A New Window on Exoplanet Atmospheres: Observations and Instrumentation in the Near-Infrared

A PhD Thesis Proposal for the University of Toronto's Graduate Program in Astronomy & Astrophysics

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Abstract

Over four thousand exoplanets have been discovered, but relatively little is known about their atmospheric properties and compositions. Characterizing exoplanet atmospheres is the most promising avenue through which we can learn more about exoplanets themselves, and high-resolution spectroscopy is currently one of the best methods by which this can be accomplished. In this thesis, I will use state-of-the-art ground-based spectrographs in the near-infrared wavelength regime to detect, characterize, and understand the atmospheres of exoplanets, with a particular focus on super-Earths and hot Jupiters, for which there are no Solar System analogues and which remain poorly understood. This work will provide important insights on theories of planet formation and evolution, and shed light on the dynamics and chemical compositions of planetary atmospheres.

1 Introduction

1.1 Open Questions in the Study of Exoplanets

Characterizing and understanding exoplanets, many of which are entirely unlike the planets in our own Solar System, are some of the major goals of modern astronomy. The physical and chemical processes that govern planet formation and evolution are complex and poorly understood, but undoubtedly play crucial roles in the determination of the bulk compositions, surface features, and atmospheric makeup of exoplanets. Studying and constraining these physical and chemical mechanisms will allow for a more detailed understanding of the more than 4000 exoplanets that have been discovered to date, shedding light on their formation and evolutionary histories and placing our own planet Earth in the greater context of planetary systems throughout the Galaxy.

Spectroscopic observations of exoplanet atmospheres are a key tool with which we can begin to tackle these goals and shed light on the diverse characteristics of exoplanets. In particular, optical and infrared transit and eclipse spectroscopy can yield insights into the compositions, dynamics, and thermal transport processes of exoplanet atmospheres, potentially answering such key questions as:

- are the gaseous envelopes of rocky planets acquired through impact accretion or outgassing, and are these retained or eroded over the planets' lifetimes?
- what determines the boundary between rocky terrestrial planets and gas-rich giants, and what kind of planets, if any, can be found in the intermediate regime between super-Earths and mini-Neptunes?
- what are the bulk compositions of different classes of exoplanets, and how does an exoplanet's interior composition reveal itself in the exoplanet's atmosphere?
- which exoplanets are likely to be habitable, and how can we work towards detecting and identifying habitable worlds?

1.2 Thesis Objectives

With these broad questions in mind, the aims of this thesis are twofold: first, to explore a diverse range of exoplanet atmospheres in the optical and near-infrared wavelength regimes; and second, to characterize and test novel instruments designed explicitly to observe exoplanet atmospheres.

While previous work in the field has focused on those exoplanets whose atmospheres are easiest to characterize — massive hot Jupiters on extremely short orbits with highly inflated radii — the study of exoplanet atmospheres is in the midst of a shift to studies of smaller, cooler, and more elusive targets. To truly begin to understand the diverse physical and chemical mechanisms that govern planet formation and evolution, we must focus our observational efforts on an equally diverse demographic of exoplanet targets from across a range of physical and orbital parameters, and for a diverse set of host stars. It will only be through creating such a census of diverse exoplanet atmospheres that we will be able to reveal new insights into the formation and evolution of exoplanets, as well as the physical and chemical mechanisms responsible for these processes.

1.2.1 Observations of Exoplanet Atmospheres

To this end, the first aim of my thesis will be to explore observations of exoplanet atmospheres in the optical and near-infrared regimes, with the goal of pushing current methods to both longer wavelengths and smaller exoplanets on wider orbits. While optical observations of hot Jupiter atmospheres have proven successful in the past, truly understanding the full diversity of exoplanet atmospheres will require extending our methods to terrestrial planets, as well as planets located at further distances from their host stars which are subject to less irradiation than the well-studied hot Jupiter population. This will also require extending our observations into the NIR, as (i) molecules such as water, methane, carbon dioxide, and carbon monoxide, which are expected to be found in exoplanet atmospheres, have the majority of their spectral features in the NIR; (ii) the blackbodies of M-dwarfs, which host a large fraction of known exoplanets and which provide the lowest contrast between planet and host star, peak in the NIR; and (iii) emission from the exoplanets themselves is likewise strongest in the NIR, allowing for complementary observations of exoplanets in both transmission and emission.

Although a complete catalogue of exoplanet atmospheres across all possible physical and orbital parameters is beyond the scope of this thesis, the work undertaken for this thesis will contribute to such a catalogue, as is already being assembled by the wider scientific community. Being able to draw informed conclusions about the physical and chemical mechanisms inherent to planet formation and evolution will require observations of a large number of exoplanets across a wide range of physical and orbital parameter space, and the work I plan to undertake on smaller, cooler exoplanets in the NIR regime will help contribute to this goal.

Of particular interest in the context of the goals of this thesis are two classes of exoplanets for which there exist no Solar System analogues: hot Jupiters, which are Jupiter-sized exoplanets at orbital periods of less than ten days, and which tend to have inflated radii; and super-Earths, which exist in the region between Earth- and Neptune-sized exoplanets, and which may allow us to investigate the transitional regime between rocky terrestrial exoplanets and gas-rich giants. Furthermore, observations of young planetary systems will help shed light on earlier stages of planet formation and evolution, which similarly cannot be directly observed in Solar System planets.

Hot Jupiters

A great deal of focus has been placed on observations of hot Jupiter atmospheres over the past several years. The fact that these exoplanets are hot, close in to their host stars, and large — often with inflated atmospheres extending through an appreciable percentage of their radii — means that atmospheric features are readily detectable. Yet despite this, key questions remain unanswered about this class of exoplanets: in particular, how exactly they form, and what mechanism results in a subset of them possessing highly-extended radii.

While the core nucleated accretion model for giant planet formation (i.e. the idea that giant planet formation is seeded by the growth of a solid core that eventually reaches a critical mass after which runaway nebular gas accretion may occur) posited by Pollack et al. (1996) is generally accepted within the field, several questions remain as to how exactly this mechanism proceeds. In particular, while the fact that gias giant envelopes are though to form via runaway accretion of nebular gas implies that the atmospheric compositions of gas giants should be relatively similar to those of their host stars, various processes may cause these compositions to differ. Solid cores that form in protoplanetary disks will likely sequester heavier elements, leaving the remaining gas deficient in these compared to the host star. Additionally, migration pathways of gas giants may lead to accretion from different parts of the disk. This is of particular interest in the case of hot Jupiters, which are likely to have formed *ex situ*[1] and migrate inwards by either gas disk migration (e.g. Goldreich & Tremaine 1980; Ida & Lin 2008, among others) or high-eccentricity tidal migration caused by e.g. planet-planet scattering (e.g. Rasio & Ford 1996; Chatterjee et al. 2008, among others) or secular interactions (e.g. models put forth by Petrovich 2015; Wu & Lithwick 2011, or Kozai-Lidov cycles e.g. Kozai 1962; Lidov 1962; Naoz 2016).

By studying the atmospheric compositions of hot Jupiters — and, in particular, how these compositions differ from those of their host stars — we can potentially determine the migration histories of these exoplanets, thus shedding further light on their formation mechanism. For example, Madhusudhan et al. (2014) show that while observations of eccentricities and spin-orbit misalignments of hot Jupiters have been unable to differentiate between disk and tide migration pathways, chemical depletions in hot Jupiter atmospheres may be able to constrain their migration mechanisms. Furthermore, measurements of the C/O ratio in hot Jupiter atmospheres can be obtained through observations of major carbon- and oxygen-bearing species such as CO, CH_4, and CO_2, among others (Madhusudhan 2012). These measurements can then be used to explore and constrain the different chemistries present in hot Jupiter atmospheres, investigate the effects of the C/O ratio on thermal inversions (Madhusudhan et al. 2011), and shed light on formation pathways (Öberg et al. 2011).

Although a significant amount of observational work has been done on the atmospheres of hot Jupiters, in Deibert et al. (2019a) (see also section 2.1) I investigated a smaller subset of the hot Jupiter population (referred to in Deibert et al. (2019a) as "warm Saturns") that had not previously been observed at high spectral resolutions, providing further insight on the atmospheric properties of this enigmatic class of exoplanets. Additional work on unique subsets of the hot Jupiter population, as well as observations across a wider range of wavelengths, will further help to elucidate this population's atmospheric properties.

Super-Earths

On the other hand, super-Earths are also of particular interest in the study of exoplanet atmospheres, and it is only with the advent of novel observational techniques and/or state-of-the-art high-resolution spectrographs that this population is now beginning to be observed in detail.

NASA's *Kepler* mission revealed super-Earths — e.g. planets with radii between $1-4R_\oplus$ with periods less than 100 days (Morbidelli & Raymond 2016) — to be ubiquitous in the Galaxy (e.g. Mayor et al. 2011; Petigura et al. 2013). However, such exoplanets were unexpected and challenged models of planetary formation. *In situ* formation of super-Earths would require the minimum-mass extrasolar nebula (i.e. the structure representing the least amount of initial material required to form an exoplanetary system, e.g. Kuchner 2004) to be extremely dense ($\sim 10-100$ times denser than that of the Solar System or those of other young stellar systems; e.g. Raymond et al. 2008; Chiang & Laughlin 2013; Schlichting 2014).

Furthermore, while the core masses of super-Earths are typically large enough for runaway gas accretion to occur, the atmospheres that these planets have accreted typically only represent a few percent of their total masses. Various theories have been proposed to explain this in the context of super-Earth formation;

[1]Note that *in situ* formation of hot Jupiters is largely considered unlikely: in the case of core accretion models, it has been shown that the available disk mass and opening of disk gaps likely preclude the formation of hot Jupiters (e.g. Rafikov 2006); and in the case of disk instability models, processes such as viscous heating and stellar irradiation cause the gas to cool too slowly for bound clumps to form (e.g. Matzner & Levin 2005; Rafikov 2005).

for example, Lee et al. (2014) and Lee & Chiang (2016) suggest that super-Earths may have formed at a later stage, in transition-like disks, once the gas disks had begun to clear. Alessi et al. (2017) investigate the possibility that super-Earths formed in short-lived (i.e. ≤ 2 Myr) disks in which photo-evaporation is completed while the planets are still slowly accreting gas.

While many theories have been proposed as to the formation pathways of super-Earths, however, the relative importance of processes such as gas accretion onto smaller cores, degassing of volatiles, and accretion of ice-rich material remain unconstrained. Additionally, the bulk density measurements that have been made for ~ 100 super-Earths (Marcy et al. 2014) have shown that many of these planets have low densities, and are perhaps more like "mini-Neptunes" than "super-Earths" in nature.

Observing the atmospheres of these exoplanets will allow for further constrains to be placed on their formation, evolution, and composition. In particular, this will allow us to answer such questions as what masses and insolations are required in order for a planet to retain a hydrogen-rich atmosphere; what roles outgassing, accretion, and atmospheric escape play in the formation of super-Earths or mini-Neptunes; and what are the bulk compositions of super-Earths, among others.

While previous work on the atmospheres of super-Earths has largely revealed featureless transmission spectra resulting from aerosol-dominated atmospheres (e.g. Kreidberg et al. 2014; Knutson et al. 2014), more recent observations have resulted in detections of molecular species in the atmospheres of Neptunes and super-Earths (e.g. Tsiaras et al. 2018; Benneke et al. 2019a; Tsiaras et al. 2019; Benneke et al. 2019b). In the future, observations of super-Earth atmospheres at high spectral resolutions, and across broader wavelength ranges, may be able to see through any obscuring aerosols and yield additional detections which will shed light on the questions outlined above.

In Deibert et al. (2019b), I analyzed the atmosphere of 55 Cancri e, a hot super-Earth orbiting a bright G8-dwarf that is particularly amenable to atmospheric characterization. This analysis made use of NIR data, which contains a larger number of molecular absorption features from species such as water and hydrogen cyanide than previous observations of this exoplanet with optical data (e.g. Esteves et al. 2017; Jindal et al. 2019). I investigated a potential detection of hydrogen cyanide in the atmosphere of 55 Cancri e by Tsiaras et al. (2016), as well as other species that have been suggested to be present by models (e.g. Hammond & Pierrehumbert 2017; Angelo & Hu 2017; Miguel 2019). This work provides insights on super-Earth atmospheres, and will help guide future observations of similar exoplanets.

Throughout the remainder of my thesis, I plan to carry out additional work on super-Earth atmospheres. These observations will help inform theories of planet formation and evolution, and will shed further light on the properties of clouds and aerosols present in exoplanet atmospheres. The details of this planned work are described in greater detail in section 4.

Young Planetary Systems

Of further interest in better understanding planetary formation and evolution are young planetary systems. Young exoplanets orbiting pre-main-sequence stars can shed light on physical processes integral to planet formation and evolution which remain poorly understood, as has been discussed above. For example, processes such as photo-evaporation (Owen & Wu 2013; Lopez & Fortney 2013), planetary impacts (Schlichting 2018), and core-envelope interactions (Ginzburg et al. 2018) — all of which result in net atmospheric loss — are likely contributors to the radius gap observed between super-Earths and mini-Neptunes (Fulton et al. 2017; Fulton & Petigura 2018, and see above section on super-Earths), but the relative importance of each mechanism is unknown. In the case of giant planets, observations of young systems may held shed light on how planets accrete gaseous envelopes, as well as whether or not these planets harbour rocky cores (Baraffe et al. 2003; Marley et al. 2007). Evolutionary processes such as orbital migration and radiative cooling likewise remain poorly understood, but are undoubtedly crucial aspects of the evolutionary histories of the exoplanet systems we observe today.

While several hot Jupiters have previously been reported around young stars, those systems are non-transiting and thus their atmospheres cannot easily be characterized with current instrumental capabilities. It is only within the last several months that the atmosphere of a young exoplanet has been probed (Flagg et al. 2019); however, future discoveries of young transiting exoplanets will offer far greater opportunities for detailed atmospheric characterization, and are therefore of great interest.

By observing the atmospheres of young exoplanets, we may be able to distinguish between formation via gravitational instability, which would produce hot planets, and formation via core accretion, which would produce comparatively cooler planets (Marley et al. 2007, see also Flagg et al. 2019)[2]. Additionally, while spectroscopy during transit or eclipse has revealed evaporating atmospheres in a few old (i.e. more evolved) exoplanets (e.g. Vidal-Madjar et al. 2004; Spake et al. 2018), similar detections of planets at a much younger age would provide valuable insights into an earlier stage of planetary evolution.

Historically, detecting planets around young stars has proven to be challenging. Young stars are typically more active than their main-sequence counterparts (e.g. Jeffers et al. 2013, 2014) which makes detection via radial velocity (RV) or transit signals difficult. Despite these challenges, several young planetary systems have been reported in the past several years (e.g. CI Tau b (Johns-Krull et al. 2016), V830 Tau b (Donati et al. 2016), and V1298 Tau b (David et al. 2019b), among others).

Flagg et al. (2019) demonstrated the efficacy of the Doppler cross-correlation technique traditionally used to study exoplanet atmospheres at high spectral resolution (Snellen et al. 2010; see also for e.g. Deibert et al. 2019a or section 2.1) in characterizing the atmosphere of a young exoplanet. They used high-resolution NIR observations to detect CO in the atmosphere of the young $\sim 10M_J$ exoplanet CI Tau b, both allowing them to constrain the formation mechanism of this exoplanet as well as yielding a directly determined, model-independent dynamical mass and an absolute magnitude estimate of the exoplanet in the K-band.

Such techniques could be similarly applied to other young planetary systems, providing further insight into planet formation mechanisms. Of interest would be observations of exoplanets across a range of ages, which would allow for various stages of planetary formation and evolution to be tracked and better constrained.

A side project that I plan to complete during my thesis invovles observing the atmosphere of the young exoplanet V1298 Tau c (David et al. 2019b). This project will provide an important insight into early stages of atmospheric evolution, and is described in greater detail in section 5.

1.2.2 Instrumentation

The second aim of this thesis will involve the characterization and testing of novel instruments designed to explore the diversity of exoplanet atmospheres. While a number of instruments have been highly successful in characterizing the atmospheres of various exoplanets, the majority of these were not specifically designed with this purpose in mind. To this end, I aim to make observations with a new instrument focused explicitly on exoplanet science: the MMT Adaptive Optics Exoplanet Characterization System, or MAPS. I also propose a side project that involves testing and characterizing a new photonics concept that will undertake atmospheric characterization methods optically, rather than after spectra have been obtained.

The MAPS project, which is currently underway and slated to be operational by the end of 2020, is a technical upgrade to the existing Arizona Infrared Echelle Imager and Spectrometer (ARIES) and MMT Adaptive Secondary Mirror (ASM)-based Adaptive Optics (AO) system. The new MAPS instrument will be composed of two high-resolution modes: MAPS65, which will have instantaneous spectral coverage from $1-5\mu$m with a resolution of $R = 65,000$; and MAPS120, which will deliver a resolution of $R = 120,000$ over a 1.5 μm subset of the full $1 - 5\mu$m band. The primary science goal of this upgrade will be characterizing the atmospheric composition of exoplanets, and by doing so it will serve as the definitive high-resolution spectroscopic follow-up counterpart to *Kepler*, TESS, and eventually JWST.

Observations at longer (i.e. $2.5 - 5\mu$m) wavelengths are of particular interest, as the current suite of high-resolution spectrographs amenable to observations of exoplanet atmospheres don't extend this far into the NIR.

[2]Note, however, that more recent theories suggest that core accretion may also be able to produce so-called "hot start" exoplanets, e.g. as in Berardo & Cumming (2017).

Furthermore, the AO system will correct for turbulence in the Earth's atmosphere and aim to deliver diffraction-limited observations, which can aid in suppressing light from the host star and reducing the contrast between the host star and the exoplanet. This will allow for observations of exoplanets on wider separations from their host stars, further expanding the range of exoplanet atmospheres that can be probed at high spectral resolution. Additionally, the use of an AO system results in less background noise both from background stars (due to the fact that a smaller slit can be used than a non-AO assisted spectrograph) as well as from the instrument itself, as less mirrors are used than in a traditional non-AO system. This is particularly important for long-wavelength IR observations, where components of the instrument typically radiate.

The new photonics instrument that I plan to work on during this thesis will carry out the Doppler cross-correlation technique (Snellen et al. 2010, see also section 2.1) — which has been widely successful in characterizing exoplanet atmospheres — optically, instead of after the spectra have been obtained from the telescope. Narrow-band notch filters will be designed to match template molecular features expected to be found in exoplanet atmospheres, allowing these features to be detected in the optical output of the device. The result will be a simpler, less costly, and potentially much more sensitive method of detecting molecular features in exoplanet atmospheres, and offers the possibility to push to much fainter targets than is currently possible with classical spectrographs.

Altogether, my work on these two new instruments will not only allow me to obtain unique, unprecedented observations of exoplanet atmospheres in the NIR, but will also allow me to gain valuable knowledge as to how astronomical instruments are prototyped, designed, tested, and ultimately validated.

1.3 Summary of Proposal

This thesis will be built upon two distinct yet complementary aims: first, observing and characterizing a diverse range of exoplanet atmospheres in the optical and near-infrared wavelength regimes, with a particular focus on exoplanet populations for which there are no Solar System analogues; and second, characterizing and testing novel near-infrared instruments designed explicitly to observe exoplanet atmospheres.

Nominally, this thesis will be comprised of three primary chapters and two additional chapters, which are described in greater detail in the following sections but will be summarized briefly here.

My first thesis chapter ("High-Resolution Transit Spectroscopy of Warm Saturns") has already been published in *The Astronomical Journal* (Deibert et al. 2019a, see also section 2.1). This chapter explored high-resolution optical observations of hot Jupiter atmospheres, and allowed me to familiarize myself with analysis techniques currently being employed while simultaneously carrying out my goal of characterizing exoplanets for which there are no Solar System analogues, i.e. the hot Jupiters HAT-P-12b and WASP-69b.

My second thesis chapter ("Near-Infrared Transit Spectroscopy of 55 Cancri e") is currently in preparation and will be ready for submission to *The Astronomical Journal* imminently. Towards my goal of observing super-Earth atmospheres in the near-infrared regime, I focused this chapter on an analysis of high-resolution NIR observations of the hot super-Earth 55 Cancri e, another exoplanet for which there is no Solar System analogue.

The remainder of my thesis will consist mainly of carrying out a survey of exoplanet atmospheres with the MMT Adaptive Optics Exoplanet Characterization System (MAPS). This will involve observing the atmospheres of a range of exoplanets, including both hot Jupiters and super-Earths, from $1 - 5\mu$m at high-resolution. A representative sample of planets will be chosen based on the latest discoveries from TESS and from the *One Hit Wonders* survey (see section 4.1.2).

This proposal also includes descriptions of an additional two/three thesis chapters that can be focused on in greater detail if there are technical delays in the MAPS project. The first project (which may consist of two chapters) involves constraining the ephemerides of a young planetary system, and subsequently carrying out follow-up ground-based observations at high spectral resolution to probe these young planets' atmospheres. The second supplementary project involves testing a novel photonics instrument designed to carry out the Doppler cross-correlation analysis technique for exoplanet atmospheres at the instrument, as opposed to in post.

2 Completed Work

2.1 High-Resolution Transit Spectroscopy of Warm Saturns

Towards my goal of observing a diverse range exoplanet atmospheres at high spectral resolution, my work in Deibert et al. (2019a) includes an analysis of high-resolution optical data from the High-Dispersion Spectrograph (HDS) at the Subaru Telescope and the GRACES instrument at the Canada-France-Hawaii Telescope. In this paper, we used the Doppler cross-correlation technique pioneered by Snellen et al. (2010) which has been successful in characterizing the atmospheres of large hot Jupiters with highly extended atmospheres (see Fig. 1). We pushed this technique to a new regime by observing transits of two so-called "warm Saturns": Saturn-mass exoplanets at several-day orbits. The two planets considered in this work (HAT-P-12b and WASP-69b) were ideal targets for extending this previously-proven method to a new class of targets, because both possess highly extended atmospheres and are thus well-suited to atmospheric characterization.

My analysis made use of model transmission spectra that had been calculated specifically for each planet to search for the absorption signatures of atomic sodium, atomic potassium, and water vapour. I was able to make a tentative (3.2σ) detection of sodium in the atmosphere of HAT-P-12b — a feature that had not been detected in previous analyses — as well as place stringent constraints on the atmospheres of both planets.

In addition to this, my work in Deibert et al. (2019a) involved an innovative analysis of the presence of clouds in the atmosphere of WASP-69b. Recent work in the field has shown clouds to be common, if not ubiquitous, in exoplanet atmospheres, and to result in flat, essentially featureless spectra (see for e.g. Kreidberg et al. 2014; Sing et al. 2016). In Deibert et al. (2019a) we found that water vapour, if present in the atmosphere of WASP-69b, would result in an extremely strong detection; however, if a cloud deck were located at increasingly higher heights in the atmosphere, this feature would become masked. We used this information to place a constraint on where a cloud deck could possibly exist in the atmosphere of WASP-69b. This result is shown in Fig. 2.

3 Current Work

3.1 Near-Infrared Transit Spectroscopy of 55 Cancri e

In addition to the work described in section 2.1, I have also made progress towards my goal of observing the atmospheres of super-Earths in the NIR. In Deibert et al. (2019b), we analyze high-resolution NIR spectra during transits of the hot super-Earth 55 Cancri e from both the Calar Alto high-Resolution search for M dwarfs with Exoearths with Near-infrared and optical Échelle Spectrographs (CARMENES; Quirrenbach et al. 2014) at the Calar Alto Astronomical Observatory and the SpectroPolarimètre Infra-Rouge (SPIRou; Artigau et al. 2014) at the Canada France Hawai'i Telescope (CFHT).

55 Cancri e (hereafter referred to as 55 Cnc e) is a nearby transiting exoplanet of $\sim 8M_\oplus$ and $\sim 2R_\oplus$ (Bourrier et al. 2018) that orbits its bright (V=5.95) G8 dwarf host star with a period of 17.7h. Its ultra-short orbital period results in an extremely hot equilibrium temperature in excess of 2000 K, potentially leading to exotic atmospheric properties.

While this exoplanet's bulk density indicates that it likely has an atmosphere (see for e.g. Gillon et al. 2012; Bourrier et al. 2018), several observational attempts have not been able to definitively detect its presence. In particular, Ehrenreich et al. (2012) found no evidence for an extended hydrogen atmosphere. Esteves et al. (2017) used high-resolution ground-based spectroscopy to derive limits of water absorption consistent with the exoplanet having either a hydrogen-poor atmosphere or a hydrogen-rich atmosphere that is significantly depleted in water vapour, and Jindal et al. (2019) further refined these limits. Demory et al. (2016) measured the photometric phase-curve of 55 Cnc e at 4.5 μm with the Spitzer Space Telescope, and found a large temperature contrast between the exoplanet's permanent day and night sides. They also found that the hottest longitude on the exoplanets dayside was shifted by 40° from the substellar point.

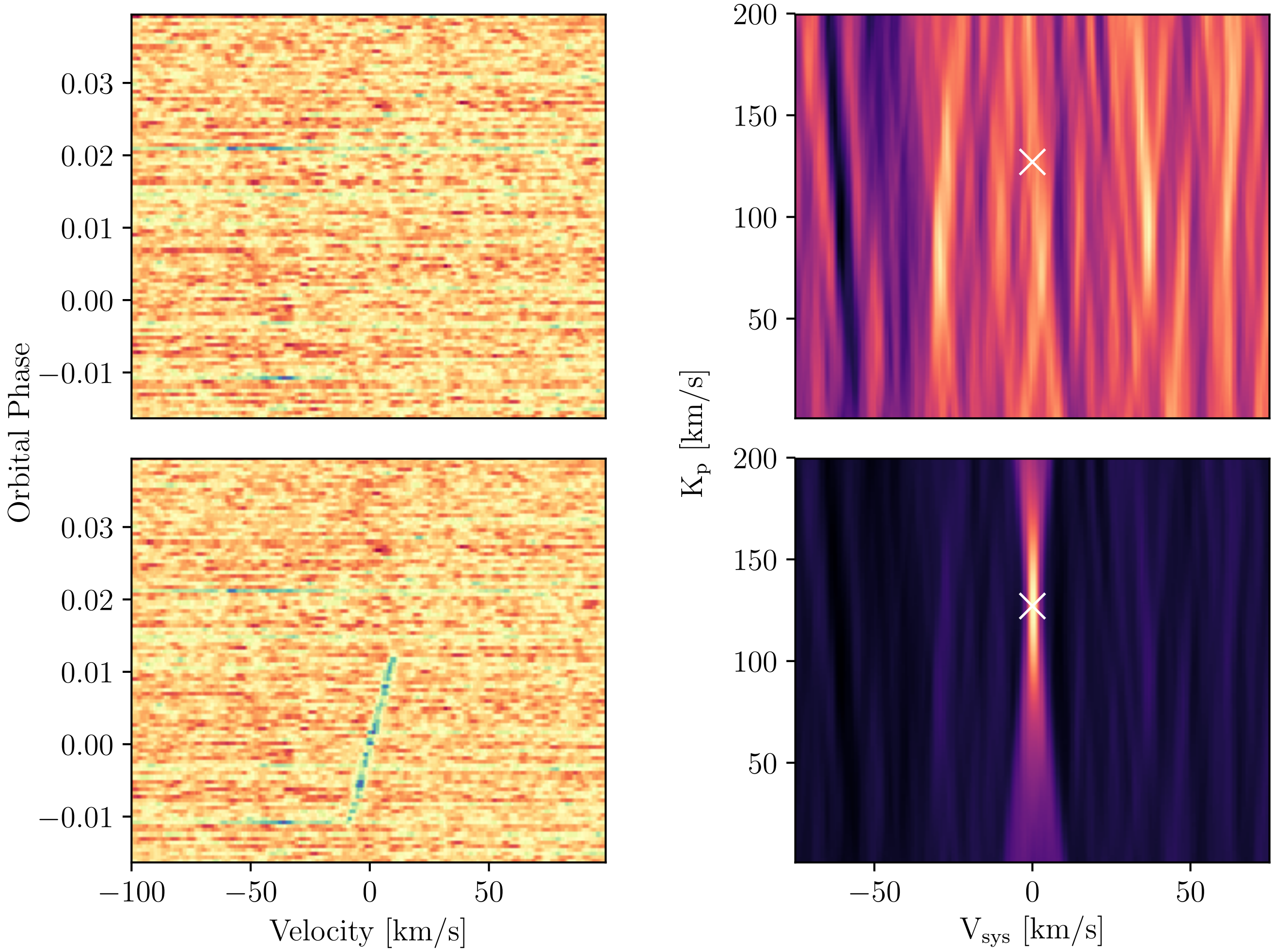

Figure 1: An example of the Doppler cross-correlation technique (Snellen et al. 2010). The left panels show correlation maps, and the right panels show correlations that have been phase-folded to the systemic velocity of the planet. These were obtained by cross-correlating thousands of water absorption lines across each spectrum of WASP-69b observations analyzed in Deibert et al. (2019a) with atmospheric models at Doppler shifts of between -100 km/s to +100 km/s. The colour represents the correlation strength. The top panels show the analysis process for the data, and the bottom panels show the same process repeated on the data with a water model injected. The signal from water is visible in the bottom-left panel as a diagonal line across the in-transit portion of the map, corresponding to roughly -0.01 to + 0.01 orbital phase. Likewise, the signal is visible at the Keplerian velocity of the exoplanet in the bottom-right panel, at the expected V_{sys} and K_p of the planet: 0 km/s and $\sim$ 127 km/s respectively. The cross indicates this position in both panels. The fact that no similar signal is visible in the original analysis of the data indicates that water is not present in the atmosphere of WASP-69b at the strength of the injected model. Figure from Deibert et al. (2019a).

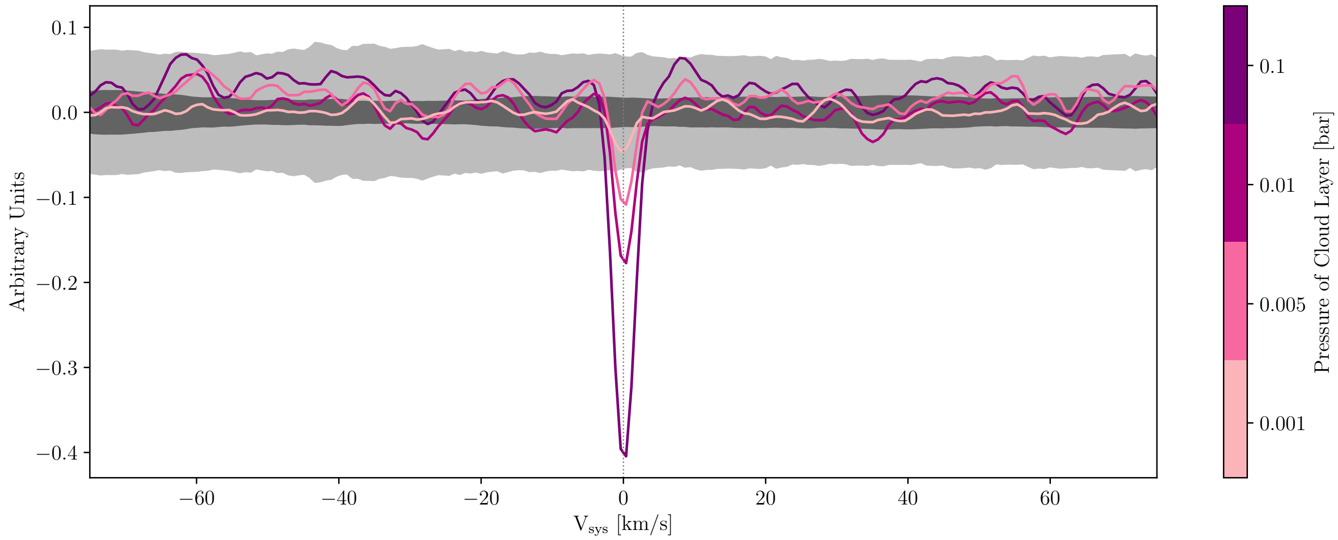

Figure 2: The figure shows the results of injecting model spectra with cloud layers at various pressures into our WASP-69 data. The pressures corresponding to each layer are indicated in the colour bar, while the dark- and light-grey contours represent 1- and 3-σ confidence levels respectively. This analysis was performed using models containing only water absorption features. We see that at a pressure of 1 mbar, the injected signal is no longer detectable in the data. Figure from Deibert et al. (2019a).

Using data from the Wide Field Camera 3 (WFC3) aboard the Hubble Space Telescope (HST), Tsiaras et al. (2016) reported the potential detection of an atmosphere around 55 Cnc e, and suggested that this atmosphere is likely hydrogen-rich, with a large scale height and high C/O ratio. They indicated that HCN is the most likely molecular candidate able to explain features detected at 1.42 and 1.54 μm. Together, these results suggest that the planet's atmosphere may well be carbon-rich. However, Tsiaras et al. (2016) cautioned that additional observations at high spectral resolution are needed to confirm these results.

Recent theoretical work by Miguel (2019) has additionally revealed that transmission spectra of 55 Cnc e should show strong absorption features of HCN and NH_3, but that these may weaken (while CO, CO_2, and H_2O features will increase in strength) if the presumed N/O ratio is decreased.

In Deibert et al. 2019b, I present high-resolution spectroscopy of 55 Cnc e in the near-infrared wavelength range, focusing on absorption features due to CO, CO_2, H_2O, HCN, and NH_3. My analysis takes advantage of two facets of my observations: first, the wide combined wavelength coverage of both Calar Alto/CARMENES and CFHT/SPIRou, which together span thousands of absorption features of both water and various carbon-rich molecules; and second, the extremely high resolutions of both instruments used, which allows me to individually resolve these thousands of absorption features.

While my preliminary analysis doesn't result in a detection of atmospheric absorption from any of the species listed above, I am able to place constraints on the presence of these species in 55 Cnc e's atmosphere, and therefore better constrain the composition of this super-Earth. Notably, I do not detect HCN in the atmosphere of 55 Cnc e, despite the fact that Tsiaras et al. (2016) tentatively claimed to have detected this molecule in a previous analysis. I am able to rule out a number of models consistent with the Tsiaras et al. (2016) analysis (see Fig. 3; however, I cannot rule out all models that are allowed by their observations and thus conclude that HCN may be present at a low volume mixing ratio in the exoplanet's atmosphere.

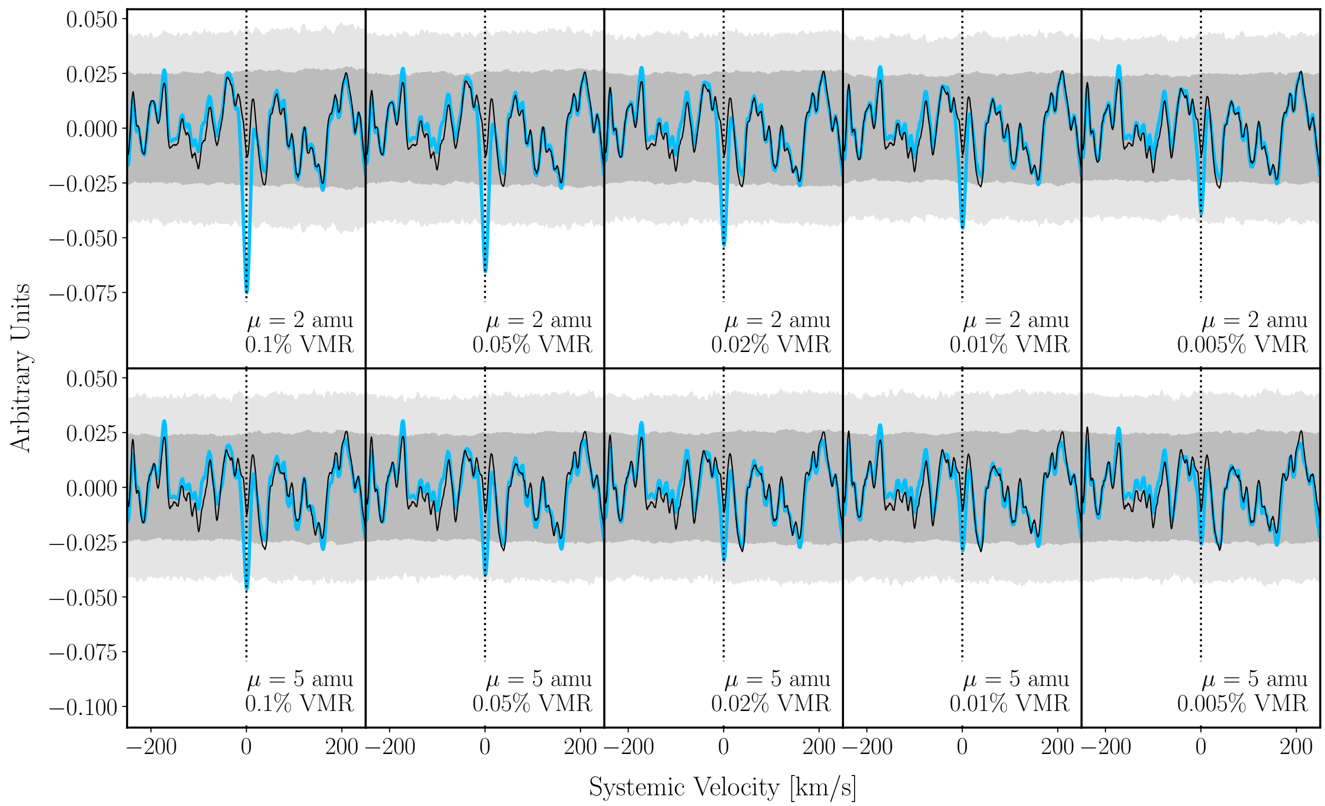

Figure 3: The figure shows the results of injecting model spectra containing HCN into the CARMENES and SPIRou datasets. The blue lines represent spectra with models injected, while the black lines represent the data alone. The dark- and light-grey contours correspond to 1- and 3-σ confidence levels, respectively. The mean molecular weight (μ) and volume mixing ratio (VMR) of each model is shown in the bottom right of each panel. Each model is consistent with the analysis of Tsiaras et al. (2016). While models with low mean molecular weights and high volume mixing ratios can be ruled out, these observations were not sufficient to rule out models with lower volume mixing ratios. Figure from Deibert et al. (2019b).

4 Future Work

While the work outlined in sections 2 and 3 highlights my extensive experience analyzing observations of exoplanet atmospheres, the next several years will be focused on the second goal of my thesis: namely, gaining experience observing exoplanet atmospheres with novel NIR instruments.

4.1 A Survey of Exoplanet Atmospheres from $1 - 5\mu$m

To achieve my goal of studying the atmospheres of exoplanets in the NIR, I plan to be involved in the initial observations taken with the MMT Adaptive Optics Exoplanet Characterization System (MAPS) at the University of Arizona's MMT Observatory. As mentioned in section 1.2.2, the MAPS project is an upgrade to the currently-existing Arizona Infrared Echelle Imager and Spectrometer (ARIES) and MMT Adaptive Secondary Mirror (ASM)-based Adaptive Optics (AO) system. The upgrade is currently underway, with an engineering deadline set for July of 2020 and preliminary observations slated to be taken shortly after this.

The observations I plan to take will consist of both a systematic, comparative study of Jovian atmospheres, as well as detailed observations of individual super-Earths and mini-Neptunes. By studying planets over a range of masses, temperatures, and orbital properties, I will be able to constrain the roles that these properties play in the formation, evolution, and regulation of atmospheres. Furthermore, I hope to be able to make one of the first definitive detections of molecular species in a super-Earth atmosphere at high spectral resolution.

Ideally, many of the planets I observe will be chosen from the sample discovered by the *One Hit Wonders* survey (Ziegler et al. 2019; see also section 4.1.2 below), the goal of which is to follow-up on single-transiting planets detected by TESS. In doing so, the survey will yield a population of long-period exoplanets around M-dwarfs that will fill a region of parameter space that has to date remained unexplored with high-resolution spectroscopy. As a co-investigator on the *One Hit Wonders* survey, I will have immediate knowledge of and access to these planets, and can quickly schedule follow-up observations of their atmospheres at high spectral resolution.

Although the exact details of these observations will be determined closer to the instrument's first light, they will nominally consist of at least two observations of each planet, and will include a range of both transmission and emission observations. For wavelengths longer than $\sim 1\mu$m, thermal emission typically dominates the planetary signal over e.g. reflected light (García Muñoz 2017). In the case of hot Jupiters, I plan to observe planets spanning a range of semi-major axes and temperatures, including both extremely hot, highly-irradiated hot Jupiters as well as cooler planets on longer (~ 10 day or slightly longer) orbits. This will allow me to shed light on the effects of planetary temperature and stellar irradiation on hot Jupiter atmospheres, and will additionally allow me to investigate a range of C/O ratios (Madhusudhan 2012).

4.1.1 The MMT Adaptive Optics Exoplanet Characterization System

MAPS will be composed of two unpredented high-resolution modes: MAPS65, which will provide instantaneous spectral coverage from $1-5\mu$m at a resolution of $R = 65,000$; and MAPS120, which will provide a resolution of $R = 120,000$ over a 1.5 μm subset of the full $1-5\mu$m band. MAPS will make use of AO-assisted high-resolution spectroscopy to allow for unprecedented observations of exoplanet atmospheres in the NIR. The power of high-resolution spectroscopy increases with the number of resolved spectral lines, and MAPS will take advantage of a combination of (1) a high spectral resolution, which will allow for a greater number of individual lines to be resolved; (2) a large (6.5 m) collecting area; and (3) a wide instantaneous spectral coverage, which will allow for simultaneous coverage of multiple molecular bandheads of a particular species. Overall, this will result in a maximal number of individual spectral lines that can be resolved in a measured spectrum. As the signal-to-noise of a line profile is boosted by the square-root of the number of detected spectral lines, these design considerations make MAPS ideal for detecting and characterizing exoplanet atmospheres, and will position MAPS as the definitive high-resolution follow-up counterpart to *Kepler*, TESS, and eventually JWST.

MAPS will also benefit from its unique infrared wave-front sensor. The use of AO with an IR wave-front sensor will allow for guiding on fainter, redder stars than would otherwise be possible, opening the door to observations of systems that can't be observed with other spectrographs. This is particularly important for observing M-dwarfs, which comprise a large fraction of both the TESS and *One Hit Wonders* samples.

The core science project of MAPS will focus on exoplanet characterization, with a goal of carrying out a comprehensive survey of exoplanet atmosphere abundance patterns, chemistry, and dynamics. The project will focus on a wide variety of exoplanets spanning a range of orbital semimajor axes, ages, and masses. In particular, since the high-resolution spectroscopic techniques that MAPS will make use of can be applied to both transiting and non-transiting systems, as well as close-in and spatially-resolved wide-orbit systems, this survey won't be limited to a particular class of exoplanets and will allow for comparative studies of atmospheres across a range of parameters.

The wavelength range of MAPS will allow for unique opportunities to constrain the C/O abundance of exoplanet atmospheres, which is important for theories of planet formation and evolution (see section 1.2.1). The major carbon- and oxygen-bearing species in the atmospheres of gas giants are water, methane, carbon monoxide, and carbon dioxide (e.g. Moses et al. 2013), and the relative abundances of these gases are dependent on the planet's temperature and C/O ratio. In cooler planets with C/O< 1, for example, methane dominates over carbon monoxide (Madhusudhan 2012). The wavelength coverage of MAPS

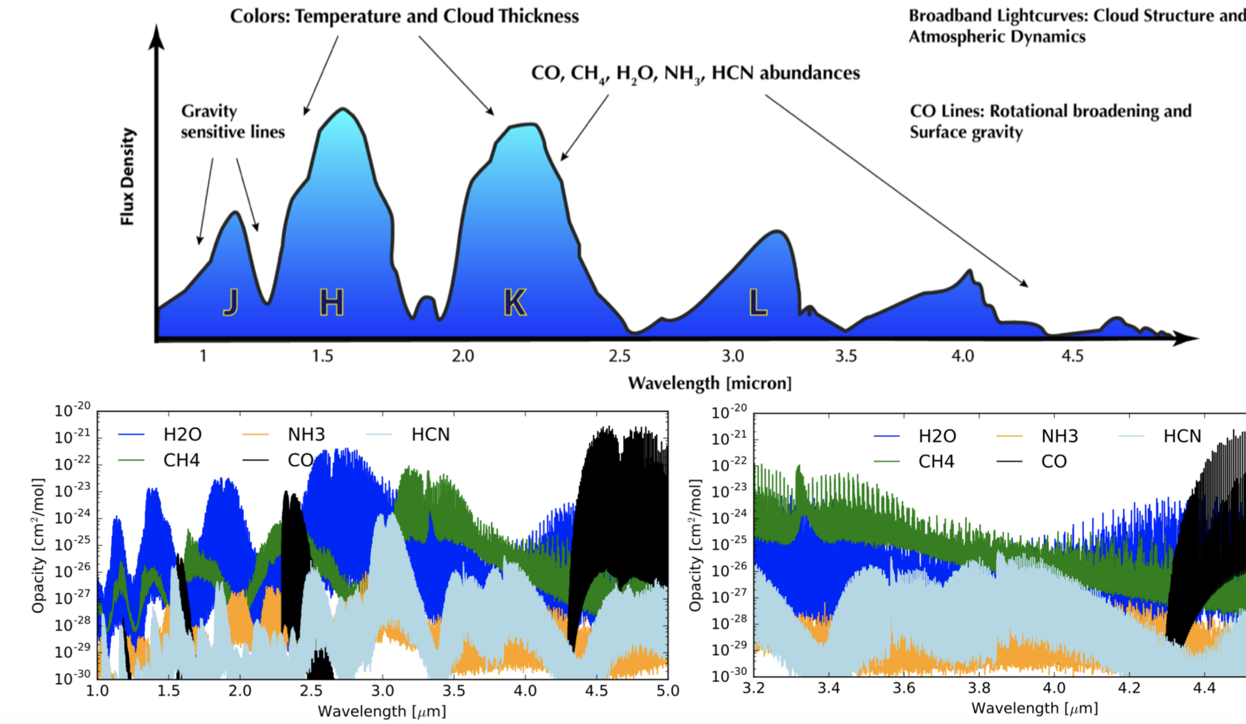

Figure 4: **Top**: Schematic of expected planetary features within the spectral range of MAPS120. **Bottom**: Abundance weighted cross-sections for prominent molecules in a $\sim$ 1000 K atmosphere plotted for the MAPS65 mode (**left**) and a subset of the red channel of the MAPS120 mode (**right**). Figure from the MAPS NSF Project Description.

($1 - 5\mu$m) is uniquely suited to probing these molecular species, as the majority of their spectral features are present in this wavelength range (see Fig. 4). The broad wavelength range of MAPS will vastly increase the number of lines that can be resolved, also allowing for the detection of less-abundant species such as HCN.

The core science program of MAPS is comprised of two complementary observing programs: first, a program that aims to characterize close-in exoplanets (both transiting and non-transiting); and second, a program that aims to characterize young, giant exoplanets (as well as brown dwarfs) on much wider orbits. The work I propose for this thesis will primarily overlap with that of the first observing program, which I briefly describe below. A discussion of the second observing program is available in the MAPS NSF Project Description.

The MAPS65 mode will provide both day- and night-side observations of close-in, non-transiting hot Jupiters and super-Earths, and will allow for studies of the atmospheric chemistry, structure, and circulation of these exoplanets.

From a sensitivity estimate of the expected SNR for thermal emission from an exoplanet's day-side, the MAPS Science Team has put together a sample of known planets that will be observable with MAPS65. These include both hot Jupiters and super-Earths, among other populations (e.g. cold gas giants). In particular, it is estimated that if 55 Cnc e has an atmosphere containing water, MAPS65 will be able to detect it in day-side emission at a SNR of 10 in one full night of observation.

Transiting planets will also be studied in transmission with MAPS120. These high-resolution observations will provide insight into the composition, cloud properties, atmospheric dynamics, and rotation of a wide range of exoplanets, including mini-Neptunes and super-Earths.

Finally, while a subset of targets have been selected from the currently-known exoplanets, a minimum

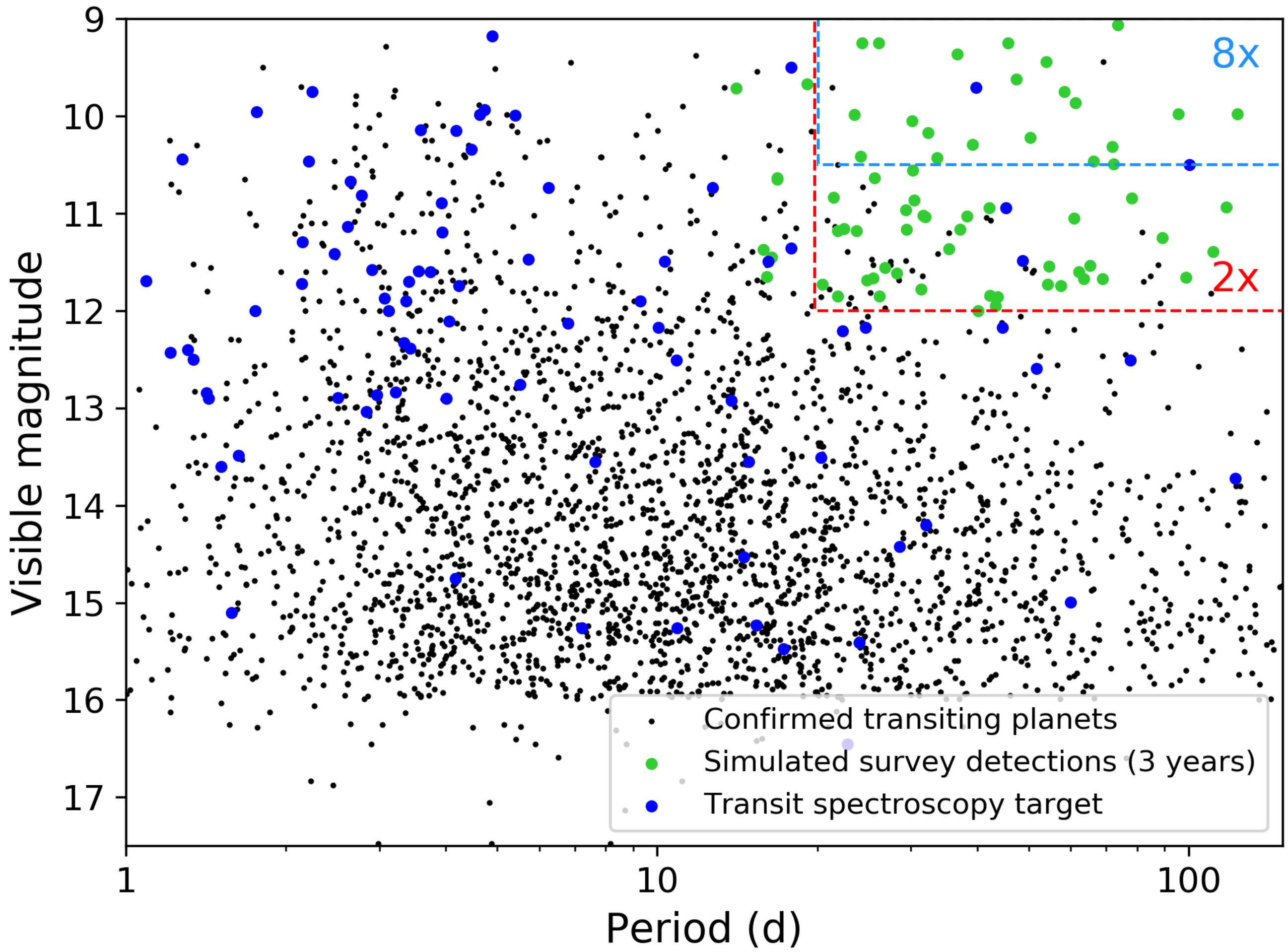

Figure 5: The period and visible magnitude of confirmed transiting exoplanets and the simulated survey detections from the *One Hit Wonders* survey over three years. *One Hit Wonders* can potentially vastly increase the number of long-period planets orbiting bright stars. The potential enrichment by the *One Hit Wonders* yield over currently known systems is shown in two bins. Planets which have had their atmospheres previously studied through transmission spectroscopy are also shown. Figure from Ziegler et al. (2019).

of 16 observing nights have been allocated to discoveries from TESS (and other facilities) that will be made in the coming years. I hope to focus my thesis work on these targets, as described in the following section. In total, at least 40 nights of MAPS time has been allocated to studying exoplanet atmospheres.

4.1.2 Unique Follow-Up Opportunities with the *One Hit Wonders* Survey

While the core science project of MAPS will include follow-up of select *Kepler*/*K2* targets that have been pre-selected, as well as upcoming TESS targets, my thesis work will focus on an additional unique follow-up opportunity: TESS planets confirmed by the *One Hit Wonders*[3] survey based out of the Dunlap Institute.

The goal of the *One Hit Wonders* survey will be to use an autonomous half-meter telescope to follow up on the thousands of single-transit events that will be detected (but not confirmed) by TESS (Sullivan et al. 2015; Villanueva et al. 2018). In doing so, this survey will yield a population of long-period exoplanets that will fill a region of parameter space that has to date been unexplored with high-resolution spectroscopy,

[3]https://onehitwonders.space/

as shown in Fig. 5. As a co-investigator on the survey, I will have immediate and unparalleled access to these targets, which can be explored at high spectral resolution with MAPS.

These targets will be of interest with regards to the science goals outlined in section 1.2.1. Due to the fact that they will be orbiting bright host stars, these single-transit planets will be ideal candidates for atmospheric characterization, and will represent an unexplored area of parameter space: exoplanets with orbits of $\sim$ 10s of days.

Some of these exoplanets, at orbits of $\sim 14 - 20$ days, will be interesting targets for characterization with the MAPS instrument. In particular, MAPS will allow for observations of thermal emission from the day-side of these planets. The fact that these targets will be cooler than the majority of exoplanets which have been observed at high spectral resolution is also of particular interest. Observations of hot Jupiter and super-Earth atmospheres have revealed clouds and condensate hazes — which act to obscure all but the upper atmosphere — to be commonplace (e.g. Marley et al. 2013), and although the exact mechanism behind these features remains poorly understood, there is evidence to suggest that they are caused by scattering from small particles (Dragomir et al. 2015) or equilibrium condensates such as water, salt, sulfides, or silicates (Wakeford et al. 2017). In planets with lower equilibrium temperatures, however, these particles will condense out and appear deeper in the atmosphere. This means that clouds/hazes will likely occur at lower levels than in previously-studied exoplanets, increasing the probability of detecting molecular species.

The *One Hit Wonders* survey is expected to confirm approximately 20 long-period planets in its first year (Ziegler et al. 2019), with approximately 2–4 of these expected to be located in their host stars' habitable zones. The telescope has recently been moved to its permanent location at the Deep Sky West observing site in New Mexico, and has begun operations as of September 2019, with several transits of various non-single-transiting TESS candidates already observed. As soon as TESS single-transit candidates are released for the Northern hemisphere, the survey will begin yielding targets.

The timeline of the *One Hit Wonders* survey complements that of MAPS. *One Hit Wonders* is nominally slated to be operational for a one-year survey, and is expected to confirm $\sim$ 20 single-transit TESS targets during this time (Ziegler et al. 2019). With the nominal one-year survey finishing in September 2020 and the MAPS engineering deadline occurring towards the end of summer 2020, MAPS will ideally be operational and ready for preliminary observations by the time many of the *One Hit Wonders* targets have been confirmed.

4.1.3 Selecting a Sample of Exoplanets to be Observed

Preliminary sensitivity calculations obtained for MAPS (see the MAPS NSF Project Description) indicate that water, as an example, should be detectable at a significance of $> 5\sigma$ with the MAPS65 observing mode, requiring one hour of observing time for host stars with a K-band magnitude of 9, and one night of observing time for host stars with a K-band magnitude as low as 13. These estimates were obtained by modelling the expected sky and telescope background, instrument throughput, detector read noise, host star noise, and number of spectral lines expected to be detectable.

In the case of hot Jupiters, it would be most interesting to observe slightly cooler, longer-period exoplanets than have been traditionally probed with high-resolution spectroscopy. My work in Deibert et al. (2019a) focused on this goal by observing two hot Jupiters at slightly longer ($\sim$ 3 day) orbital periods, thereby shedding light on the properties of cooler, less irradiated atmospheres. Observations of even cooler gas giants at high spectral resolution are difficult to obtain with current facilities, but the wide wavelength coverage and high spectral resolution of MAPS would lend itself well to such observations. Many of the planets expected to be detected with the *One Hit Wonders* survey will be longer-period Jovian planets around bright stars (Ziegler et al. 2019), and will thus fit these criteria well.

A sample set of hot Jupiters to be observed could then range from newly-discovered extremely hot Jupiters from TESS on orbital periods of $\sim$ 1 day, to cooler hot Jupiters from the *One Hit Wonders* survey on orbital periods as long as $\sim$ 10 days, or potentially longer. By probing the C/O ratio for such a range of planets, we could shed light on theories of hot Jupiter formation and migration. For example, planets forming exterior to the water ice line are predicted to have super-stellar C/O ratios due to the segregation of oxygen into ices (Öberg et al. 2011) under the core-accretion paradigm, whereas disk instability models predict a more homogeneous, stellar C/O ratio (Boss 1997). Additionally in the case of core-accretion, formation further out in the disk results in a higher C/O ratio (Eistrup et al. 2018). Measurements of C/O ratios across a range of orbital separations are therefore crucial in better understanding hot Jupiter formation scenarios.

Observations of major carbon- and oxygen-bearing species will be of particular interest in hot Jupiters on slightly wider separations, as fewer such observations exist. The prevalence of various species over others can be used to constrain the C/O ratio (Madhusudhan 2012) which, again, can help constrain formation theories. In this case, the redder wavelengths offered by MAPS will be of particular interest, as they will allow for more detailed observations of e.g. CO relative to other species (see Fig. 4).

Of interest would be observations in both transmission and emission, as these probe different parts of the atmosphere. While transmission spectroscopy probes lower pressures (i.e. higher altitudes) and therefore facilitates easier detections (especially in the presence of clouds, aerosols, or hazes), emission spectroscopy allows for an examination of the temperature structure of the atmosphere (Kreidberg 2018). For example, if a thermal inversion is present (i.e. the temperature increases with altitude), certain spectral features may be seen in emission rather than absorption.

The reddest wavelengths offered by MAPS will be of particular interest for emission spectroscopy. This is because the typical size of the emission feature can be predicted from (Kreidberg 2018):

$$\frac{F_p}{F_*} = \frac{B(\lambda, T_{\rm eq})}{B(\lambda, T_*)} \left(\frac{R_p}{R_*}\right)^2, \tag{1}$$

where F_p/F_* is the planet-to-star flux ratio, $B(\lambda, T)$ is the blackbody spectral radiance at a given temperature T, and R_p/R_* is the planet-to-star radius ratio. Since the planets are cooler than the stars they orbit, the planet-to-star flux ratio will naturally become larger at redder wavelengths.

At the same time, the easiest planets to observe in transmission will be those with large atmospheric scale heights, i.e. high temperatures and low surface gravities. The amplitude of spectral features seen in transmission is given by (Kreidberg 2018):

$$\delta_\lambda = \frac{(R_p + nH)^2}{R_*^2} - \left(\frac{R_p}{R_*}\right)^2 \sim 2\frac{nR_pH}{R_*^2}, \text{ where } H = \frac{K_b T_{\rm eq}}{\mu g} \tag{2}$$

Here, H is the atmospheric scale height, μ is the mean molecular weight, g is the surface gravity, and n is the number of scale heights crossed at wavelengths for high opacity.

Sample sensitivity calculations obtained for MAPS suggest that in the case of transmission spectroscopy, 1 hour of observations will be sufficient to make $\sim$ 5-σ detections for each planet for which the planet-to-star contrast ratio exceeds $\sim 3 \times 10^{-4}$ (at a K-band magnitude down to 9). However, as previous work has revealed cases where atmospheric detections cannot be produced in subsequent observations (e.g. Ridden-Harper et al. 2016; Herman et al. 2019), I will aim to observe at least two transits for each planet. Likewise, the MAPS sample sensitivity calculations suggest that only $\sim$ 1 hour of emission observations will be necessary to make $\sim$ 5-σ detections for similar targets; I will ideally obtain at least two such observations for each target in order to confirm any detections.

I therefore propose to observe a sample of 5–10 Jupiter-sized exoplanets with periods ranging from $\sim$ 1–20 days in order to characterize the C/O ratios of giant planets across a range of temperatures. In the case of planets on shorter orbital periods (e.g. $\lesssim$ 3 days), an estimate of the planet-to-star flux ratio obtained using Eq. 1 suggests that a single hour of observing time is needed to achieve detections of 5-σ for a 1 $R_{\rm Jupiter}$ exoplanet (based on the MAPS sensitivity estimates provided in the MAPS NSF Project Description). This is shown in Fig. 6 for a planet orbiting an M-dwarf, and 7 for a planet orbiting a solar-type star. In the case of planets on longer orbits, increasingly more observing time is needed, but with no more than one night of observations necessary. Larger and/or hotter (i.e. due to a greater amount

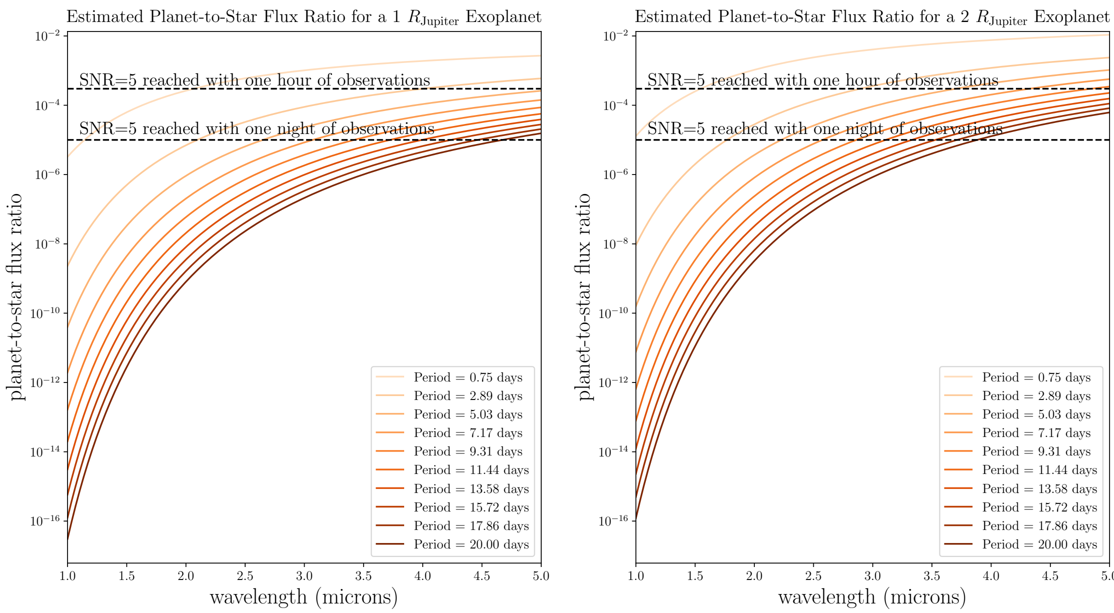

Figure 6: An estimate of the planet-to-star flux ratio for a $1R_{\mathrm{Jupiter}}$ exoplanet (left) and a $2R_{\mathrm{Jupiter}}$ exoplanet (right) orbiting a typical red dwarf star. The estimates of the planet-to-star flux ratio were obtained using Eq. 1, where T_{eq} of the planet was estimated by $T^4 = \frac{L_*}{16\pi d^2 \sigma_{\mathrm{SB}}}$. The dashed lines represent minimum flux ratios accessible for SNR detections of 5-σ with one hour and one night of observations, and are based off of estimates presented in the MAPS NSF Project Description. Note that these estimates also depend on the brightness of the star, and although including that information in these plots is beyond the scope of this simple estimate, it suffices to say that brighter stars generally require less observing time.

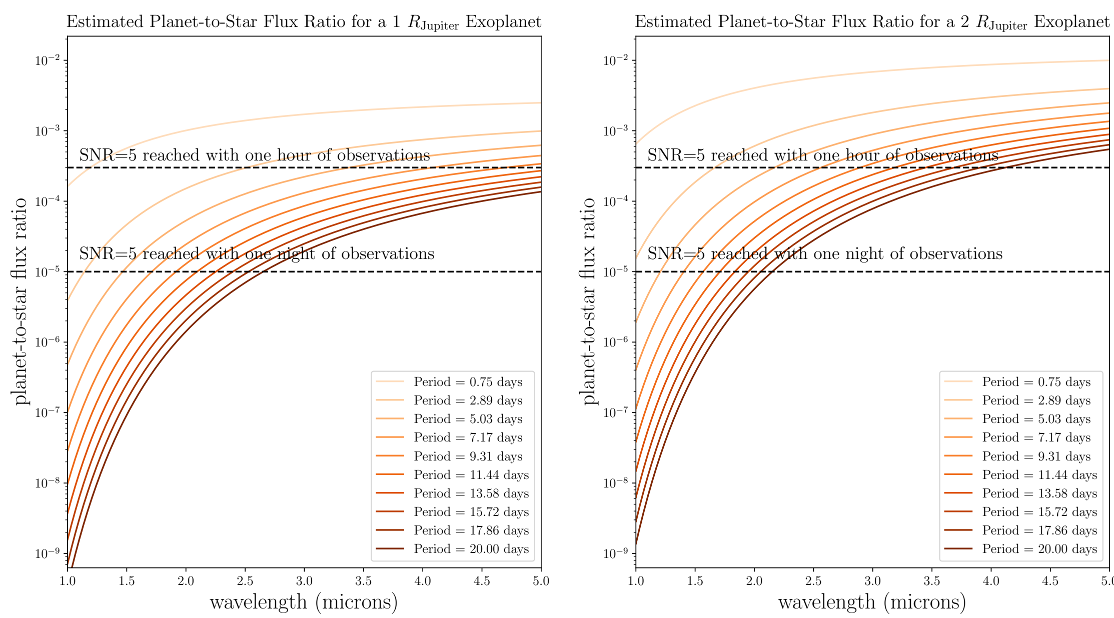

Figure 7: An estimate of the planet-to-star flux ratio for a $1R_{\mathrm{Jupiter}}$ exoplanet (left) and a $2R_{\mathrm{Jupiter}}$ exoplanet (right) orbiting a solar-type star. The figures are as described in Fig. 6.

of irradiation) planets would result in less required observing time for longer-period exoplanets (see Figs. 6 and 7), and would thus be of interest.

Overall, my proposed observations thus require ~ 4 hours (two hours of transmission and two hours of emission) for close-in planets and up to four nights for planets on longer orbits. However, I would selectively choose to observe only large planets with high temperatures at large orbital separations, in order to decrease the amount of observing time required for each target. This would then result in a more realistic estimate of slightly more than 4 hours for planets at larger orbital separations. Conservatively assuming that 8 hours are necessary for these longer-period targets, this would result in a total of several full nights of observations for a small sample of hot Jupiters ranging in orbital separation.

In the case of smaller planets (e.g. ranging in size from mini-Neptunes to super-Earths), I propose to observe a few carefully selected targets for which strong atmospheric features are expected to be present. To date, observations of super-Earths have largely revealed featureless spectra masked by clouds/hazes, except notably in the case of K12-18b (Tsiaras et al. 2019; Benneke et al. 2019b). No definitive detections of molecular features in super-Earth atmospheres at high spectral resolutions have previously been obtained. With the extra wavelength coverage provided by MAPS, however, I will be able to resolve significantly more spectral lines and greatly increase the strength of any planetary signal present. Furthermore, the molecular species that are expected to be present in super-Earths that have atmospheres produced via outgassing — CO, CO_2, H_2O, and HCN, among others (Deming & Seager 2017) — have a large number of atmospheric features in the redder end of the MAPS spectrum, which is currently inaccessible by other high-resolution spectrographs (see Fig. 4).

From the MAPS sensitivity estimates, a full night of observations is required to detect water at a SNR of 10 in emission from 55 Cnc e, if water exists in this planet's atmosphere. I thus propose to observe 4 full nights of emission spectra from 2 mini-Neptunes or super-Earths discovered by TESS. Ideally these will be planets on short orbits comparable to 55 Cancri e, and orbiting bright, nearby host stars.

Finally, I note that a significant portion of my thesis will be spent on carrying out sensitivity estimates in far greater detail than the illustrative estimates which have been presented in this proposal. Doing this will require calculating model spectra for the planets I plan to observe, and from these, determining an average line depth of atmospheric features. I will also need to make SNR estimates for the host stars, and use e.g. Eqs. 1 or 2 to determine the expected SNR of the planet. This can be accomplished using (Birkby 2018):

$$\mathrm{SNR_{planet}} = \frac{\mathrm{S_p}\sqrt{\mathrm{N_{lines}}}}{\sqrt{\mathrm{S_*} + \sigma_{\mathrm{bg}}^2 + \sigma_{\mathrm{read}}^2 + \sigma_{\mathrm{dark}}^2}} \approx \left(\frac{\mathrm{S_p}}{\mathrm{S_*}}\right) \mathrm{SNR_*}\sqrt{\mathrm{N_{lines}}} \tag{3}$$

Here, $\frac{\mathrm{S_p}}{\mathrm{S_*}}$ is the star-to-planet flux ratio or the amplitude of the expected transmission signal (e.g. Eqs. 1 and 2).

4.1.4 Comparable Facilities

With its wide spectral resolution and dedicated exoplanet science goals, the MAPS project will be unique among comparable near-infrared spectrometers. Nevertheless, it is valuable to place MAPS within the context of comparable existing or planned high-resolution NIR facilities, as shown in Fig. 8.

Fig. 8 uses an instrument capability metric defined by Crossfield (2016) which combines spectral resolution (R), collecting area (D^2), and simultaneous wavelength coverage ($\Delta\lambda/\lambda_{\mathrm{max}}$) in order to assess the efficacy of various spectrographs. While MAPS65 and MAPS120 have higher capabilities than similar instruments when measured with this metric, it is worthwhile as well to assess and compare MAPS and other instruments in terms of each of these parameters individually. These are summarized in Table 4.1.4.

Several of the existing and planned NIR spectrographs shown in Fig. 8 possess comparable or higher resolutions to MAPS65/MAPS120. Among these are CRIRES+/VLT, which will have a resolution of $R = 100,000$; IRD/Subaru, which has a resolution of $R = 70,000$, CARMENES/Calar Alto, which has a resolution of $R = 80,400$ in the NIR (see also section 3.1); SPIRou/CFHT, which has a resolution of

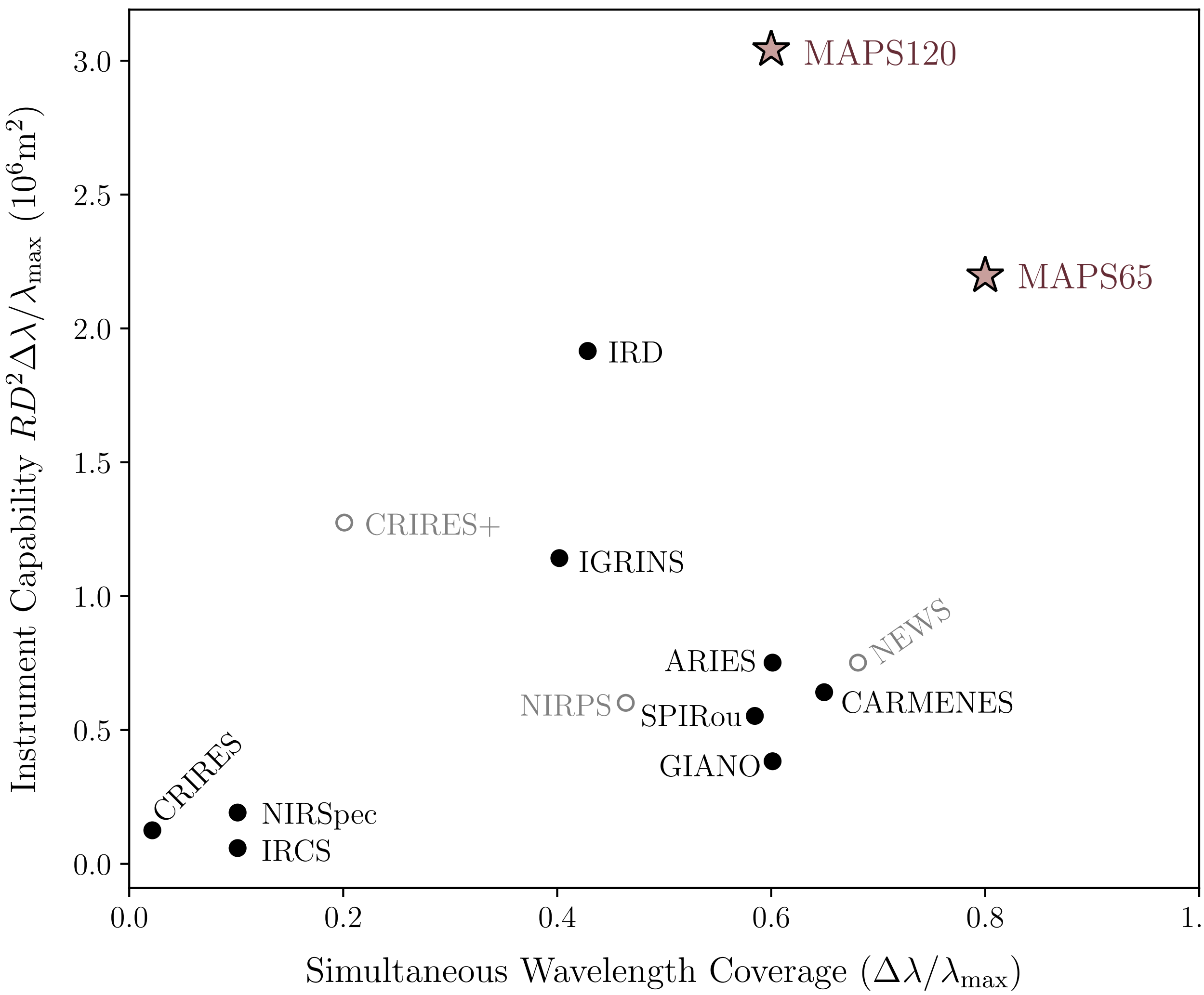

Figure 8: A comparison of existing (filled circles) and planned (unfilled circles) near-infrared spectrographs. The instrument capability metric shown on the y-axis combines the spectral resolution (R), collecting area (D^2), and simultaneous wavelength coverage ($\Delta\lambda/\lambda_{\mathrm{max}}$) in order to quantify the efficacy of each instrument at performing high-resolution spectroscopy (Crossfield 2016). The MAPS instrument provides a dramatic increase in instrument capability compared to all other existing and planned spectrographs in this wavelength regime. Figure adapted from the MAPS NSF Project Description.

$R = 75,000$ (see also section 3.1); and NIRPS/La Silla, which will have a resolution of $R = 100,000$. Obtaining a high spectral resolution is of particular importance in the study of exoplanet atmospheres, as it is only with high spectral resolutions that we are able to resolve individual lines from atmospheric molecular species, and an increase in the number of lines that can be resolved results in an increased detection strength.

At the same time, only a subset of the spectrographs mentioned above extend as far into the NIR as MAPS will. IRCS/Subaru has a wavelength coverage of 0.9-5.6 μm, while NIRSPEC/Keck has a wavelength coverage of 0.96-5.5 μm; however, the maximum spectral resolutions of these instruments (20,000 and 25,000 respectively) are not comparable to those of MAPS65/MAPS120, and are thus not ideally suited to high-resolution atmospheric characterization in the same way that MAPS is. In fact, of the spectrographs listed above with comparable resolutions to MAPS, only CRIRES+ has a comparable wavelength range, from 0.92–5.2 μm. These redder wavelengths are of great interest in the study of exoplanet atmospheres because

Instrument	Facility	Wavelength Range (μm)	Resolution
MAPS65	MMT	1–5	65,000
MAPS120	MMT	1–5	120,000
IRD	Subaru	0.970–1.75	70,000
IRCS	Subaru	0.9–5.6	20,000
CRIRES+	VLT	0.92–5.2	100,000
IGRINS	Various	1.45–2.5	45,000
CARMENES	Calar Alto	0.96–1.71	80,400
GIANO	TNG	0.95–2.45	50,000
SPIRou	CFHT	0.95–2.35	75,000
NIRSPEC	Keck	0.96–5.5	25,000
NIRPS	La Silla	0.95–1.8	100,000

Table 1: A summary of existing and planned high-resolution NIR spectrographs.

the exoplanets themselves emit at these wavelengths, and because a number of molecules that are expected to be present in exoplanet atmospheres have strong absorption features here (see for e.g. Fig. 4).

A main difference between the MAPS modes and CRIRES+ is the instantaneous spectral coverage of each. While CRIRES+ can achieve instantaneous coverage of the Y-band in a single exposure, additional exposures are needed at increasingly redder wavelengths, with 5 exposures needed for the M-band (Oliva et al. 2014). With MAPS, on the other hand, there is the option to achieve instantaneous spectral coverage from 1–5 μm at a reduced, but still high, spectral resolution (i.e. with MAPS65). Furthermore, MAPS120 offers instantaneous coverage over 1.5 μm at a resolution of 120,000, which is nearly an order of magnitude more than the instantaneous coverage offered by CRIRES+ from 0.96–1.13 μm at a resolution of 100,000. On the other hand, however, CRIRES+ will operate with a larger collecting area (the 8.2m diameter of the VLT) than MAPS (the 6.5m diameter of the MMT).

Overall, MAPS will likely serve as a Northern-hemisphere counterpart to CRIRES+ in the Southern hemisphere. Like MAPS, one of the main science goals of CRIRES+ will be atmospheric characterization of transiting exoplanets, focusing on molecular gases such as CO, NH_3, CH_4, etc. (Follert et al. 2014). MAPS will be ideal for my thesis work, however, because it will have access to Northern-hemisphere targets obtained through the *One Hit Wonders* survey, as described above.

4.1.5 Contingency Plan

As is the case with any observational-based thesis—especially one for which the instruments to be used are not currently operational—there is a risk of either not obtaining data due to unforeseen circumstances or not being able to access desired instruments before the nominal thesis end date. In the event that MAPS is not operational within the timeline of my thesis, there are a number of other avenues I can explore.

By submitting observing proposals to currently-operations instruments — for example, SPIRou, for which I have already successfully proposed and obtained observations (see section 3.1) — I can carry out additional projects similar to the work I did in Deibert et al. (2019a) and Deibert et al. (2019b). Despite not extending as far into the NIR as MAPS, SPIRou still extends further than the majority of currently-operational high-resolution NIR spectrographs (see Table 4.1.4), and thus offers interesting opportunities to probe exoplanet atmospheres in both transmission and emission.

Another possibility will be to carry out observations with the currently-planned NIRPS instrument at La Silla. My supervisor Ray Jayawardhana and committee member Diana Valencia are both members of the science team for this instrument, which may offer me unique opportunities for early observations. While NIRPS doesn't extend as far into the NIR as MAPS will (see Table 4.1.4), its high spectral resolution ($R = 100,000$) is ideal for atmospheric characterization.

Alternately, in the case that the *One Hit Wonders* survey doesn't yield as many planets as expected, or doesn't yield planets that are amenable to atmospheric characterization, I can instead observe newly-discovered planets from TESS, or previously-known planets from *Kepler* or other surveys, with MAPS. In this case, I would carry out a similar survey of planets across a range of orbital and planetary parameters, focusing on the unique impact each of these parameters has on the planets' atmospheric properties.

In the case that I am unable to obtain data through any of the means described above, there are ample unexplored archival observations available for various instruments that I can use to carry out additional projects. As an example of this, Nortmann et al. 2018 recently used archival CARMENES observations of the warm Saturn WASP-69b to detect an extended helium atmosphere.

Finally, I have proposed a number of side projects (see section 5) that support the main goals of my thesis, and which could become a larger focus of my dissertation in the event that MAPS is not operational before my nominal thesis end date.

5 Potential Side Projects

In addition to the main project of my thesis described in section 4, I also anticipate being able to complete several side projects that will further support my goal of characterizing exoplanet atmospheres in the NIR.

5.1 Characterizing Atmospheres in the Young Planetary System V1298 Tau

As mentioned previously, young planetary systems are of particular interest in better understanding planet formation and evolution. Observations of the atmospheres of young exoplanets would help shed light on an earlier stage of planet evolution, perhaps revealing which processes and physical mechanisms are most important in the formation and retention of planetary atmospheres.

It is clear that observations of a young, transiting exoplanet system are of interest in the study of exoplanets. The newly-discovered V1298 Tau multi-planet system (David et al. 2019b) offers the first opportunity to observe the atmosphere of a young, transiting exoplanet, and thus constitutes a truly compelling target for follow-up. The star is a young (20-30 Myr) solar analog that is known to host a Jupiter-sized exoplanet on a 24 day orbit, and has more recently been found to host three additional planets between the size of Neptune and Saturn on ~ 8, 12, and > 36 day orbits (David et al. 2019a). This system is likely a precursor to the compact multi-planet systems revealed to be common by NASA's *Kepler* mission (Lissauer et al. 2011), but the planets around V1298 Tau are much larger than those in typical *Kepler* multi-planet systems, suggesting that these planets are still undergoing contraction due to radiative cooling or photo-evaporative mass loss. Follow-up observations of the atmospheres of these planets can provide valuable insight on the evolutionary histories of their more evolved counterparts.

In order to schedule ground-based observations for follow-up atmospheric characterization, however, more stringent constraints on the ephemerides of the system are required. The transit times of each of the planets are currently only predictable to within several hours; in particular, the transit midpoints of the inner two planets have uncertainties of $\sim$ 3-4 hours (David et al. 2019a), due to the fact that the K2 data used to detect the planets originate from early 2015. Additionally, as the inner two planets are close to a 3:2 resonance, transit timing variations (TTVs) may exist with amplitudes of $\sim$ 0.5–5 hours. Furthermore, the transits are relatively long, between 4.7 and 7.5 hours in duration (David et al. 2019a), making it difficult to observe them in totality from the ground.

5.1.1 Constraining the Ephemerides of the V1298 Tau System

To constrain the ephemerides of this system and therefore be able to schedule follow-up observations from the ground, I recently submitted an observing proposal to NEOSSat (Laurin et al. 2008), a Canadian microsatellite designed to detect and track asteroids and satellites. NEOSSat has previously carried out proof-of-concept photometric observations of known exoplanet systems, and offers near-continuous monitoring which is ideal for obtaining additional transits of the V1298 Tau planets.

My proposal consisted of two-day windows around the expected transit times of each of the inner three planets in the system. This not only offers us the chance to observe the planets' transits and therefore better constrain their ephemerides, but also provides us with out-of-transit data with which we can model the variability of the host star.

This proposal was accepted by NEOSSat, and at least one observation consisting of transits of both planets c and d has been scheduled, with additional observations to be scheduled in the future.

Our goal with this work will be to measure transits of the inner three planets in the system, therefore better constraining their ephemerides. However, there is also a fourth planet in the system for which only one transit was observed with *Kepler*, meaning that only a lower limit of 36 days can be placed on its period. However, by assuming that this planet may be orbiting in either a 3:2 or 2:1 resonance with the inner plants (as is typical of compact *Kepler* systems), we were able to strategically schedule observations that would yield the highest probability of additionally detecting a transit of planet e. Observing a transit of planet e would allow for a more stringent upper limit to be placed on the planet's period, and aid in future follow-up photometric observations of the system.

Finally, our observations will also enable us to constrain the masses of the planets through observations of transit timing variations (TTVs) caused by gravitational interactions between the planets in this compact system. As a compact, multi-planet system with members close to a mean-motion resonance, V1298 Tau represents an ideal target for TTV observations (Agol & Fabrycky 2018). By observing multiple transits of the V1298 Tau planets and measuring the variation in time between consecutive orbits, we will be able to measure, for the first time, the masses of planets c and d. These measurements will also allow us to infer the densities, thus bulk compositions, of these planets, providing insights that can be used to guide future spectroscopic observations of their atmospheres.

5.1.2 Atmospheric Characterization of V1298 Tau c

Of the four currently-known planets in the V1298 Tau system, V1298 Tau c has the shortest orbital period, at roughly 8 days (David et al. 2019a). Its radius is approximately half that of Jupiter, and it takes approximately 4.5 hours to transit its host star.

Based on this, V1298 Tau c represents an extremely interesting target for follow-up spectroscopic observations at high spectral resolution. To date only one young exoplanet, CI Tau b, has had its atmosphere observed (Flagg et al. 2019); however, this was not a transiting planet and thus did not allow for the option of transmission spectroscopy. V1298 Tau c is similar in both radius and orbital period to CI Tau b; likewise, the host star V1298 Tau is comparable in magnitude to CI Tau. The analysis presented in Flagg et al. (2019) can thus serve as a proof-of-concept of the feasibility of observing the atmosphere of V1298 Tau c. While Flagg et al. (2019) used moderate-resolution observations spanning $1.45 - 2.5\mu$m, however, I aim to observe V1298 Tau c at a resolution of 65,000 in the full MAPS wavelength range ($1 - 5\mu$m) in order to better constrain the planet's C/O ratio and resolve a larger number of individual lines in its spectrum. This will allow me to investigate the planet's formation mechanism in a similar manner to the analysis presented in Flagg et al. (2019), and will provide one of the first observations of a young exoplanet's atmosphere in transmission.

5.2 A Photonics Solution for the Doppler Cross-Correlation Method

The final project I propose to work on for my thesis involves exploratory work into a novel instrument concept that will make use of a photonics solution to carry out the Doppler cross-correlation technique (Snellen et al. 2010) optically, rather than after spectra have been obtained. The instrument itself will be made of narrow-band notch filters that will be designed explicitly to match template molecular features expected to be found in exoplanet atmospheres. The filters will be modulated in wavelength to perform the cross-correlation either through localized heating or through stretching. The cross-correlation will therefore be encoded in the optical output of the device, resulting in a simpler and less costly method of detecting molecular features in exoplanet atmospheres. Furthermore, since the light is not dispersed within this device, we may potentially be able to greatly increase the sensitivity for detection of exoplanet atmospheres. The device has already been designed and is currently being prototyped.

My role in this project will be to help determine what we can expect to achieve with such a device, and potentially test initial observations taken in this way.

Towards this goal, I was recently involved in an OPTICON Proposal to observe Venus, Mars, and Jupiter with GIARPS (GIANO + HARPS) at the TNG in semester 2020A. If successful, these observations will be taken at high spectral resolution in the wavelength range of the instrument prototype, and will be used to carry out predictive simulations of the prototype's behaviour. As these data will directly include effects such as telluric absorption and radial velocity changes of the planets between epochs, they will be useful for predicting and simulating the expected behaviour of this new instrument concept.

6 Proposed Timeline

A proposed timeline towards completing this thesis by the end of August 2022 is presented in Fig. 9. Major projects are indicated by coloured bars, and various project milestones indicated by stars. Today's date is also marked.

With the publication of one thesis chapter already complete (Deibert et al. 2019a; see also section 2) and an additional chapter nearing completion/subsequent publication (Deibert et al. 2019b; see also section 3) my dissertation is well on its way to being completed by my nominal program completion date. The projects outlined in section 4 will comprise the remaining chapters of my dissertation.

7 Conclusion

The goal of the thesis presented in this proposal will be to characterize a diversity of exoplanet atmospheres at high-spectral resolution in the near-infrared regime. This will be accomplished using both existing instruments (e.g. CARMENES and SPIRou) and the soon-to-be-operational MAPS instrument at the MMT observatory. The result will be a large-scale survey of exoplanet atmospheres across an unprecedented area of parameter space, with a particular focus on populations of exoplanets for which we lack a Solar System analogue — e.g. hot Jupiters, super-Earths, and young exoplanet systems. This work will provide important insights on theories of planet formation and evolution, and shed light on the dynamics and chemical composition of planetary atmospheres.

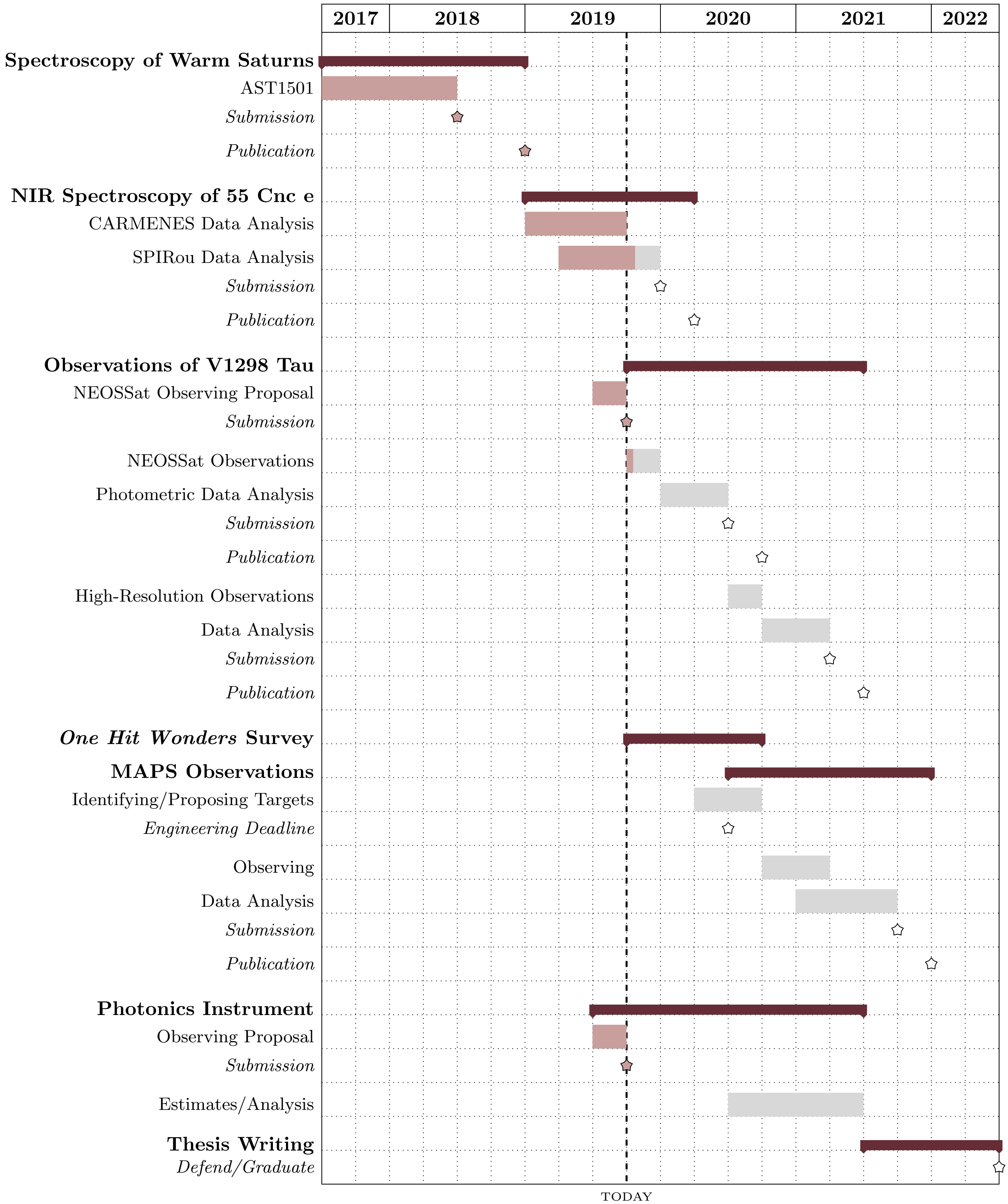

Figure 9: A visualization of the the timeline for this thesis, with specific goals based on the work described above. The shaded regions correspond to the amount of each goal that has been completed to date, and the stars correspond to various progress milestones, with coloured stars corresponding to completed milestones.

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