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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 4.9-28.8 μm . 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 and Queloz) 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 and Queloz) 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 (Chauvin2004). 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. The parameters of some directly imaged exoplanets are summarized in table 1

Name
2M1207b
β Pic b
HR8799b
HR8799c
HR8799d
HR8799e
Fomalhaut b
2M J044144b
LkCa 15b
HD 95086b
Gliese 504b
51 Eridani b
PDS 70b
PDS 70c

Table 1: Summary of directly imaged planet parameters [Bowler](#) and references therein.

(Beichman et al., “Direct Imaging and Spectroscopy of Exoplanets with the James Webb Space Telescope”) ([Lagage2015](#)) ([Macintosh et al.](#)) ([Macintosh et al.](#))

Beta Pictoris b

Discovered in 2008 ([Lagrange et al.](#)), β Pic b is one of the most well-studied exoplanet systems ([Hoeihmakers2018](#); [Quanz et al.](#) [Chilcote et al.](#) [Chilcote et al.](#)). Due to its young age of 23 ± 3 Myr ([Mamajek2014](#)) and high mass of $12.9 M_J$ ([Chilcote et al.](#)) it remains hot, between 1590K and 1847K ([Nowak2019](#)). Combined with its typically wide separation on its 9.2AU orbit ([Chauvin2012](#)), this allows for relatively easy imaging and spectroscopy in the near infrared. Recent RV observations indicate the possibility of an additional planet at 2.3 AU ([Lagrange2019](#)).

The quantity and quality of spectral data for β Pic b has allowed for the study and characterization of its atmosphere: measurements of its metallicity and C/O ratio can trace the formation history of the planet ([Nowak2019](#); [Chilcote et al.](#)). It also provides insight into its current atmospheric structure and composition, which can in turn inform models of exoplanet atmospheres.

HR 8799 System

PDS 70 b,c

1.2 BROWN DWARFS

([Oliveira](#)) ([Helling and Casewell](#)) ([Cooper2014](#)) ([Madhusudhan and Seager](#)) ([Burrows, Sudarsky, and Lunine](#)) ([Marley2014](#)) ([Manjavacas](#)) ([B. Biller](#)) ([Faherty et al.](#)) ([Morley et al.](#))

1.2.1 Physics

1.2.2 Observational Properties

T-Type

L-Type

Y-Type

1.3 MOTIVATION

1.3.1 Current Status of Atmospheric Characterization

(Kreidberg)(B. A. Biller and Bonnefoy, “Exoplanet Atmosphere Measurements from Direct Imaging”) (Bozza, Mancini, and Sozzetti) (Danielski et al.) (Madhusudhan et al.)

Transmission Spectroscopy

(Lee, Fletcher, and P. G. Irwin) (MacDonald and Madhusudhan) (Madhusudhan et al.)

Emission Spectroscopy

1.3.2 JWST Studies

(Beichman et al., “Direct Imaging and Spectroscopy of Exoplanets with the James Webb Space Telescope”)

1.3.3 Biosignatures and Future Missions

1.4 THESIS OVERVIEW

2

MIRI: THE MID-INFRARED INSTRUMENT

MIRI is an imaging and spectroscopic instrument on board the James Webb Space Telescope (JWST). It will operate at a temperature of 6.7K to reduce instrumental backgrounds over its wavelength range of 4.8-28.8 μ m. Rieke et al., "The Mid-Infrared Instrument for the James Webb Space Telescope , I: Introduction " Kendrew2015

2.1 JWST

JWST is a 6.5m space based observatory that will be located 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.

2.2 MRS

Wells et al.

2.2.1 Integrated Field Spectroscopy

2.2.2 Optical Systems

Channels, bands, etc Chen et al., "Habitability and Spectroscopic Observability of Warm M-dwarf Exoplanets Evaluated with a 3D Chemistry-Climate Model"

2.2.3 Detectors

2.3 COORDINATES

2.4 OBSERVATIONS

2.4.1 Dithering

2.4.2 Readout Modes

2.4.3 Exposure time calculations

3

FRINGING EFFECTS IN MIRISIM

3.1 FRINGING

- FRINGING REQUIREMENTS FOR MIRI - context - sub percent residuals
- is this true and if so how much does it impact real spectral features? - What has been done so far - fitting, optical modelling - only for some channels - Might remove actual spectral features as well - justification for this work (especially re posn dependence) - need to reproduce plots from fringing white paper - explain why point sources are harder (angle => optical thickness => large phase shift) - [Lahuis2018](#)

3.2 MIRISIM

Consortium, “[MIRISim Documentation](#)” [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 2.2. 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

3.2.2 Data Products

3.2.3 Instrumental effects

3.2.4 Fringing

[Lahuis and Boogert VanderPlas](#) 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 2 and illustrated in Fig. 1.

Thin film interference occurs when light is coherently reflected at the boundary between two layers and interferes with the incident light. This

Figure 1

Table 2

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:

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

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

Figure 2

a more complete model along with additional calibration data to constrain the detector layer parameters.

FM Data

CV Data

3.2.5 Implementation

3.2.6 JWST Pipeline

Bushouse, Droettboom, and Greenfield Labiano-Ortega et al., “The MIRI Medium Resolution Spectrometer calibration pipeline”

Stage 1 Processing

Stage 2 Processing

Fringing correction

Carnall

Aperture Photometry

3.2.7 Cross-Correlation

I. Snellen et al. Simkin1974 Tonry1979 Petermann Bodis2007 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 as 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 Mollière et al., 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.

3.2.8 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.

3.3 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.

3.3.1 Effects of fringing on spectral extraction

4

ATMOSPHERIC RETRIVALS

Schlawin et al. Madhusudhan, “Atmospheric Retrieval of Exoplanets” Fisher et al. Oreshenko2019 Barman et al. Benneke and Seager Benneke and Seager Blanco-Cuaresma2018 Konopacky et al. Morley2018 Lupu et al. Gandhi and Madhusudhan Baudino et al. Line et al. Madhusudhan2018b P. G. Irwin et al. Robinson, Stapelfeldt, and Marley Waldmann et al. Waldmann et al. Line et al. “Uniform Atmospheric Retrieval Analysis of Ultracool Dwarfs. II. Properties of 11 T dwarfs” Zalesky et al.

4.1 INTRODUCTION

Batalha et al. Feng et al. Mollière et al.

4.2 ATMOSPHERIC MODELING

Behmard, Petigura, and Howard Guillot, “On the radiative equilibrium of irradiated planetary atmospheres” Chen et al., “Habitability and Spectroscopic Observability of Warm M-dwarf Exoplanets Evaluated with a 3D Chemistry-Climate Model” Mollière et al.

M. Zhang et al.

4.2.1 petitRadTrans

Mollière et al.

Radiative Transfer

Line-by-line

Correlated K

Goody et al. Lacis and Oinas

Clouds

Line and Parmentier Faherty et al. Morley et al.

4.3 BAYESIAN METHODS

Lavie et al.

4.3.1 MCMC

Foreman-Mackey et al. Speagle MacKay2003

4.3.2 Nested Sampling

Skilling Feroz2007 Feroz and Hobson Feroz2014 Feroz et al.

4.3.3 multineest

Hyperparameters

4.3.4 Prior choice

4.3.5 Bayesian Model Selection

4.4 TARGETS

4.4.1 Atmospheric Parameters

Madhusudhan, “C/O ratio as a dimension for characterizing exoplanetary atmospheres”Moses2012Garland and P. G. J. Irwin Bowler Fegley1994 Tokunaga

4.4.2 petitRadTrans

4.5 RESULTS

4.5.1 Posterior Distributions

5 | CONCLUSIONS

A | APPENDICES

A.1 PACKAGE REQUIREMENTS

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


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