrieval. Model atmospheres will be generated using PetitRadTrans, and processed using MIRISIM and the JWST pipeline to produce a mock observation. An atmospheric retrieval will be performed, demonstrating to what extent MIRI will be able to retrieve atmospheric parameters such as temperature, pressure and composition. The posterior distributions of these parameters are compared with and without the fringing removal, again demonstrating the importance of correcting for this effect.

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Since the first detection of a planet around a sun-like star (Mayor et al., 1995) the field of exoplanets has evolved rapidly. Thousands of companions have been identified using the radial velocity and transit detection methods, and a handful have been imaged directly using both ground and space based observatories. In the last decade, many advances have been made that allow us to begin to characterize the properties of a few of these planets using spectroscopy. With the launch of the James Webb Space Telescope (JWST) in 2021, and the dawn of the era of extremely large telescopes, we will be able to peer deeper into these planets and further constrain atmospheric or geological properties, allowing us to answer questions about their formation history, climate, and even the prospects for habitability and life.

JWST will operate in near to mid infrared wavelengths, which will provide a new window into studying the atmospheres of exoplanets and brown dwarfs. The Mid Infrared Instrument (MIRI) will provide unprecedented spectral resolution in the mid infrared, allowing for the measurement of composition, pressure and temperature. Novel instrumentation does not come without challenges. Optical and instrumental effects will constrain the ability to which we can measure spectral features, which will ultimately limit the science that can be accomplished.

In this thesis, we will measure the impact of thin-film fringing in the layers of the detectors in the MIRI Medium-Resolution Spectrometer on measurements of atmospheric parameters of brown dwarfs and exoplanets. This will provide a baseline for determining the level of correction necessary to minimize the impact of fringing, as well as providing a first look into the ability of the MRS to characterize atmospheres.

1.1 EXOPLANETS

The last quarter century of observations has revealed the diversity of exoplanets and extra-solar systems. Both the architecture and individual planetary characteristics vary greatly when compared to each other, as well as to our own solar system. From the hot Jupiters initially found by Mayor and Queloz (Mayor et al., 1995) to the thousands of planets discovered by the Kepler mission, the variety in exoplanets has raised questions about their formation and development, as well as their present day structure, climate, and even prospects for life. Improvements to observational techniques have allowed us to improve our understanding of these planets. Secondary eclipse and transmission spectroscopy has opened the door to the study of planets in close orbits to their host stars, while emission spectroscopy of young planet has allowed for constraints on models of planet formation. Over the next decades, new instruments will be developed that improve sensitivity,

allowing us to study smaller, colder and fainter planets: with the ultimate goal of studying atmospheric and surface features of an earth-like planet.

Of particular interest are observable features that allow us to measure physical properties of exoplanets. The radial velocity (RV) method provides a measure of the planet mass, while a transit can constrain the radius. Already these properties tell us something about the overall structure of the planet. Spectroscopy can provide insight into the composition of the planet's atmosphere, as well as its temperature and pressure. These properties are linked to its age and location of formation in the circumstellar disk. The atmosphere, combined with the distance between the planet and its star determine the climate of the planet.

Direct Imaging

While the majority of exoplanet detections have been made using the radial velocity or transit techniques, direct imaging opens up the possibility of collecting light from the planet itself. This provides a window into the planet's atmosphere and surface. Most direct imaging to date has used near-to-mid infrared wavelengths, where the contrast between the thermal emission from the planet and the star is at a minimum. This has its drawbacks: we are so far only able to image young planets that have retained some of the heat from their formation.

Direct imaging can make use of both ground and space based observatories. However, the high spatial resolution required drives the need for a large primary mirror, limiting the possibilities of space-based telescopes. On the other hand, atmospheric turbulence necessitates the use of an adaptive optics equipped facility to observe from the ground. Atmospheric absorption due to telluric lines (absorption lines of Earth's atmosphere) also restrict infrared observations to narrow bands.

In addition to the requiring high spatial resolution, it is also challenging to separate the light emitted by the planet from that of the star. Imaging techniques such as Angular Differential Imaging (ADI) (Marois2007) and Reference Differential Imaging (RDI) (Lefreniere2009; Soummer2012) provide methods for reducing the stellar point-spread-function (PSF). Coronagraphs are optical elements which suppress the stellar PSF through self-destructive interference or physical occultation, depending on the position in the optical path. The difference in spectra between the planet and the star can also be used to separate the two sources.

Presently, 10m class telescopes such as the Very Large Telescope (VLT) in Paranal, Chile or the Gemini Observatory split between Hawaii and Chile provide the best combination of resolution and instrumentation to perform direct imaging of exoplanets. The NACO instrument at the VLT provided the first image of an exoplanet in 2004 (Chauvin et al., 2004). These observatories are among those equipped with an adaptive optics system, coronagraphic instrumentation and near to mid infrared imaging and spectroscopic capabilities to directly image exoplanets, with several exemplar systems becoming standard objects of interest. While it's terribly interesting to explore the details of each of these objects, we will focus our discussion on objects will be used further in this study, due to their scheduled observation as part

of the JWST GTO and Early Release Science (ERS) programs (Charles A. Beichman et al., 2019c). The parameters of these and other directly imaged exoplanets and brown dwarfs are summarized in table 1.

Name	d [pc]	Mass [M_{Jup}]	Sep [au]	Sep ["]	Age [Myr]	$\log(L_{bol}/L_{\odot})$	T_{eff} [K]	References
Widely separated companions								
VHS 1256b	12.7 ± 1.0	2 ± 1	102	8.1	$10^3 - 10^4$	-5.05 ± 0.22	880	(Gauza et al., 2015a)
Fomalhaut b	7.704 ± 0.028	≤ 2	119	13	440 ± 40	...	1600 ± 100	
Close in companions								
2M1207b	152.4 ± 1.1	2 ± 1	41	0.8	10 ± 3	-4.68 ± 0.05	1600 ± 100	
51 Eridani b	29.4 ± 0.3	2 ± 1	13	0.45	23 ± 3	-5.06 ± 0.2	700	(Macintosh et al., 2015)
β Pic b	19.3 ± 0.2	2 ± 1	9	0.4	23 ± 3	-3.78 ± 0.03	1600 ± 100	(Quanz et al., 2010)
GJ 504b	17.56 ± 0.08	$3 - 30$	44	2.5	$100 - 6500$	-6.13 ± 0.03	544	(Skemer et al., 2016a)
HD 95086b	90.4 ± 3.3	5 ± 2	56	0.6	17 ± 4	-4.96 ± 0.10	1050	(De Rosa et al., 2016)
HR8799b	39.4 ± 1.0	5 ± 1	68	1.7	40 ± 5	-5.1 ± 0.1	870^{+30}_{-70}	(Marois et al., 2008; Skemer et al., 2012)
HR8799c	39.4 ± 1.0	7 ± 2	38	0.95	40 ± 5	-4.7 ± 0.1	1090^{+10}_{-90}	(Marois et al., 2008; Skemer et al., 2012)
HR8799d	39.4 ± 1.0	7 ± 2	24	0.62	40 ± 5	-4.7 ± 0.2	1090^{+10}_{-90}	(Marois et al., 2008; Skemer et al., 2012)
HR8799e	39.4 ± 1.0	7 ± 2	14	0.38	40 ± 5	-4.7 ± 0.2	1000	(Marois et al., 2008; Skemer et al., 2012)
LkCa 15b	145 ± 15	6 ± 4	20	0.08	2 ± 1	
PDS 70b	113.43 ± 0.52	7 ± 2	23	0.19	5 ± 1	...	900	(Haffert et al., 2019)
PDS 70c	113.43 ± 0.52	4.4 ± 1	30	0.24	5 ± 1	...	10^4	(Haffert et al., 2019)
Nearby Brown Dwarfs								
WISE o855	2.2 ± 0.2	$3 - 10$	$10^3 - 10^4$	-10.5	$225 - 260$	(Luhman, 2014; Tinney et al., 2014)
Luhman 16B	1.998 ± 0.0004	28.6 ± 0.3	$600 - 800$	-4.68	1201	(Garcia et al., 2017; Sahlmann et al., 2015)

Table 1: Summary of directly imaged planet and brown dwarf parameters based on (Bowler, 2016) and references therein. Luminosity for WISE o855 is calculated in H band.

(Lagage2015)

VHS 1256 b

2M1207b

1.2 BROWN DWARFS

(Oliveira) (Helling et al., 2014)(Cooper2014) (Nikku Madhusudhan et al., 2018) (Burrows2003) (Marley2014) (Manjavacas, 2014) (B. Biller, 2017) (Jacqueline K Faherty et al., 2018) (Morley et al., 2014)

1.2.1 Physics

1.2.2 Observational Properties

T-Type

L-Type

Luhman 16B

Y-Type

WISE 0855-0714

1.3 MOTIVATION

1.3.1 Current Status of Atmospheric Characterization

(Kreidberg, 2018)(B. A. Biller et al., 2018) (Bozza et al., nodate) (Danielski et al., 2018) (Nikku Madhusudhan et al., 2016)

Transmission Spectroscopy

(Lee et al., 2012) (MacDonald et al., 2017) (Madhusudhan)

Emission Spectroscopy

1.3.2 JWST Studies

(Charles A Beichman et al., 2019c)

1.3.3 Biosignatures and Future Missions

1.4 THESIS OVERVIEW

2

MIRI: THE MID-INFRARED INSTRUMENT

MIRI is an instrument that will provide unique capabilities for studying exoplanets and other cold and distant objects. This chapter will provide a detailed overview of the technical details and capabilities of the instrument. A complete description of MIRI is provided in (Boccaletti et al., 2015; Bouchet et al., 2015; Glasse et al., 2015; P. Lagage et al., 2015; Ressler et al., 2015; Rieke et al., 2015b,c; Wells et al., 2015; Wright et al., 2015)

2.1 THE JAMES WEBB SPACE TELESCOPE

JWST is a 6.5m space based observatory built in collaboration between NASA, ESA and CSA that will be located in a halo orbit at the L2 Earth-Sun Lagrange point. As the successor to the Hubble Space Telescope and the Spitzer Space Telescope, it will provide a new perspective for infrared astronomy. It is currently scheduled to launch in March 2021.

James Webb is fully optimized for infrared astronomy. To reduce instrumental thermal background, the entire telescope will operate at cryogenic temperatures. A large sun-shield will help block solar infrared radiation. The lightweight beryllium mirrors are coated in gold to maximize reflectivity out to the mid infrared.

Of key interest to exoplanet science is the both the sensitivity and spatial resolution of the instrument. With its 6.5m primary, JWST will have a spatial resolution from 0.01" at 0.6 micron to 0.92" at 29 micron. The increase in sensitivity is due in part to the larger collecting area, but also to advances in detector technology since the previous generation of infrared observatories. For example, the MIRI instrument will have a minimum detectable flux of 0.13 μ Jy at 5.6 micron, or roughly a factor of 1000 better than what was possible with the Spitzer Space Telescope (Glasse et al., 2015).

There are four primary instruments that constitute the Integrated Science Instrument Module (ISIM). Near-Infrared Camera (NIRCam), which provides imaging with coronagraphic capabilities from 0.6-5 micron. The Near-Infrared Spectrograph (NIRSpec) provides fixed slit and integrated field unit spectroscopy capable of analyzing multiple objects simultaneously, and operates in the same wavelength range as NIRCam. The Fine Guidance Sensor/ Near-Infrared Imager and Slitless Spectrograph (FGS/NIRISS) allows for low and medium resolution spectroscopy with high photometric stability, as well as aperture masking interferometry. The final instrument, MIRI, is the subject of this thesis.



Figure 1: The James Webb Space Telescope during integration of the telescope into the Spacecraft Element (**assembled**).

Subsystem
Imaging
4QPM Coronagraphic Imaging
Lyot Coronagraphic Imaging
Low Resolution Spectroscopy
Medium Resolution Spectroscopy

Table 2: Summary of MIRI observing modes.

2.2 MIRI

The Mid-Infrared Instrument (MIRI) provides imaging, fixed slit and integrated field spectroscopy between 4.8 and 28 micron (**Rieke2015**). It will operate at a temperature of 6.7K to reduce instrumental backgrounds over its wavelength range of 0.6-28.8 micron.

(**Kendrew2015**)

2.3 THE MEDIUM RESOLUTION SPECTROGRAPH

The Medium Resolution Spectrograph (MRS) consists of four integrated field spectrographs projected onto two detectors, covering 4.8-28 micron with a spectral resolution varying from $R=1700$ to $R=3500$.

(**Wells2015**)

Channel	Sub-band	Band	Detector	λ Range [μm]	FOV [as]	$\lambda/\Delta\lambda$
1	Short	1A	SW	4.83 - 5.82	3.46×3.72	3500
	Medium	1B		5.62 - 6.73	3.46×3.72	3500
	Long	1C		6.46 - 7.76	3.41×3.72	3300
2	Short	2A	SW	7.44 - 8.90	4.16×4.76	3000
	Medium	2B		8.61 - 10.28	4.16×4.76	3000
	Long	2C		9.94 - 11.87	4.12×4.76	3000
3	Short	3A	LW	11.47 - 13.67	6.00×6.24	2700
	Medium	3B		13.25 - 15.80	5.96×6.24	2300
	Long	3C		15.30 - 18.24	5.91×6.24	2300
4	Short	3A	LW	17.54 - 21.10	7.14×7.87	1700
	Medium	3B		20.44 - 24.72	7.06×7.06	1700
	Long	3C		23.84 - 28.82	6.99×7.87	1500

Table 3: Properties of the MIRI MRS channels (Wells et al., 2015).

2.3.1 Coordinates

There are three primary coordinate systems in use with JWST/MIRI-MRS, of which two will be relevant for this thesis, with the detector and local MRS coordinates described in Fig. 2 (Argyriou et al., nodate).

The detector coordinate grid is formed by counting x/y pixels, as well as the slice number. Each of the two MRS detectors is an array of 1032×1024 pixels, though only 1024 are photosensitive in the horizontal direction. Each image slice from the IFU appears as a curved stripe on the detector, though neighboring stripes on the detector do not correspond to neighbouring slices of the image.

The local MRS coordinate system is described in terms of α , β and λ . The continuous α coordinate is the along slice direction, while β is perpendicular and discrete, corresponding to the slice number. λ is the wavelength. Both α and λ are fit by a second order polynomial to account for along and across slice distortion (Wells et al., 2015). Each detector sub array has its own mapping to α , β , λ space, due to the differences in FoV, slice count, distortion and spectral resolution.

The third coordinate frame is the global coordinate system of JWST itself, V_1, V_2, V_3 . The V_1 coordinate refers to the symmetry axis of the telescope, V_3 points towards the foldable secondary mirror support structure strut. V_2 completes the coordinate system, being orthogonal to V_1 and V_3 . This coordinate system will not be used in this thesis.

2.3.2 Integrated Field Spectroscopy

2.3.3 Optical Systems

Channels, bands, etc ref:Chen2019

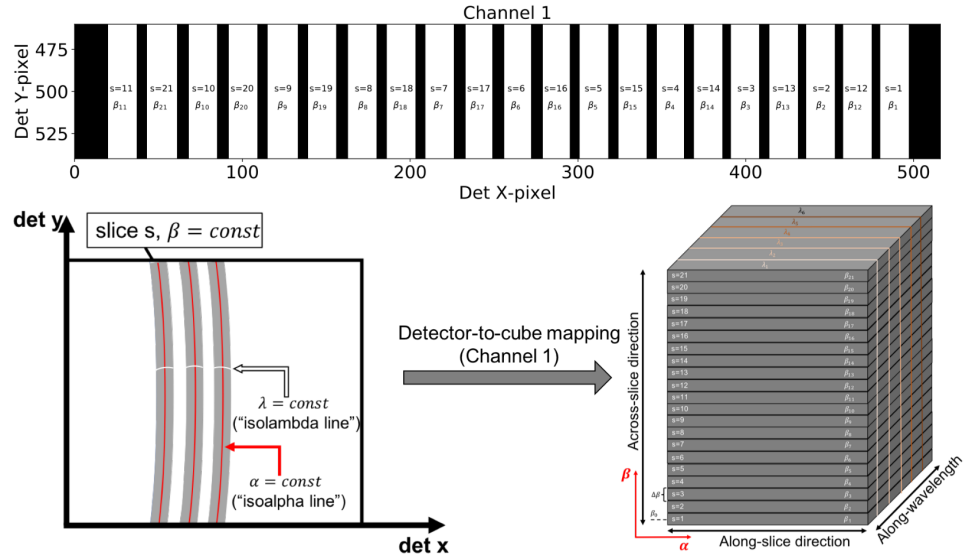


Figure 2: Description of the MRS detector (x, y, s) coordinate system to the local MRS (α, β, λ) cube coordinates. **Top:** Detector coordinates. Note that the consecutive stripe numbers s_i, s_{i+1} correspond to neighbouring image slices. **Bottom:** Description of the (invertible) detector-to-cube transformation (Argyriou et al., [nodate](#)).

Figure 3: Detector images of a spatially and spectrally flat calibration source for the SW detector (left) and LW detector (right).

2.3.4 Detectors

Readout Modes

2.4 OBSERVATIONS

2.4.1 Dithering

2.4.2 Exposure time calculations

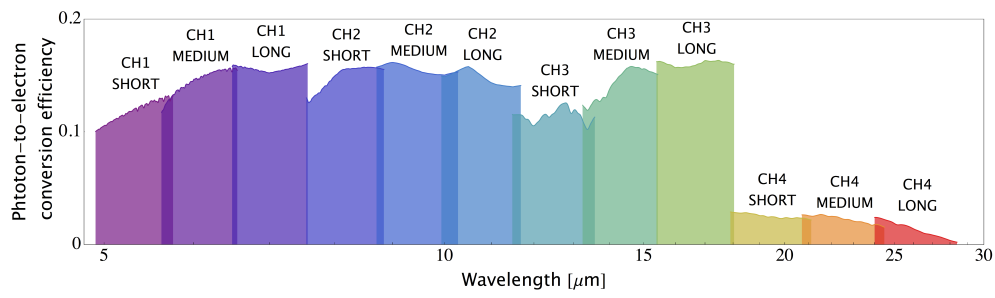


Figure 4: Average photon-to-electron conversion efficiencies for the MIRI MRS detectors

Understanding optical and instrumental effects is critical for creating accurate simulated observations and for characterizing systematics. These systematics and uncertainties in turn impact the potential science results from any instrument by biasing measurements, reducing the signal to noise ratio of measurements or by injecting non-physical signals and correlations. The aim of this chapter is to examine fringing in the MIRI detectors and how this effect is modeled in the instrumental simulator (MIRISIM).

3.1 FRINGING

Thin film interference occurs when light is coherently reflected at the boundary between two layers and interferes with the incident light. This is the principle on which Fabry-Pérot interferometers function. As we wish to determine the effect of fringing on the amplitude of the signal received by the detector, we are effectively interested in the transmittance of a series of Fabry-Pérot interferometers. Assuming an ideal plane-parallel optical cavity with a reflectance R at both boundaries, thickness D , and an angle θ at which the light travels within the cavity, we can compute the transmittance as:

$$T_c = \frac{1}{1 + \frac{4R}{(1-R)^2} \sin^2\left(\frac{\delta}{2}\right)} \quad (1)$$

Where the phase δ at half a wavelength ($\phi = \pi$), with wavenumber σ is:

$$\delta = 4\pi\sigma D \cos \theta - (\phi - \pi) \quad (2)$$

Systems with a spacing on the order of millimeters produces significant interference for infrared light (Lahuis et al., 2003).

The detectors of the MRS consist of several layers, as shown in Fig. 5, with a characteristic thickness of $500\mu\text{m}$, which results in significant (10%-30%) ‘fringing’ in a spectrally flat signal - visible in Fig. 3. While this is typical for infrared detectors such as those in the Spitzer Space Telescope (Lahuis et al., 2003) or in the Space Telescope Imaging Spectrograph on board HST (Malumuth2003), the sensitivity and spectral resolution of the MRS increase the significance of this issue. The MIRI consortium has stated that the error budget for all detector effects must be 3.3% or less. Present fringing corrections result in a 5% deviation from a photometrically accurate signal, and can introduce correlated noise which will degrade any measured spectrum. Therefore it is critical to examine the impact of fringing on a signal, the parameters that influence the fringing strength and phase, and possible solutions for fringe correction. While a more complete treatment of proposed fringe correction can be found in (Argyriou2020), this work will examine the implementation of fringing into the MIRI instrumental simulator and

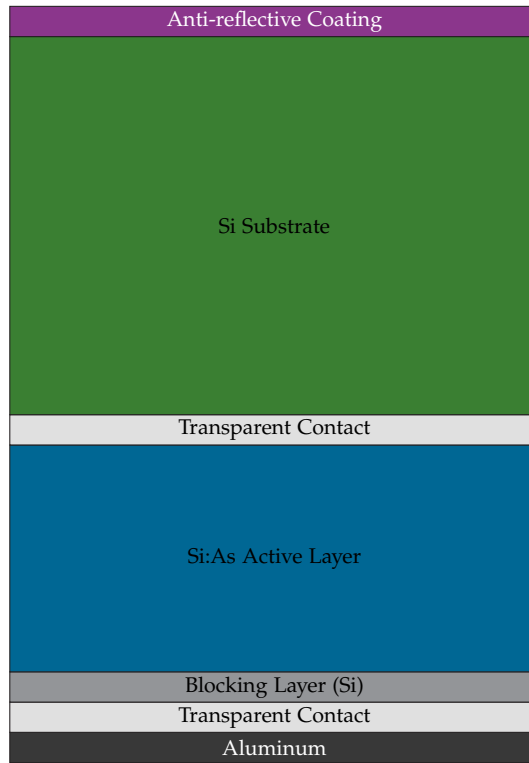


Figure 5: Layers of the MIRI MRS detectors. Note that thicknesses are not to scale (Rieke et al., 2015c).

address the current state of fringe correction in the JWST Data Calibration Pipeline.

Fred Lahuis et al., 2018

3.2 MIRISIM

Consortium2018 Cossou2019 The MIRI instrument has been modeled in python as a program known as MIRISIM. This program takes in an astronomical ‘scene’ along with some configuration parameters to output a detector data product, similar to what will be produced by the actual instrument. This is relatively full-featured simulator, modelling the instrumental PSF, various noise sources and distortion maps, among other effects. While MIRISIM is functional for all of the MIRI sub-instruments, this report will only deal with the Medium-Resolution Spectrometer (MRS) sub instrument, described in section 2.3. The goal of this section is to describe the implementation and testing of an updated optical model of the ‘fringing’ effect - an optical effect caused by thin film interference from the multiple layers of the detector.

3.2.1 Architecture

SCENE - SEDs SIMULATOR PYSPECSIM

Figure 6

Table 4

3.2.2 Data Products

3.2.3 Instrumental effects

3.2.4 Fringing

Lahuis et al., 2003 VanderPlas, 2018 A key effect on spectral data is fringing, described in ref:Argyriou2018. MIRI uses a total of three Si:As impurity band conduction detector arrays, two of which are used by the MRS. These detectors consist of 7 layers, listed in table 4 and illustrated in Fig. 5.

If all of the parameters were known, this would be sufficient to numerically solve for the fringing pattern within MIRI. Unfortunately, uncertainties in the thickness in the detector layers, variations in the layer deposition thickness, and the uncertainty of transmittance and reflectance of the materials used at cryogenic temperatures prevents the implementation of such a numerical model.

Instead, we turn to calibration data taken to characterize the fringing pattern.

DESCRIBE CURRENT MODEL - GENERIC FRINGING

However, due to the dependance of fringing on the incident angle of the light, a single model of fringing is insufficient to describe the full effect. Therefore, we use data taken in XXXXXXXXXX at various points across the detector and quantify how this changes the extracted spectra after processing in the JWST pipeline.

DESCRIBE HOW THE DATA WAS TAKEN HERE. - Problems with point vs extended sources - multiple collection runs

Ultimately this data collection produced a series of 'fringe-flats' of an almost point like at various position across the detector and in each channel. We implemented a new routine into the pySpecSim portion of MIRISIM to read in the location of point sources within a scene, and apply the correct position dependent fringe flat. This implementation comes with several caveats: namely that the fringing model is not yet fully developed, so it can only be considered accurate for point sources located at the same (α, β) location as the source used to produce the fringe flat. Additionally, the source used to generate the data is not a true point source, nor are there fringe flats produced for the full MRS wavelength range. We stress that the goal of this testing is to demonstrate the significance of this effect to justify the need for a more complete model along with additional calibration data to constrain the detector layer parameters.

*FM Data**CV Data*

3.2.5 Fringing Implementation

3.3 JWST PIPELINE

Bushouse et al., 2015 Labiano-Ortega2016

3.3.1 Stage 1 Processing

3.3.2 Stage 2 Processing

Photometric Calibration

Photometric calibration is the process of removing detector and optical biases to ensure that the measured output corresponds to the true flux incident onto the telescope. This process occurs in the PHOTOM step of the JWST pipeline, and uses reference files which store per-pixel photon-to-electron conversion efficiencies to transform the count rate data product to a flux measurement. This corrects for the wavelength dependent bias shown in Fig. 4.

However, this step remains under development, and does not produce absolutely calibrated images. In particular, even using the most up to date reference files (v8D.04.00) there remains discontinuities between channels, and poorly calibrated slopes.

Fringing correction

Carnall, 2017

*Cube Building**Aperture Photometry*

Once the data from the pipeline has been transformed into a spectral cube, we can perform aperture photometry using the photutils package to extract a 1D spectrum of the source. For each frame in each sub-band the coordinates of the spaxel at which the peak flux is detected using photutils find_peaks, which provides the location for the center of a circular aperture. A radius of 5 spaxels is used to encompass the entire PSF for a point source. If the files have already been photometrically calibrated, measuring the flux requires just adding the flux from each spaxel within the defined radius for each frame. While optimal extraction techniques exist, given our known input signal and background, this procedure is adequate for producing a spectrum in each sub-band, which can then be combined into a single spectrum for all measured sub-band.

Unfortunately, due to the issues described above with the PHOTOM step of the JWST pipeline, the spectrum built using aperture photometry does not accurately reflect the input spectrum in slope or absolute photometry. Therefore, we correct the extracted spectrum channel by channel. We fit a cubic

polynomial to a median filtered copy of both the template spectrum and the extracted spectra. The cubic fit to the extracted spectra is subtracted from the data, and the fit to the template is added. Thus this procedure corrects the slope and median flux value, but does not affect high frequency noise or signals. Fig. 7 shows an example of the results of this procedure. We believe that this is a justified measure, as the errors with photometric calibration in the pipeline should be resolved before first light of the telescope.

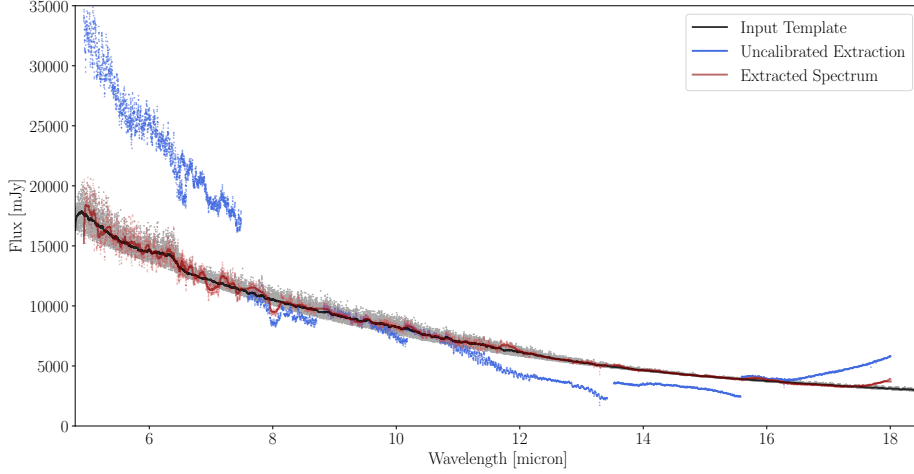


Figure 7: Comparison of an input spectrum generated using petitRadTrans and the empirically calibrated output spectrum after extraction from the cube produced by the JWST pipeline.

3.3.3 Cross-Correlation

Ignas Snellen et al., 2014 Simkin, 1974 Tonry 1979 Petermann, 2019 Bodis, 2007 To quantify the similarity of the spectrum output by the JWST pipeline to the input into MIRISIM, we rely on the technique of cross correlation. For two arbitrary, complex-valued functions $f(t)$ and $g(t)$, we can compute the cross correlation as a function of the shift τ between the functions (typically in time or velocity space):

$$(f \star g)(\tau) \equiv \int_{-\infty}^{\infty} f^*(t)g(t + \tau)dt \quad (3)$$

Our signals of interest are astrophysical spectra, measured in a finite number of discrete wavelength bins. For such a signal with M bins:

$$(f \star g)[n] \equiv \sum_{m=0}^M f^*[m]g[m + n] \quad (4)$$

Care must be taken when cross-correlating signals, as differences in normalization can result in changes in the correlation coefficient. Our procedure takes in two spectra. The first is an emission spectrum produced by the petitRadTrans program P. Mollière et al., 2019, which provides our forward model with which we compare our data spectrum. Our data is the result of

passing the template spectrum through MIRISIM, and extracting it from the resulting detector image using the JWST pipeline. We then rebin the high-resolution input spectrum to the same wavelength bins as the data spectrum, using the `spectres` package. Prior to normalization, we remove any outliers from the spectrum (due to binning errors or instrumental effects) by setting any data points separater by more than 15 standard deviations from the mean to the median value of the spectrum. For each spectrum, we subtract the minimum value to remove any offset in the spectrum, and divide by the maximum value to restrict the range to $[0,1]$. We then use apply a Savitzky-Golay filter with a window of $1/4$ the length of the spectrum and a polynomial order of 3, which we then subtract from the unfiltered spectrum. This removes the continuum emission from the spectrum, and centers it around 0. We then renormalize the spectrum by dividing by the maximum absolute value such that the range is in $[-1,1]$. The cross correlation between the forward model and itself is computed, excluding the region of interest around 0 offset. This 'autocorrelation' is subtracted from the cross correlation between the forward model and the data spectrum in order to remove secondary peaks. Finally, we normalize the cross correlation by the standard deviation of the cross correlation (excluding the central peak), giving an output measured as a signal to noise ratio.

3.3.4 Residual Statistics

In addition to computing the cross correlation between the forward model and the data spectrum, we also examine the residuals between the two spectra. Here we can see any unexpected variations between the two (periodic signals, offsets or other features). We can also examine a histogram of the residuals, normalized by the standard deviation of the data spectrum. This provides us with a distribution which should have a mean of 0 and unit width if the data are unbiased and share a distribution with the true input spectrum.

3.4 FRINGING RESULTS

1. A stronger input signal results in a stronger correlation.
2. Fringing does NOT necessarily degrade the cross correlation SNR, but rather increases it. The scale of this increase seems to depend on the absolute magnitude of the correlation (ie, a larger increase at higher SNR)
3. The residuals from subtracting the template from the data has structure.
4. If the residuals are histogrammed (and normalized by the standard deviation of the data), the width of the distribution may correspond to the cross correlation SNR (wider distribution = lower SNR)
5. Only when strongly increasing the fringing effect does the SNR decrease.
6. Correcting for fringing using the standard JWST fringe map decreases the SNR when compared to the case of fringing with no correction, but is typically still above the no-fringing case.
7. The JWST correction performs worse in the off axis case, as the fringe pattern begins to vary more when compared to the CV fringing model.

3.4.1 Effects of fringing on spectral extraction

Everything photon of light that we receive from an exoplanet will interact with its atmosphere, and will therefore provide us with a hint of what that atmosphere may look like. An atmospheric retrieval is the process of reconstructing the atmosphere of an object based on an observed spectrum. This process relies heavily on having accurate models which can be parameterized by the physical quantities we are interested in: generally the temperature, pressure and composition (Nikku Madhusudhan, 2018). As these models cover a very large parameter space (>10 parameters, each covering several orders of magnitude), it is necessary to have an efficient method for sampling this space, computing a model and comparing this model to the data (Bjoern Benneke et al., 2012).

This chapter will outline the process of an atmospheric retrieval from modelling to marginalization of posteriors, and will examine the impact that the instrumental effects described in chapter 3 have on the retrieved parameters. Additionally, this will provide an example of how the MIRI MRS can be used to explore exoplanet and brown dwarf atmospheres, and what observational parameters should be considered when studying these objects.

Schlawin et al., 2018 Fisher et al., 2019 Oreshenko2019 Barman et al., 2015 Björn Benneke, 2013 Bjoern Benneke et al., 2012 Blanco-Cuaresma2018 Konopacky et al., 2013

(Morley et al., 2018) Lupu et al., 2016 Gandhi et al., 2018 Baudino et al., 2017 Line et al., 2013 Madhusudhan2018b Irwin et al., 2008 Robinson et al., 2016 Waldmann et al., 2015b Waldmann et al., 2015a Line et al., 2015, 2017; Zalesky et al., 2019

Batalha et al., 2018 Feng et al., 2018 P. Mollière et al., 2019

Atmospheric Modeling

Atmospheric modelling is the task of creating an spectra based on the physical properties of the atmosphere. This is a broad task that can range from a 3D Global Circulation Model (GCM) which accounts for self-consistent atmospheric chemistry (Chen et al., 2019) to a 1D model based around an empirical temperature-pressure profile (P. Mollière et al., 2019). The choice of model depends largely on the requirements for accuracy and computational cost. Considering the potentially millions of possible atmospheres that must be examined in a retrieval problem, whatever model is used must be computationally efficient above all else.

4.1 PETITRADTRANS

For this work we chose to use the petitRADTRANS package due to its user-friendly python implementation, high speed computation for retrieval

Property	Description
Temperature	Parameterized, e.g. (Guillot, 2010)
Abundances	Parameterized, e.g. vertically constant
Scattering	Cloud scattering, transmission spectra only
Clouds	Power law and condensation clouds
Cloud particle size	f_{SED} and K_{ZZ} or parameterized
Particle size distribution	log-normal, variable width
Cloud abundance	Parameterized
Wavelength spacing	$R=1000$ (c-k), 10^6 (lbl)
Valid emission spectra	Clear, from NIR and longer

Table 5: Description of the parameters available in petitRADTRANS. For cloud particles, f_{SED} is the mass-averaged ratio of the cloud particle settling speed and mixing velocity. K_{ZZ} is the atmospheric eddy diffusion coefficient (Ackerman et al., 2001)

use and extensive high resolution, line-by-line spectral library for generating planetary spectra (P. Mollière et al., 2019). It is a 1D, radiative transfer package with many parameters options, described in table 5. PetitRADTRANS can compute both emission and transmission spectra, with an output spectral resolution of $R=1000$ in correlated k mode, or $R=1\,000\,000$ in line-by-line mode.

Note that much of the following sections applies to many other similar 1D radiative transfer atmospheric modelling programs such as ATMO (Goyal2018), Planetary Spectrum Generator (Villanueva2018), HELIOS (Malik et al., 2017, 2019) and others. Many (or even most) of these programs rely on the same set of high-resolution molecular line lists, including HITRAN/HITEMP (Rothman1973; Gordon et al., 2017; Rothman et al., 2010), ExoMol/ExoCross (Tennyson2016a; Tennyson et al., 2016; Yurchenko et al., 2018) and others.

4.1.1 Radiative Transfer

In order to compute the emission spectrum an initial featureless black-body spectrum $B(T_{int})$ is passed through multiple discrete layers of the atmosphere, parameterized by their temperature, pressure, and the opacities of each of the species present in a given layer. Modeling each layer as plane parallel, the intensity is computed as in (Irwin et al., 2008; P. Mollière et al., 2017, 2019)

$$I_{top} = B(T_{int})\mathcal{T}^{atmo} + \frac{1}{2} \sum_{i=0}^{N_L-1} \left[B(T^i) + B(T^{i+1}) \right] \left(\mathcal{T}^i - \mathcal{T}^{i+1} \right) \quad (5)$$

N_L is the number of layers in the atmosphere, and \mathcal{T} is the transmission from a given layer to the top of the atmosphere. All quantities are averaged per wavelength bin in c-k mode, while they are evaluated at each wavelength point in line-by-line mode.

(Guillot, 2010)

4.1.2 Opacity Sources

To compute the emission spectra of an atmosphere, petitRADTRANS accounts for various opacity contributions including absorption and emission lines, collisionally induced absorption, cloud opacity and scattering and Rayleigh scattering cross sections. These sources are described in detail in (P. Mollière et al., 2019), summarized in tables 2 and 3. For this work we consider only the case of a cloud-free atmosphere due to the complexity of realistic cloud modeling.

Line-by-line

In its high resolution line-by-line mode, petitRADTRANS computes emission spectra with $R=10^6$. These spectra are computed using opacity sources for molecular and atomic lines from ExoMol/ExoCross library (Yurchenko et al., 2018). Pressure broadening is taken into account using the coefficients from HITRAN/HITEMP (Rothman et al., 2010, 2013) or from (Sharp2007) (Eqn. 15). The line opacities are computed from 80-3000K, and from 0.3-28 μ m in high resolution mode.

Correlated K

The low resolution mode of petitRADTRANS uses the correlated-k (c-k) method of computing line opacities (Fu et al., 1992; Goody et al., 1989; Lacis et al., 1991). This method for calculating emission and absorption features assumes that the opacity distribution functions between differing species are uncorrelated, which permits simple computation of overlapping features. While petitRADTRANS implements a c-k method with a spectral resolution of 1000, in principle it is accurate to much higher resolutions. However, the principle utility of the c-k method is in the dramatic reduction in computational cost for computing a spectra such that petitRADTRANS can be used as the foundation for an atmospheric retrieval code requiring hundreds of thousands or millions of models to be generated. (P. Mollière et al., 2019) discusses the variations between the results of the line-by-line method and the c-k method, finding discrepancy of at most 6%. Typical variation is much lower, as seen in Fig. 2 of (P. Mollière et al., 2019).

Clouds

Line et al., 2016 Jacqueline K Faherty et al., 2018 Morley et al., 2014 Lavie et al., 2017

4.2 BAYESIAN INFERENCE

An atmospheric retrieval is the process of extracting information about physical parameters from a measured spectrum. In general this procedure involves comparing the data to a series of template spectra with known parameters and identifying the best fit model. Unfortunately for astronomers, atmospheres are complicated: typical one 1D models still require many (>15)

parameters to generate a somewhat realistic model. This results in a very large parameter space in which to search for the correct set of properties that describe our measurement.

Monte Carlo methods, including Nested Sampling, are used to effectively search this large space using the Bayesian evidence as a goodness-of-fit metric. Here we will follow (Joshua S. Speagle, 2019) to provide a brief overview of Bayesian inference.

To measure the likelihood of a given model, we turn to Bayes' Theorem:

$$P(\Theta_M|\mathbf{D}, M) = \frac{P(\mathbf{D}|\Theta, M)P(\Theta|M)}{P(\mathbf{D}|M)} \quad (6)$$

In our notation, Θ is the set of parameters that describe a model M , that is fit to the data \mathbf{D} . Bayes' theorem asks what is the probability that the parameters Θ are true given the data and model. The distributions for each parameter are the **posterior** distributions.

This is then related to the **likelihood** $P(\mathbf{D}|\Theta, M)$ of measuring the data given the model, the **prior** probability $P(\Theta|M)$ which describes our degree of belief in our model and the **evidence** $P(\mathbf{D}|M)$, which is marginalized over all possible Θ and quantifies how well the model describes the data. To simplify notation, we adopt the following convention for Bayes' theorem:

$$\mathcal{P}(\Theta) = \frac{\mathcal{L}(\Theta)\pi(\Theta)}{\mathcal{Z}} \quad (7)$$

In general, the goal of an atmospheric retrieval is to find the best fit model by maximizing the evidence \mathcal{Z} , and as a by product finding the marginalized posterior distributions for each parameter. This comes with many challenges, especially when dealing with large numbers of parameters. Selection of the priors and model will determine the extent to which a result can be interpreted, while sampling large parameter spaces and computing likelihoods introduces substantial numerical challenges. The Markov Chain Monte Carlo method and the Nested Sampling method described below attempt to solve the challenges of exploring a large parameter space.

4.2.1 MCMC

Foreman-Mackey et al., 2013 MacKay, 2003

4.2.2 Nested Sampling

Nested sampling attempts to address several of the shortcomings of MCMC methods while simultaneously improving computational efficiency (Skilling, 2004). MCMC methods generate samples 'proportional to' the true posterior distributions, which lead to difficulties in computing the evidence \mathcal{Z} (Joshua S Speagle, 2020). In contrast, nested sampling puts the evidence first and provides estimates of the posterior distributions from the importance weights of the final set of samples. First described in (Skilling, 2004), nested sampling has been adopted as the sampling algorithm of choice within the astrophysics community (Buchner et al., 2014; F. Feroz et al., 2009; Farhan Feroz et al., 2019; Joshua S Speagle, 2020).

With the goal of parameter estimation, nested sampling attempts to estimate the evidence \mathcal{Z} rather than directly sampling the posteriors (Skilling, 2004). This is done by integrating over the entire parameter space of Θ

$$\mathcal{Z} = \int_{\Omega_{\Theta}} \mathcal{L}(\Theta) \pi(\Theta) d\Theta \quad (8)$$

This is difficult.

Rather than attempting to directly solve the entire multidimensional integral, nested sampling transforms this into an integration over the *prior* volume X :

$$\mathcal{Z} = \int_{\Omega_{\Theta}} \mathcal{L}(\Theta) \pi(\Theta) d\Theta = \int_0^1 \mathcal{L}(X) dX \quad (9)$$

This is now a contour integral over isocontours $\mathcal{L}(X)$ which bound the prior volume

$$X(\lambda) = \int_{\Omega_{\Theta}: \mathcal{L}(\Theta) \geq \lambda} \pi(\Theta) d\Theta \quad (10)$$

which is the fraction of the prior where the likelihood of the data given the model is above some threshold λ . The integration is now simplified into a 1D integration over X , given proper prior selection.

Method

Consider a parameter space with D dimensions. We will describe this space as a unit hypercube, where each parameter runs from 0 to 1. Priors are thus transformations from this space to a physical parameter space. Often the prior is a uniform distribution, which simply scales the space, but it may also be an informative prior such as a normal distribution centered at an expected physical value. In order to sample this space, N_L ‘live points’ are generated, each of which provides a set of parameters Θ . N_L must be greater than $D + 1$, and typically values on the order of $50 \times D$ are used (F. Feroz et al., 2009). Using a likelihood function $\mathcal{L}(\Theta)$, the evidence \mathcal{Z} can be computed by comparing the model to the data. Having computed the evidence at each point, the live points are then sorted and the point with the lowest evidence is discarded. A set of ellipsoids is drawn around the remaining points. The procedure for computing these ellipsoids is given in (F. Feroz et al., 2008, 2009). By using a set of ellipsoids, multiple modes in the parameter space can be encompassed. Once the ellipsoids bounding the remaining points are drawn, a new sample is drawn from within the restricted sample space. The evidence for the new point is computed, and it is accepted if the evidence is greater than the minimum evidence of the previous remaining set of points. The entire procedure is repeated until some convergence criteria is satisfied, with each iteration resulting in a smaller volume being encompassed by the ellipsoids, nested within the previous volume.

This procedure can be improved in many ways, including importance nested sampling (Farhan Feroz et al., 2019) and dynamic nested sampling (Joshua S Speagle, 2020).

Parameter	Prior	Constraints
$\log \delta$	$\mathcal{N}(-5.5, 2.5)$	
$\log \gamma$	$\mathcal{N}(0, 2)$	
T_{int}	$\mathcal{U}(0, 3500)$	
T_{equ}	$\mathcal{U}(0, 30)$	
$\log P_{Trans}$	$\mathcal{N}(-3, 3)$	
α	$\mathcal{N}(0.25, 0.4)$	$\alpha < 1$
$\log g$	$\mathcal{U}(2.0, 4.5)$	
$\log P_0$	$\mathcal{U}(-5, 2)$	
$\ln(X_i)$	$\mathcal{U}(-18, 0)$	$\sum X_i < 1$

Table 6: Prior choices for atmospheric retrievals. $\mathcal{U}(a, b)$ is a uniform distribution from a to b . $\mathcal{N}(\mu, \sigma)$ is a normal distribution. T_{int} corresponds to the effective temperature of an object, while T_{equ} is the equilibrium temperature between an object and a host star. For free floating objects, T_{equ} is set to 3.4K, justifying the small range of the prior. δ is in units of bar^{-1} , temperatures are in K, and pressures in bar.

4.2.3 Multinest

For our implementation of an atmospheric retrieval code, we chose to use the Multinest algorithm (F. Feroz et al., 2009) using the pyMultinest wrapper (Buchner et al., 2014) and using importance nested sampling to improve the accuracy of the Bayesian evidence calculation (Farhan Feroz et al., 2019). This particular implementation of nested sampling is commonly used in atmospheric retrieval codes due to its fast Fortran implementation, though it was initially developed for cosmological problems.

Using the pyMultinest package, we implemented the required log-prior function which transforms the unit hypercube to physical parameter space and the log-likelihood function used to compare the model to the data. The full code is available at <https://github.com/nenasedk/petitRetrieval>, and is based of the emission spectrum retrieval described in (P. Mollière et al., 2019). Retrievals were typically performed using 500 or 1000 live points, with the convergence criteria

$$\Delta \ln \mathcal{Z} = \ln Z_i - Z_{i+1} \quad (11)$$

set to 0.3 for parameter estimation and 0.8 for model comparison, as suggested in the pyMultinest documentation.

4.2.4 Prior choice

4.2.5 Bayesian Model Selection

4.3 TARGETS

4.3.1 Atmospheric Parameters

Nikku Madhusudhan, 2012 Moses2012Garland et al., 2019 Bowler, 2016 Fegley et al., 1994 Tokunaga, 1983

4.3.2 petitRadTrans

4.4 RESULTS

4.4.1 Posterior Distributions

5 | CONCLUSIONS

A | APPENDICES

A.1 PACKAGE REQUIREMENTS

```
numpy=1.4.0  
scipy=1.5
```


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