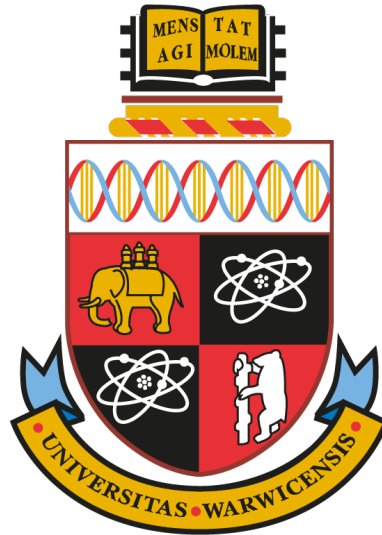




# Planet Detection in the Era of Extreme Precision

by

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*“You are a lot less cool now than when you started this PhD”*

JAMIE WILLIAMS, 2026

# Declarations

I declare that this thesis is my own work except where explicitly stated otherwise.  
This thesis has not been submitted to this or any other academic institution for any other degree or qualification.

# Abstract

The detection and characterisation of exoplanets increasingly demands precision at the level where variability on the surface of the host star becomes a dominant source of noise. This thesis addresses both the discovery of new exoplanets and the fundamental limitations imposed by stellar surface convection on high-precision spectroscopic measurements.

In the first part of this work, I present the discovery and characterisation of a transiting exoplanet located within the Neptune desert, a sparsely populated region of parameter space defined by a deficit of intermediate-mass planets at short orbital periods. The planet was identified using photometric observations from the Transiting Exoplanet Survey Satellite (TESS) and confirmed through ground-based follow-up, including high-resolution spectroscopy with HARPS. A joint analysis of the photometric and radial velocity data was performed using a Bayesian framework, enabling precise constraints on the planetary mass, radius, and orbital parameters. The resulting system provides a valuable contribution to the population of planets within the Neptune desert, offering insight into the physical processes governing atmospheric loss and planetary migration.

The second part of this thesis focuses on the impact of stellar granulation on spectroscopic observables, a key limiting factor in the detection of low-mass exoplanets. I develop a novel parameterisation framework to isolate and model granulation-driven variability using three-dimensional hydrodynamic simulations of the solar photosphere. Spectral line profiles are synthesised using radiative transfer, and subsequently decomposed into physically motivated surface components. This enables the statistical reconstruction of disk-resolved line profiles across the stellar surface without requiring the full simulation data.

Building on this framework, I introduce a method for generating time-varying, disk-integrated stellar absorption line profiles that isolate granulation as the sole source of variability. This approach produces an effectively unlimited set of physically consistent synthetic observations, allowing a detailed investigation of line-by-line granulation-induced variability. I demonstrate that granulation-induced radial velocity scatter varies between spectral lines, with amplitudes of order  $0.16\text{--}0.21\text{ m s}^{-1}$  under idealised conditions. Furthermore, I explore correlations between line-shape diagnostics and convective velocity shifts, highlighting the potential for mitigating granulation signals in high-precision radial velocity measurements.



# Abbreviations and quantities

## Abbreviations

**CCF** Cross Correlation Function

**CLV** Centre-to-Limb Variations

**EPRV** Extreme Precision Radial Velocity

**ESPRESSO** Echelle SPectrograph for Rocky Exoplanets and Stable Spectroscopic Observations

**EW** Equivalent Width

**ExoFOP** Exoplanet Follow-up Observing Program

**FAP** False Alarm Probability

**FFI** Full Frame Image

**FPP** False Positive Probability

**FWHM** Full-Width Half Maximum

**GP** Gaussian Process

**GRASS** GRanulation And Spectrum Simulator

**GT** Granular Top

**HARPS** High Accuracy Radial velocity Planet Searcher

**HD** Hydrodynamic

**HMC** Hamiltonian Monte Carlo

**IgL** Intergranular Lane

**LCOGT** Las Cumbres Observatory Global Telescope

**LTE** Local Thermodynamic Equilibrium

**MCMC** Markov Chain Monte Carlo

**MHD** Magneto-hydrodynamic

**MURaM** The Max-Planck-Institute for Aeronomy/ University of Chicago Radiation Magneto-hydrodynamics code

**NUTS** No-U-Turn Sampler

**OGR** Outer Granular Region

**p-mode** Pressure mode

**PDC(SAP)** Pre-search Data Conditioning (Simple Aperture Photometry)

**PLATO** PLAnetary Transits and Oscillations of stars

**RM** Rossiter-McLaughlin effect

**rms** Root Mean Square Error

**RT** Radiative Transfer

**RV** Radial Velocity

**SAP** Simple Aperture Photometry

**SNR** Signal-to-Noise Ratio

**SPOC** Science Processing Operations Centre

**TBJD** TESS Barycentric Julian Date

**TESS** Transiting Exoplanet Survey Satellite

**TOI** TESS Object of Interest

**TPF** Target Pixel File

**TSM** Transmission Spectroscopy Metric

**TTV** Transit Timing Variation

## Quantities

**$R_{\oplus}$**  Earth radius: 6371 km

**$M_{\oplus}$**  Earth mass:  $5.972 \times 10^{24}$  kg

**$R_{\odot}$**  Solar radius: 695,000 km

**$M_{\odot}$**  Solar mass:  $1.988 \times 10^{30}$  kg

**AU** Astronomical unit:  $1.496 \times 10^8$  km

**G** Gravitational constant:  $6.674 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$

**k** Boltzmann constant:  $1.381 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$

**$\hbar$**  Reduced Planck constant:  $1.054 \times 10^{-34} \text{ m}^2 \text{ kg s}^{-1}$

**c** Speed of light:  $2.998 \times 10^8 \text{ m s}^{-1}$

## Part I

# Exoplanet detection and characterisation

# Chapter 1

## An Introduction to Exoplanets

*“The universe is a pretty big place. If it’s just us, seems like an awful waste of space.”*

---

*Carl Sagan, Contact*

### 1.1 In Pursuit of Other Worlds

In 1584, the Italian philosopher Giordano Bruno wrote of “innumerable suns” surrounded by “innumerable Earths,” each perhaps hosting life of its own [Dick, 1980]. His vision, radical for its time, placed humanity within an infinite cosmos populated by other worlds. Although Bruno spoke from intuition rather than evidence, the idea that the Universe might contain countless planetary systems persisted for centuries, inspiring both speculation and scientific inquiry. Today, more than four centuries later, astronomy has finally attained the tools needed to test the possibility he could only imagine: that worlds beyond our own not only exist, but may be common.

For most of human history, the question of other worlds remained firmly in the realm of philosophy. It was only in the late 20th century that technology finally caught up with imagination. The first detections of exoplanets in the 1990s, most famously the discovery by Mayor & Queloz [1995] of a Jupiter-mass companion orbiting the Sun-like star 51 Pegasi, transformed Bruno’s conjecture into an empirical reality. In the decades since, advances in Doppler spectroscopy, transit photometry, and direct imaging have revealed that planets are not rare anomalies, but common outcomes of star formation. As of December 10<sup>th</sup> 2025, exoplanet.eu [Schneider et al., 2011] lists 7891 known exoplanets that span a vast range of sizes, compositions, and orbital

architectures. What was once a speculative philosophical idea has become a mature and rapidly expanding empirical discipline.

The remaining question therefore lies not in whether other worlds exist, but in how they compare to our own. One longstanding motivation for this comparison is the possibility of life beyond Earth. From early philosophical musings to modern interdisciplinary research, the possibility that life might have arisen beyond Earth has shaped the trajectory of planetary science, astrobiology, and observational astronomy. Assessing habitability requires knowledge of planetary masses, radii, temperatures, and atmospheres, as well as the influence of their host stars, all quantities that can be constrained only through careful observations.

A second important motivation is the desire to understand our own Solar System in its broader cosmic context. By studying the architectures, compositions, and dynamical histories of other planetary systems, we gain insight into whether the Solar System represents a typical outcome of planet formation or a more unusual configuration. Comparisons across systems help inform models of disc evolution, migration, and atmospheric development, and provide a framework for interpreting the origins and characteristics of our own planets.

Both motivations rely on a robust empirical foundation. Each method used to detect exoplanets offers access to different orbital periods, masses, radii, equilibrium temperatures, all the while introducing its own selection effects and uncertainties. Together, these techniques define the parameter space within which we can study planetary systems.

The next subsection reviews the principal detection methods, outlining the information each provides and the constraints they impose on our understanding of exoplanets and their hosts.

## **1.2 Exoplanet Detection methods**

### **1.2.1 The Transit Method**

The transit method detects exoplanets by measuring the periodic diminution of a star’s flux when a planet passes (“transits”) in front of the stellar disc as seen from

Earth. The fractional loss of light (the *transit depth*) at mid-transit is, to first order,

$$\delta \approx \left( \frac{R_p}{R_\star} \right)^2, \quad (1.1)$$

where  $R_p$  is the planet radius and  $R_\star$  the stellar radius; this relation makes transit photometry a direct probe of planetary size [Winn, 2010].

Determining the absolute planetary radius requires an independent estimate of the stellar radius. In practice, this is obtained through stellar characterisation using spectroscopic and photometric observations, typically by fitting inferred stellar parameters (e.g. effective temperature, surface gravity, and metallicity) to stellar evolution models [Torres et al., 2010]. For well-characterised nearby stars, additional constraints such as parallaxes (e.g. from *Gaia*) and spectral energy distribution fitting can further refine radius estimates [Berger et al., 2020]. A detailed treatment of stellar parameter inference is beyond the scope of this work; however, it is important to note that uncertainties in  $R_\star$  directly propagate into the derived planetary radius.

From an observed sequence of transits one can directly measure the orbital period  $P$  and, combined with the transit duration and shape, place constraints on the scaled semi-major axis  $a/R_\star$ , the orbital inclination  $i$ , and the impact parameter  $b$  (and thus the geometry of the system). Under favourable conditions (good signal-to-noise and knowledge of stellar parameters) there is a unique solution for  $R_p/R_\star$ ,  $a/R_\star$ , and  $b$  from a high-quality transit light curve [Seager & Mallén-Ornelas, 2003]. The detailed morphology of the transit is set by the four contact points ( $t_I$ ,  $t_{II}$ ,  $t_{III}$  and  $t_{IV}$ ), which mark the beginning and end of ingress and egress. First and fourth contact correspond to the moments when the planetary disc first and last touches the stellar limb, while second and third contact define the start and end of full transit. The ingress and egress durations (the time between first–second and third–fourth contact, often denoted  $\tau$ ) encode additional geometric information, being particularly sensitive to the ratio  $R_p/R_\star$  and the impact parameter, and therefore help break degeneracies in light-curve fitting [Winn, 2010]. A schematic illustrating these quantities is shown in Figure 1.1.

The transit duration  $T$  for a circular orbit may be approximated by

$$T \approx \frac{P}{\pi} \arcsin \left( \frac{\sqrt{(R_p + R_\star)^2 - b^2}}{a \sin i} \right) \quad (1.2)$$

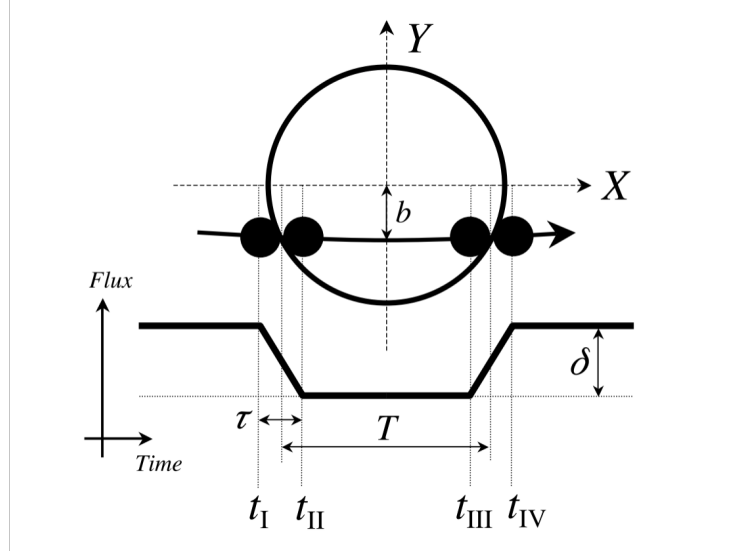


Figure 1.1: **Figure from Winn [2010]**. Schematic of a planetary transit, showing an idealised light curve with labelled parameters defined within the text of this section.

and in the small-planet limit this simplifies to standard expressions relating  $T$ ,  $P$ ,  $a/R_\star$  and  $b$  used in light-curve fitting. These formulae (and their generalisations to eccentric orbits) are standard in the transit literature [Seager & Mallén-Ornelas, 2003].

#### What transits measure:

- **Planet radius.** From  $\delta$  and an estimate of  $R_\star$  (e.g: Charbonneau et al. [2000]).
- **Orbital period.** From the cadence of repeated transits.
- **Orbital geometry.** Impact parameter and orbital inclination from transit shape and duration (e.g: Charbonneau et al. [2000]).
- **Atmospheric signatures.** Differential transit depths as a function of wavelength (transmission spectroscopy) can reveal atomic and molecular absorption in a planet's atmosphere; this technique was demonstrated on HD 209458 b and subsequently used for many planets (e.g: Charbonneau et al. [2002].)
- **Transit timing and duration variations.** Deviations from strict periodicity in the times of transit (TTVs) can indicate the presence of additional bodies in the system. Gravitational interactions between planets can produce



measurable timing offsets, even for non-transiting companions, making TTVs a powerful tool for detecting and characterising multi-planet systems and constraining planetary masses and orbital architectures [Agol et al., 2005; Holman & Murray, 2005].

**Strengths and scientific impact:** The transit method is exceptionally powerful because it yields relative planetary radii directly, and when combined with radial-velocity mass measurements can determine planetary bulk densities and constraints on composition. Large, uniform photometric surveys from space missions (most notably *Kepler* [Borucki et al., 2010] and *TESS* [Sullivan et al., 2015]) have produced the vast majority of known small exoplanets and enabled robust occurrence-rate studies. Ground-based transit surveys, such as WASP [Pollacco et al., 2006] have also played a crucial role, particularly in the discovery of short-period giant planets around bright stars, which remain favourable targets for detailed follow-up characterisation. Future missions such as *PLATO* [Rauer et al., 2025] aim to extend this legacy by providing precise stellar characterisation alongside transit detections, enabling improved constraints on planetary radii and ages.

#### Limitations:

- **Geometric bias.** Only systems with orbital inclinations such that the planet transits the stellar disc are detectable; the transit probability scales roughly as  $R_{\star}/a$ , so short-period planets are far easier to find.
- **Stellar noise and systematics.** Stellar variability (discussed in detail in Chapter 4) and instrumental systematics can both reduce sensitivity and mimic transit-like signals.
- **Astrophysical false positives.** Background eclipsing binaries, hierarchical triples, and grazing eclipsing systems can produce transit-like light curves; vetting with high-resolution imaging, multi-colour photometry, centroid analysis, and spectroscopy is needed to validate candidates [Torres et al., 2011; Fressin et al., 2013].

### 1.2.2 The Radial Velocity Method

The radial velocity (RV) method is used to detect exoplanets by measuring the periodic Doppler shifts in the spectrum of a star due to the reflex motion induced by an orbiting planet. As the star moves toward or away from the observer, stellar

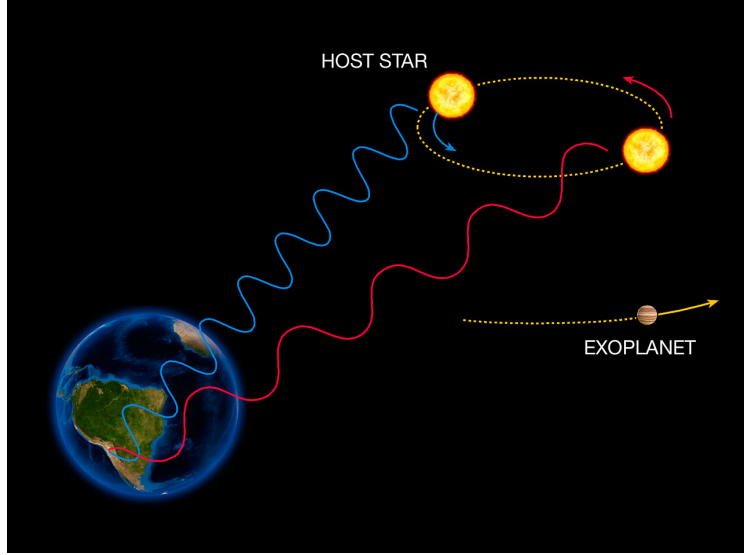


Figure 1.2: Illustration of an orbiting planet causing Doppler shifts in the spectrum of a star. Image credit: ESO.

absorption lines are shifted in wavelength according to the line-of-sight velocity. This behaviour arises from the Doppler effect, whereby motion toward the observer produces a shift to shorter wavelengths (a blueshift), while motion away from the observer results in a shift to longer wavelengths (a redshift). See Figure 1.2 for an illustration of this effect. In the non-relativistic limit, the fractional shift in wavelength is given by:

$$\frac{\Delta\lambda}{\lambda_0} = \frac{v_r}{c}, \quad (1.3)$$

where  $\Delta\lambda$  is the change in wavelength relative to the rest wavelength  $\lambda_0$ ,  $v_r$  is the radial velocity of the star, and  $c$  is the speed of light. The observed velocity amplitude therefore encodes the gravitational influence of the planet on the star [Mayor & Queloz, 1995].

For a planet of mass  $M_p$  on a Keplerian orbit around a star of mass  $M_\star$ , the radial-velocity semi-amplitude is

$$K = \left( \frac{2\pi G}{P} \right)^{1/3} \frac{M_p \sin i}{(M_\star + M_p)^{2/3}} \frac{1}{\sqrt{1 - e^2}}, \quad (1.4)$$

where  $P$  is the orbital period,  $i$  the orbital inclination, and  $e$  the orbital eccentricity.

For  $M_p \ll M_\star$ , this simplifies to

$$K \approx \left( \frac{2\pi G}{P} \right)^{1/3} \frac{M_p \sin i}{M_\star^{2/3}} \frac{1}{\sqrt{1-e^2}}. \quad (1.5)$$

**What radial velocities measure:**

- **Minimum planet mass.** From  $K$ ,  $P$ ,  $e$ , and an estimate of  $M_\star$ , one derives the minimum mass  $M_p \sin i$  (the true mass requires independent inclination constraints, e.g. from transits).
- **Orbital period.** Directly measured from the periodicity of the RV curve.
- **Orbital eccentricity and orientation.** From the shape and phase of the RV signal, both  $e$  and the argument of periastron  $\omega$  can in principle be constrained. However, accurately determining eccentricity is often challenging, particularly for low-amplitude signals or sparsely sampled data. Instrumental noise, stellar variability, and incomplete phase coverage can bias eccentricity estimates toward non-zero values, even for intrinsically circular orbits. As such, caution must be exercised when interpreting small eccentricities, and statistical model comparison or priors are often required to assess their significance [Shen & Turner, 2008; Lucy & Sweeney, 1971].
- **Multiple planets.** Superposed RV signals can reveal multi-planet systems; in such cases, the observed RV curve is the sum of multiple Keplerian components. In dynamically interacting systems, deviations from strictly Keplerian motion may arise, allowing constraints to be placed on planet–planet interactions. These interactions can provide additional information on planetary masses, orbital resonances, and long-term system stability, particularly in compact systems where gravitational coupling is strong [Wright & Howard, 2009].

**Strengths and scientific impact:** The RV method was the first successful technique for the detection of an exoplanet around a solar-like star, leading to the discovery of 51 Pegasi b [Mayor & Queloz, 1995]. It is highly versatile: sensitive to a wide range of orbital periods (from days to years) and capable of detecting planets that do not transit. When combined with transit measurements, RVs provide precise planetary densities, enabling compositional studies. Long-term RV surveys have revealed diverse planetary architectures and informed occurrence rates across stellar types [Howard et al., 2010].

### Limitations:

- **Inclination degeneracy.** RVs measure  $M_p \sin i$ ; without independent inclination constraints, only a lower limit on the planet mass can be obtained.
- **Stellar Variability.** Variability on the surface of the host star (e.g: spots, plagues, oscillations, and granulation) can induce RV variations that mimic or obscure planetary signals [Saar & Donahue, 1997]. This limitation is addressed in detail in Part II of this thesis.
- **Sensitivity bias.** The RV signal amplitude scales as  $K \propto M_p \sin i P^{-1/3}$ , making the method intrinsically more sensitive to massive planets on short-period orbits.

### 1.2.3 The Astrometric method

The astrometric method detects exoplanets by measuring the tiny reflex motion of a star on the plane of the sky induced by an orbiting companion. As a planet and star orbit their common centre of mass, the star describes an ellipse with angular semi-major axis

$$\alpha \approx \left( \frac{M_p}{M_\star} \right) \left( \frac{a}{d} \right), \quad (1.6)$$

where  $M_p$  and  $M_\star$  are the planet and stellar masses,  $a$  the orbital semi-major axis of the planet, and  $d$  the distance to the system. The signal thus grows with planetary mass and orbital separation, and decreases with distance to the star, making nearby, long-period giant planets the most accessible targets [Perryman, 2014; Lindgren et al., 2021].

Unlike radial-velocity and transit techniques, which probe the line-of-sight component of a system's geometry, astrometry directly measures two-dimensional sky-plane motion. A fully sampled astrometric orbit allows simultaneous determination of orbital inclination and longitude of the ascending node, parameters inaccessible to the radial-velocity method alone.

### What astrometry measures:

- **True planet mass.** Combining the star's angular semi-major axis  $\alpha$  with its distance yields the physical size of the stellar orbit and thus the planet's absolute mass without the  $\sin i$  degeneracy inherent in radial-velocity measurements [Perryman, 2014].

- **Full orbital geometry.** Astrometry determines orbital inclination  $i$ , longitude of the ascending node  $\Omega$ , eccentricity  $e$ , and argument of pericentre  $\omega$  directly from the sky-plane motion [Lindgren et al., 2021].
- **Long-period planets.** Sensitivity increases with  $a$ ; astrometry is therefore uniquely powerful for detecting Jupiter- to Saturn-like planets on multi-year orbits.

**Strengths and scientific impact:** Astrometry provides information that is complementary to both the radial-velocity and transit methods. Most importantly, it yields true (not minimum) planetary masses and full three-dimensional orbital solutions, enabling dynamical studies of system architectures. The European Space Agency’s *Gaia* mission represents a transformative step for astrometric exoplanet detection: its microarcsecond-level precision is expected to detect thousands of giant planets and precisely characterise the orbits of many more [Gaia Collaboration et al., 2016; Perryman, 2014].

The combination of *Gaia* astrometry with radial-velocity (RV) time series is particularly powerful. While RV measurements constrain the line-of-sight motion of the host star and provide precise orbital periods and phases, they suffer from the  $\sin i$  degeneracy and therefore yield only minimum masses. Astrometry, by contrast, measures the sky-projected motion and directly constrains the orbital inclination. Joint modelling of astrometric and RV data therefore breaks this degeneracy, yielding true planetary masses and more precise orbital parameters, particularly for long-period companions where RV phase coverage may be incomplete.

Astrometry is especially sensitive to massive planets at wide orbital separations, a population that is difficult to detect with transit surveys and often only partially sampled by RV observations. Such planets are of particular interest in the context of planet formation and evolution. In the Solar System, the giant planets contain the majority of the planetary mass and angular momentum, and are thought to play a key role in shaping system architectures through processes such as migration and dynamical scattering. Expanding the sample of long-period giant planets is therefore essential for testing models of planetary system formation and evolution.

### Limitations:

- **Small angular signals.** The astrometric reflex motion induced by orbiting planets is extremely small. Even Jupiter-mass planets around Sun-like stars at distances of tens of parsecs produce signals of only tens of microarcseconds, already requiring exceptionally precise and stable measurements. For Earth-mass planets, the signal drops to the sub-microarcsecond level ( $\sim 0.1\text{--}1\ \mu\text{as}$  for nearby systems), placing it beyond the reach of current instrumentation and making detections highly challenging.
- **Temporal baseline.** Detecting long-period planets demands time series spanning a significant fraction of their orbital periods. For planets with periods comparable to or exceeding the mission lifetime, only partial orbital arcs may be observed, leading to degeneracies between orbital parameters such as period, eccentricity, and semi-major axis. In such cases, solutions may be non-unique or biased, and combining astrometric data with complementary RV measurements is often required to recover robust orbital constraints.
- **Distance-dependent sensitivity.** Because  $\alpha \propto d^{-1}$ , astrometry is most effective for nearby stars; sensitivity declines for more distant systems.

#### 1.2.4 The Direct Imaging Method

Direct imaging detects exoplanets by resolving the light of a planet from the overwhelmingly brighter emission of its host star. Observationally, this requires extremely high contrast (up to  $10^{-10}$  for Earth-like planets around Sun-like stars) and high angular resolution to separate the planet from the stellar point spread function [Traub & Oppenheimer, 2010; Bowler, 2016].

The observable quantity is the flux from the planet at a given wavelength, which can be measured in reflected starlight at optical wavelengths [Carrión-González et al., 2020] or in thermal emission at infrared wavelengths [Wagner et al., 2016]. By obtaining photometry and, in some cases, spectroscopy, direct imaging provides information on a planet’s luminosity, effective temperature, and atmospheric composition. Imaging over multiple epochs can also trace orbital motion and constrain orbital parameters.

### What direct imaging measures:

- **Planet brightness and spectral energy distribution.** Multi-band photometry or spectroscopy allows estimates of effective temperature, radius, and atmospheric composition.
- **Orbital parameters.** Repeated imaging over time can determine inclination, semi-major axis, and eccentricity for wide-orbit planets (e.g: Lagrange et al. [2010]).
- **Multiplicity and circumplanetary environment.** Direct imaging can reveal multiple companions (e.g: Marois et al. [2008]) and circumplanetary discs or debris structures.
- **Atmospheric features.** Spectroscopic observations can detect molecular species (e.g.,  $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{CH}_4$ ) and clouds in young, self-luminous planets [Artigau et al., 2018].

**Strengths and scientific impact:** Direct imaging is unique among detection methods because it captures photons from the planet itself, enabling direct study of atmospheres, composition, and thermal evolution. It is especially sensitive to young, massive planets on wide orbits (several AU or more), which are difficult to detect with radial velocities or transits. Landmark discoveries include the HR 8799 multi-planet system [Marois et al., 2008, 2010] and Beta Pictoris b [Lagrange et al., 2010], which have provided direct constraints on planetary atmospheres and orbital architectures. Instruments such as SPHERE on the VLT, GPI on Gemini, and the upcoming ELT-class instruments are extending these capabilities [Bowler, 2016]. In space, the *Nancy Grace Roman Space Telescope* will deploy an advanced coronagraphic instrument capable of achieving contrasts of  $10^{-8}$ – $10^{-9}$ , enabling the direct detection of mature giant planets in reflected light and providing a critical technological pathfinder for future missions aiming to image Earth-like planets [Kasdin et al., 2020; Nemati et al., 2023].

#### **Limitations:**

- **High contrast requirement.** Stellar light is orders of magnitude brighter than the planet, necessitating coronagraphs, adaptive optics, and sophisticated post-processing.
- **Bias toward wide, young planets.** Planets must be sufficiently separated from the star and luminous enough to detect; old or small planets at close separations are generally inaccessible.

- **Long integration times and limited samples.** Imaging surveys are time-intensive, limiting the number of stars that can be surveyed.
- **Ambiguous masses.** Mass estimates from direct imaging are model-dependent. Reflected-light observations suffer strong degeneracies between radius, albedo, and phase, while thermal-emission measurements are more directly linked to temperature and radius but still depend on atmospheric and evolutionary models. In both cases, robust masses generally require complementary dynamical constraints.

### 1.2.5 Other Detection Methods

A number of additional techniques complement radial velocities, astrometry, and transits by probing regions of parameter space that would otherwise remain inaccessible.

**Gravitational Microlensing** Gravitational microlensing detects planets through the temporary magnification of a background source star when a foreground lens system passes close to the line of sight. Planetary companions introduce short-lived anomalies in the microlensing light curve, enabling sensitivity to cold, low-mass planets at several astronomical units from their host stars. Microlensing has revealed some of the lowest-mass and most distant planets known, including OGLE-2005-BLG-390Lb [Beaulieu et al., 2006], a  $\sim 5 M_{\oplus}$  planet at  $\sim 2.6$  au, and has even uncovered candidate free-floating planets [Sumi et al., 2011]. Although events are intrinsically rare and non-repeatable, large monitoring campaigns such as OGLE and MOA continue to expand the sample of microlensing planets.

**Pulsar Timing** Pulsar timing measures variations in the arrival times of radio pulses, which can reach microsecond precision. Orbital motion induced by planetary companions produces strictly periodic timing residuals, enabling detection of very low-mass planets. The first confirmed exoplanets were discovered via this method around the millisecond pulsar PSR B1257+12 [Wolszczan & Frail, 1992], revealing an unusual system that includes terrestrial-mass planets. While pulsar planets are rare, the method remains uniquely sensitive to Earth-mass bodies in compact orbits.

**Eclipse and Orbital Timing Variations** In eclipsing binary systems and transiting planetary systems, deviations from strictly periodic eclipse or transit times can reveal the presence of additional companions. Eclipse timing variations (ETVs) in compact binaries have revealed circumbinary planets such as Kepler-16b [Doyle



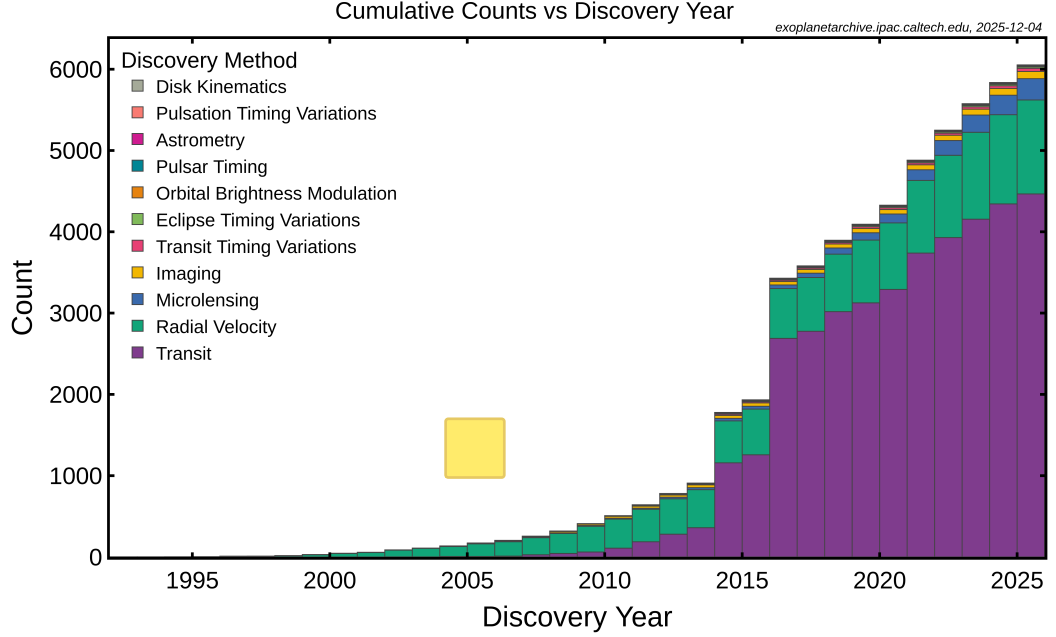


Figure 1.3: Figure from [exoplanetarchive.ipac.caltech.edu](https://exoplanetarchive.ipac.caltech.edu). Planet detection counts separated by discovery method and year.

et al., 2011]. Similarly, transit timing variations (TTVs) have enabled mass measurements and detections of non-transiting companions, famously in the Kepler-9 system [Holman et al., 2010]. These timing-based approaches are particularly powerful in multi-body systems where dynamical interactions are strong.

**Phase-Curve and Reflected-Light Modulation** High-precision space-based photometry can also detect planets by monitoring periodic brightness variations caused by reflected light, thermal emission, and ellipsoidal variations in close-in systems. The first such detection was made for the hot Jupiter HAT-P-7b using *Kepler* phase curves [Borucki et al., 2009]. Although primarily useful for short-period gas giants, these measurements provide constraints on atmospheric circulation, albedo, and day–night temperature contrasts.

Together, these methods extend exoplanet sensitivity to parameter regimes that are challenging for RVs, astrometry, or direct imaging, and they continue to play an important role in building a complete census of planetary systems.

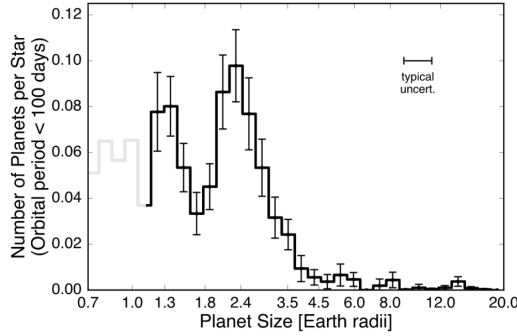


Figure 1.4: Figure from Fulton et al. [2017]. Fraction of planets found per star at various radii. The evident gap at  $\sim 1.8$  Earth radii is known as the radius valley.

### 1.3 Exoplanet Demographics

Large, homogeneous surveys, most notably those conducted by *Kepler* and *TESS*, have enabled statistical studies of planetary radii, masses, orbital periods, and host-star properties. After accounting for observational selection effects, these surveys reveal that the distribution of exoplanets is highly structured, containing distinct features such as peaks, valleys, and deserts. These features encode the imprint of planet formation and subsequent evolutionary processes, and provide some of the strongest empirical constraints on theoretical models.

Two of the most prominent and well-studied demographic features among close-in planets are the radius valley and the Neptune desert. Both occur at short orbital periods and intermediate planet sizes, and both point to the importance of atmospheric evolution in shaping the observed exoplanet population.

#### 1.3.1 The Radius Valley

One of the most striking results from the *Kepler* mission is the bimodal distribution of small planet radii at short orbital periods. When detection biases are carefully corrected, planets with radii  $\lesssim 4 R_{\oplus}$  exhibit two peaks: one centered near  $\sim 1.3 R_{\oplus}$  and another near  $\sim 2.3 R_{\oplus}$ , separated by a relative deficit of planets around  $\sim 1.8 R_{\oplus}$  (depicted in Figure 1.4). This feature, commonly referred to as the radius valley, was first clearly identified by Fulton et al. [2017] and subsequently confirmed by independent analyses [e.g. Van Eylen et al., 2018].

The location of the valley is observed to shift as a function of orbital period and

stellar mass, with the transition radius increasing at longer periods and around more massive stars [Van Eylen et al., 2018]. This behaviour strongly suggests that the valley is sculpted by evolutionary processes rather than reflecting a primordial absence of planets.

The leading explanation for the radius valley is atmospheric mass loss. In this framework, planets initially form with a range of core masses and thin hydrogen–helium envelopes. For sufficiently close-in planets, high-energy radiation from the host star (X-ray and extreme ultraviolet) can drive hydrodynamic escape, removing these envelopes on gigayear timescales. Planets that lose their envelopes entirely are left as bare, rocky super-Earths, while those that retain a fraction of their gas remain as sub-Neptunes [Owen & Wu, 2013a; Lopez & Fortney, 2013]. Alternative but related mechanisms, such as core-powered mass loss driven by a planet’s own cooling luminosity, can reproduce similar demographic features without invoking prolonged stellar irradiation [Ginzburg et al., 2018; Gupta & Schlichting, 2020a].

### 1.3.2 The Neptune Desert

The Neptune desert refers to the relative paucity of Neptune-mass or Neptune-radius planets on very short-period orbits (typically  $P \lesssim 3\text{--}5$  days), a region that is otherwise populated by both smaller super-Earths and much more massive hot Jupiters. The conspicuous demographic gap was first pointed out by Szabó & Kiss [2011] and has since become a key area of research.

In the period–mass and period–radius planes, the Neptune desert appears as a wedge-shaped region. Observationally, the desert is well established in samples combining transit and RV detections, suggesting that it is not an artefact of a single detection technique. It is worth noting that both the transit and RV detection methods actually favour close-in planets, further corroborating that this desert truly exists. Mazeh et al. [2016] derived empirical relations defining the triangular boundaries of the desert, shown in Figure 1.5. The upper boundary of the desert is typically associated with planets massive enough to resist catastrophic atmospheric loss, while the lower boundary reflects the transition to smaller, more resilient rocky or weakly enveloped planets.

Several physical mechanisms have been proposed to explain the Neptune desert. One possibility for the lower boundary is extreme atmospheric erosion: Neptune-mass planets that migrate too close to their host stars may lose their gaseous envelopes

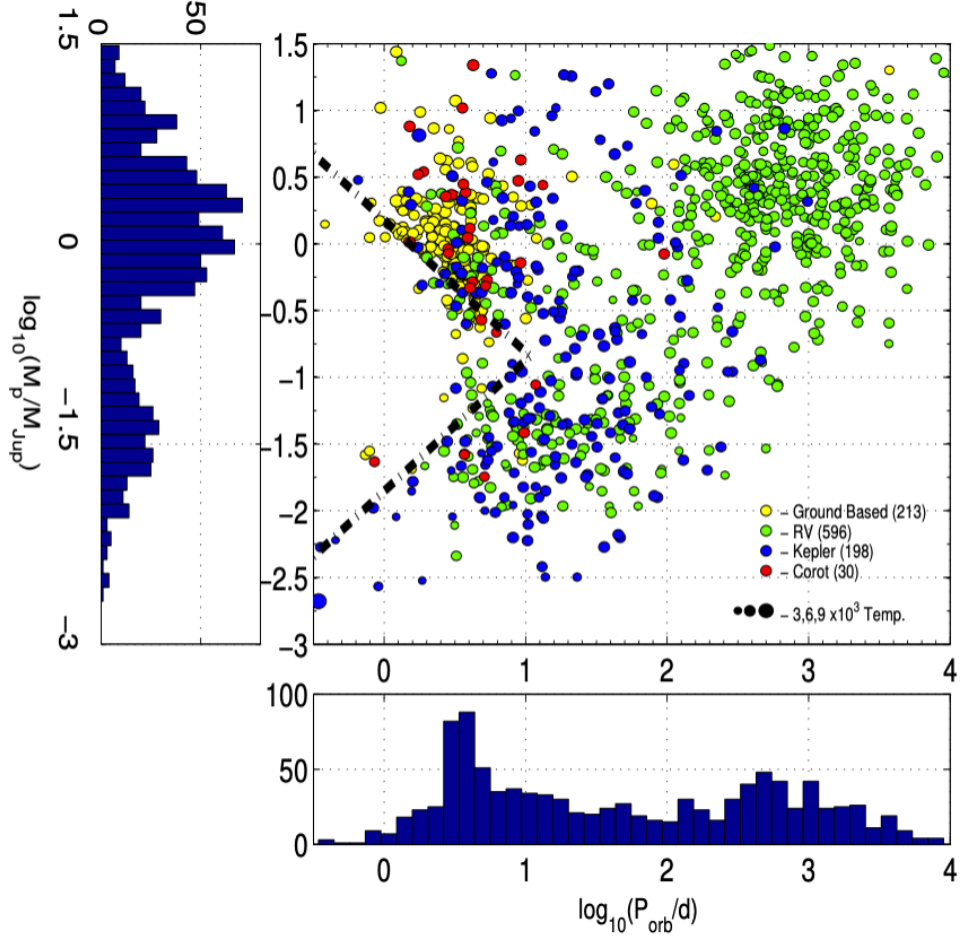


Figure 1.5: **Figure from Mazeh et al. [2016].** Planetary masses as a function of orbital periods for planets with known masses. Planets are colour coded by detection method. The black dotted lines show the boundaries of the Neptune desert, as derived by Mazeh et al. [2016].

rapidly due to intense stellar irradiation, evolving into smaller-radius planets and thereby vacating the desert region [Lammer et al., 2003; Owen & Lai, 2018a]. The upper boundary is thought to be shaped by the interplay between high-eccentricity migration and tidal disruption, whereby planets that are scattered onto highly eccentric orbits must either circularise at short periods (forming hot Jupiters) or else be tidally disrupted if their periastron lies within the Roche limit [Owen & Lai, 2018a].



## Chapter 2

# Methodology I

*“To infinity and beyond!”*

---

*Buzz Lightyear, Toy Story*

### 2.1 Photometry

Photometry is the measurement of the integrated flux of an astronomical source over a defined wavelength range, typically set by an instrumental bandpass or filter. By restricting observations to specific wavelength intervals, photometric measurements provide a coarse sampling of a source’s spectral energy distribution. Broadband filters capture flux over wide wavelength ranges and maximise signal-to-noise, while narrowband filters isolate specific spectral features at the expense of photon count. The measured flux depends on both the intrinsic luminosity of the source and the combined response of the instrument, telescope optics, and, where relevant, the Earth’s atmosphere.

Time-series photometry records flux as a function of time, enabling the detection of variability. In the context of exoplanet studies, it is used to identify transiting planets, which produce periodic dips in stellar brightness as they pass in front of their host star. The depth, duration, and shape of these transit signals encode key properties of the planetary system, including the planet-to-star radius ratio and orbital geometry, as discussed in Section 1.2.1.

In the analysis discussed in Chapter 3, photometric observations were obtained from both space-based and ground-based facilities, combining data from the Transiting



Figure 2.1: Image from [science.nasa.gov/mission/tess](https://science.nasa.gov/mission/tess). Artist's impression of the Transiting Exoplanet Survey Satellite (TESS).



Figure 2.2: Las Cumbres Observatory Global Telescope (LCOGT) 1-metre telescopes at CTIO. Credit: CTIO/NOIRLab/NSF/AURA/T. Slovinský.

Exoplanet Survey Satellite (TESS, pictured in Figure 3.1) [Ricker et al., 2015] and the Las Cumbres Observatory Global Telescope (LCOGT, pictured in Figure 3.3) network [Brown et al., 2013]. TESS is a space-based mission designed to carry out an all-sky survey for transiting exoplanets, providing high-precision, high-cadence photometry in a broad red-optical bandpass. Its observing strategy enables continuous monitoring of large sections of the sky over multi-week timescales. In contrast, LCOGT is a global network of robotic telescopes that enables flexible, targeted follow-up observations from the ground, typically in standard optical filters.

The detailed characteristics of these instruments, including detector properties, systematics, and calibration strategies, are well documented in the literature and are beyond the scope of this thesis. Comprehensive discussions of space-based transit photometry and ground-based follow-up techniques can be found in, for example,

Ricker et al. [2015], Brown et al. [2013], and related instrumentation and survey overview papers.

For the purposes of this work, the photometric data are treated as calibrated time-series flux measurements. These light curves form the basis for subsequent transit modelling, in which parameterised models of the star–planet system are fitted to the data to extract the physical and orbital properties of the planet.

## 2.2 Spectroscopy

Spectroscopy is the measurement of the intensity of light as a function of wavelength, providing a detailed view of the spectral energy distribution of an astronomical source. Unlike photometry, which integrates flux over broad wavelength ranges, spectroscopy resolves individual spectral features such as absorption and emission lines. These features arise from atomic and molecular transitions in the stellar atmosphere and encode information about the physical conditions of the star, including temperature, chemical composition, and velocity fields (this is discussed in more detail in Chapter 5).

In exoplanet studies, high-resolution spectroscopy is primarily used to measure stellar radial velocities via the Doppler shift of spectral lines. The presence of an orbiting planet induces reflex motion in the host star, resulting in periodic shifts in the observed wavelengths of absorption features. The amplitude and phase of these shifts provide constraints on the planetary mass and orbital parameters (as discussed in Section 1.2.2) complementing the geometric information obtained from transit photometry.

In this work, spectroscopic observations were obtained using the High Accuracy Radial velocity Planet Searcher (HARPS) [Pepe et al., 2002a], a fibre-fed, high-resolution echelle spectrograph designed for precise radial velocity measurements. HARPS operates at a resolving power of  $R \sim 115\,000$  and is stabilised in pressure and temperature to minimise instrumental drifts, enabling radial velocity precision at the level of  $\sim 1 \text{ m s}^{-1}$ .

The detailed design, calibration procedures, and data reduction pipelines associated with high-resolution spectrographs such as HARPS are well described in the literature (e.g. Mayor et al. 2003; Pepe et al. 2002a) and are not discussed in depth



here. In particular, radial velocities are typically extracted using cross-correlation techniques in which the observed spectrum is compared with a numerical mask to produce an average line profile, from which the velocity is derived (discussed further in Chapter 6).

In Chapter 3, the analysis uses radial velocity time series provided as reduced data products. These measurements are used in conjunction with photometric data to constrain the properties of the planetary system. In particular, radial velocity measurements provide an estimate of the planetary mass, breaking the degeneracy inherent in transit observations and enabling a full characterisation of the system.

## 2.3 Bayesian Inference and MCMC

The inference of planetary system parameters from photometric and spectroscopic observations is a statistical problem. The data are affected by measurement noise, potential systematic uncertainties, and correlated errors, while the underlying physical models are non-linear functions of their parameters. A Bayesian statistical framework enables prior knowledge about the parameters to be formally combined with the information content of the data to yield posterior probability distributions over all model parameters of interest.

### Bayes' Theorem

Given a vector of model parameters  $\boldsymbol{\theta}$  and observed data  $\mathcal{D}$ , Bayes' theorem states that

$$p(\boldsymbol{\theta} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})}{p(\mathcal{D})}, \quad (2.1)$$

where  $p(\boldsymbol{\theta} \mid \mathcal{D})$  is the posterior distribution over the parameters given the data,  $p(\mathcal{D} \mid \boldsymbol{\theta})$  is the likelihood (the probability of observing the data for a given set of parameters),  $p(\boldsymbol{\theta})$  is the prior distribution encoding knowledge or assumptions about the parameters before the data are considered, and  $p(\mathcal{D})$  is the Bayesian evidence (or marginal likelihood), defined as

$$p(\mathcal{D}) = \int p(\mathcal{D} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}. \quad (2.2)$$

The evidence acts as a normalising constant ensuring that the posterior integrates to unity and is the same for all parameter values; it therefore does not affect the shape of the posterior. In the context of Markov Chain Monte Carlo (MCMC)-based

parameter estimation, where the goal is to characterise the posterior rather than compare models, the evidence can be neglected, and Bayes' theorem is commonly written in proportional form:

$$p(\boldsymbol{\theta} \mid \mathcal{D}) \propto p(\mathcal{D} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}). \quad (2.3)$$

The posterior therefore combines two sources of information: the likelihood, which encodes what the data imply about the parameters, and the prior, which encodes any external constraints or physical expectations.

### The Likelihood Function

The likelihood  $p(\mathcal{D} \mid \boldsymbol{\theta})$  quantifies how probable the observed data are for a given model. In this work, the data consist of photometric flux measurements and radial velocity (RV) observations, each subject to independent measurement uncertainties. Assuming that these uncertainties are Gaussian and independent, the log-likelihood takes the form

$$\ln p(\mathcal{D} \mid \boldsymbol{\theta}) = -\frac{1}{2} \sum_i \left[ \frac{(d_i - m_i(\boldsymbol{\theta}))^2}{\sigma_i^2} + \ln(2\pi\sigma_i^2) \right], \quad (2.4)$$

where  $d_i$  are the observed data points,  $m_i(\boldsymbol{\theta})$  are the corresponding model predictions, and  $\sigma_i$  are the measurement uncertainties.

In practice, the formal measurement uncertainties may not fully capture all sources of noise. Astrophysical variability (such as stellar activity), instrumental systematics, or underestimated photon noise can contribute additional scatter beyond the quoted errorbars. To account for this, a per-instrument *jitter* term  $\sigma_{\text{jit}}$  is frequently included, with the total uncertainty in quadrature:

$$\sigma_{i,\text{tot}}^2 = \sigma_i^2 + \sigma_{\text{jit}}^2. \quad (2.5)$$

The jitter term is itself treated as a free parameter and inferred jointly with the physical parameters of the system.

### Prior Distributions

The prior  $p(\boldsymbol{\theta})$  encodes the state of knowledge about the parameters before the data are considered. In this work, two classes of prior are employed. Normal priors  $\mathcal{N}(\mu, \sigma)$ , with mean  $\mu$  and standard deviation  $\sigma$ , are placed on parameters for which

external constraints exist, such as stellar properties derived from spectral analysis. Uniform priors  $\mathcal{U}(a, b)$ , bounded between  $a$  and  $b$ , are placed on parameters that are essentially unconstrained within a physically motivated range.

Orbital eccentricity  $e$  and the argument of periastron  $\omega$  require special treatment. Sampling  $e$  and  $\omega$  independently can produce poor sampling geometry, since the physically meaningful quantity is the vector  $(e \cos \omega, e \sin \omega)$ , and the prior volume near  $e = 0$  is poorly represented by independent uniform priors on  $e$  and  $\omega$ . To avoid this,  $e$  and  $\omega$  are sampled jointly using `pmx.unitdisk` from PyMC3 [Salvatier et al., 2016a], which places a uniform prior on the two-dimensional unit disk in the  $(e \cos \omega, e \sin \omega)$  plane. This parameterisation ensures uniform prior probability over all physically allowed eccentricities  $e \in [0, 1)$  and arguments of periastron  $\omega \in [0, 2\pi)$ , while avoiding the degeneracy and poor geometry associated with independent sampling. The physical values of  $e$  and  $\omega$  are then recovered from the sampled Cartesian components.

The specific priors adopted for each parameter in this work are detailed in the relevant results sections (Table 3.4).

## Markov Chain Monte Carlo

For realistic exoplanet models, the posterior  $p(\boldsymbol{\theta} \mid \mathcal{D})$  is a high-dimensional, often non-Gaussian distribution that cannot be evaluated analytically or sampled directly. Instead, it can be explored numerically using Markov Chain Monte Carlo (MCMC) methods.

A Markov chain is a stochastic sequence of states  $\{\boldsymbol{\theta}_0, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots\}$  satisfying the Markov property: each state depends only on the immediately preceding state, not on the full history of the chain:

$$p(\boldsymbol{\theta}_{i+1} \mid \boldsymbol{\theta}_i, \boldsymbol{\theta}_{i-1}, \dots) = p(\boldsymbol{\theta}_{i+1} \mid \boldsymbol{\theta}_i). \quad (2.6)$$

MCMC algorithms construct such a chain whose stationary distribution is the target posterior. The empirical distribution of samples will converge to the true posterior as the chain length tends to infinity.

## Hamiltonian Monte Carlo and NUTS

Classical Metropolis–Hastings MCMC proposes new states by random walks, which become highly inefficient in high-dimensional or strongly correlated parameter spaces due to slow exploration and high rejection rates. Hamiltonian Monte Carlo (HMC) addresses this by introducing an auxiliary momentum variable  $\mathbf{p}$  and simulating Hamiltonian dynamics in the joint  $(\boldsymbol{\theta}, \mathbf{p})$  space. The Hamiltonian is defined as

$$\mathcal{H}(\boldsymbol{\theta}, \mathbf{p}) = -\ln p(\boldsymbol{\theta} \mid \mathcal{D}) + \frac{1}{2} \mathbf{p}^T \mathbf{M}^{-1} \mathbf{p}, \quad (2.7)$$

where the first term is the negative log-posterior (the “potential energy”) and the second is a kinetic energy term with mass matrix  $\mathbf{M}$ . By following the gradient of the log-posterior, HMC proposes distant states with high acceptance probability, dramatically reducing random-walk behaviour. For a more in-depth discussion on HMC, refer to Betancourt [2017].

The No-U-Turn Sampler (NUTS; Hoffman & Gelman 2011) is an adaptive extension of HMC that automatically tunes the trajectory length by terminating the simulation when the proposed trajectory begins to double back on itself. This eliminates the need to manually specify the number of leapfrog steps, which is a key tuning parameter in standard HMC and difficult to set optimally in practice. NUTS is the default sampler in PyMC and has become the standard for high-dimensional Bayesian inference in exoplanet science.

## Implementation

In this work, parameter inference is performed using the `exoplanet` Python package [Foreman-Mackey et al., 2021], which provides a probabilistic modelling environment for transiting and RV exoplanet systems, built on the PyMC framework. Transit light curves are modelled using the analytic models of Mandel & Agol [2002], as implemented in `exoplanet`, and radial velocity variations are modelled as a Keplerian orbit. Limb darkening is parameterised using the triangular sampling scheme of Kipping [2013], which ensures physically valid limb darkening coefficients are explored during sampling.

All photometric and RV data are fitted simultaneously in a joint model, ensuring that parameters shared between datasets, such as the orbital period  $P$ , the mid-transit time  $T_0$ , and the orbital eccentricity  $e$  are consistently constrained by all

available observations. Sampling is performed with NUTS, and convergence is assessed using trace plots. Parameter estimates are reported as the median of the marginal posterior distribution, with uncertainties given by the 16th and 84th percentile credible intervals (equivalent to  $\pm 1\sigma$  for a Gaussian distribution).

## Chapter 3

# TOI-2498 b: a hot bloated super-Neptune within the Neptune desert

*“My life amounts to no more than one drop in a limitless ocean. Yet what is any ocean, but a multitude of drops?”*

---

*David Mitchell, Cloud Atlas*

### Note

This chapter is a reproduction of Frame et al. [2023], originally published in July 2023 in Monthly Notices of the Royal Astronomical Society (MNRAS). The majority of writing and analysis was performed by myself. The following sections were written by co-authors: Section 3.2.2, Section 3.2.3, Section 3.2.5, Section 3.2.6, Section 3.3.1, Section 3.4.3, Section 3.4.4. Within these sections, all described analysis was performed by co-authors. All observational data collection was performed by external collaborators.

### 3.1 Introduction

Since the seminal discovery of 51 Pegasi b [Mayor & Queloz, 1995], over 5000 exoplanets have been confirmed. Our search for exoplanets has reached a stage where detection capabilities are beginning to catch up to demands, meaning that we are

able to look past detection biases and study the true exoplanet sample. This allows us to perform statistical studies on the exoplanet population, which forms a key role in gaining a better understanding of the formation of planetary systems.

The *Kepler* [Borucki et al., 2010] space mission was particularly successful in terms of the number of exoplanet detections, being responsible for over half of all confirmed exoplanets. *Kepler* was also successful in detecting smaller planets than were previously possible and found multitudes of super-Earths, filling in gaps in our knowledge of the exoplanet population. One key feature of the current exoplanet sample that was confirmed through *Kepler* discoveries is an apparent dearth of close orbit, Neptune sized planets [Szabó & Kiss, 2011; Beauge & Nesvorný, 2012; Helled et al., 2015; Lundkvist et al., 2016; Mazeh et al., 2016; Owen & Lai, 2018a].

Continuing the work of the *Kepler* space telescope, the Transiting Exoplanet Survey Satellite (*TESS*) telescope [Sullivan et al., 2015] was launched in 2018 and has since confirmed 285 exoplanets. Furthermore, *TESS* has been optimised to find planets around stars that are bright enough to be able to extract meaningful information from radial velocity observations. This enables us to be able to calculate mass and radius parameters of detected planets. Consequently, the *TESS* mission, along with spectroscopic instruments such as *HARPS* [Pepe et al., 2002a], have been integral in finding and characterising planets within the Neptune desert. In particular, the HARPS-NOMADS program endeavours to increase the number of planets in this category with precise mass and radius measurements. The objective of this pursuit is to be able to better study and understand the origins of the Neptune desert, and to better constrain the boundaries. Analysis of the boundaries of the Neptune desert could lead towards an improved understanding of formation and evolution of close orbit planets.

This chapter presents the detection of TOI-2498 b, a hot super-Neptune transiting a G type star, residing on the edge of the Neptune desert. The observations used in this work include transits from *TESS* and LCO, spectroscopy from *HARPS* and spectral imaging from SOAR. The details of these observations are outlined in Section 3.2. Analysis of these observations, including joint modelling to constrain the planetary parameters and analysis to determine stellar parameters can be found in Section 3.3. Section 3.4 contains the results of the analysis and a discussion involving the position of the planet in the Neptune desert and in mass-radius parameter space. This section also includes an analysis of the internal structure and evapo-

Table 3.1: Stellar parameters of TOI-2498

| Stellar Parameters                      | Value               | Source          |
|-----------------------------------------|---------------------|-----------------|
| <b>Identifiers</b>                      |                     |                 |
| TIC ID                                  | TIC-263179590       | TIC v8.2        |
| 2MASS ID                                | J06213989+1115062   | 2MASS           |
| Gaia ID                                 | 3330907293088717824 | <i>Gaia</i> DR3 |
| <b>Astrometric Properties</b>           |                     |                 |
| R.A. (deg)                              | 95.416220           | <i>Gaia</i> DR3 |
| DEC (deg)                               | 11.251645           | <i>Gaia</i> DR3 |
| Parallax (mas)                          | $3.61 \pm 0.05$     | <i>Gaia</i> DR3 |
| $RV_{\text{sys}}$ (km s <sup>-1</sup> ) | 8.36                | <i>Gaia</i> DR3 |
| <b>Photometric Parameters</b>           |                     |                 |
| B (mag)                                 | $12.25 \pm 0.30$    | TIC v8.2        |
| V (mag)                                 | $11.20 \pm 0.03$    | TIC v8.2        |
| G (mag)                                 | $11.27 \pm 0.00$    | <i>Gaia</i> DR3 |
| J (mag)                                 | $10.28 \pm 0.03$    | TIC v8.2        |
| H (mag)                                 | $10.00 \pm 0.02$    | TIC v8.2        |
| K (mag)                                 | $9.93 \pm 0.02$     | TIC v8.2        |
| <i>Gaia</i> BP (mag)                    | 11.61               | <i>Gaia</i> DR3 |
| <i>Gaia</i> RP (mag)                    | 10.80               | <i>Gaia</i> DR3 |

Sources: TIC v8.2 [Paegert et al., 2022], 2MASS [Skrutskie et al., 2006], Gaia Data Release 3 [Vallenari et al., 2022].

ration history of the planet. Finally the conclusions of this work can be found in Section 3.5.

## 3.2 Observations

TOI-2498 is a  $V = 11.2$ , G-type ( $T_{\text{eff}} = 5905 \pm 12$  K) solar-like star. The properties of the star are set out in Table 3.1

### 3.2.1 TESS photometry

TESS observed TOI-2498 for the first time during its primary mission (cycle 1) within sector 6, in Full Frame Images (FFIs) with a 30-min cadence. It was observed again during the first extended mission in sector 33 (cycle 3), with a 10 minute cadence FFI and a 2 minute cadence pixel stamp observation.



The candidate was alerted as a TOI [TESS Object of Interest, Guerrero et al., 2021] based on the identification of a transit signal from the SPOC pipeline [Jenkins, 2002; Jenkins et al., 2010, 2020]. This pipeline uses the PDCSAP [Presearch Data Conditioning Simple Aperture Photometry; Stumpe et al., 2012, 2014; Smith et al., 2012] light curves, which removes instrumental and some stellar trends from the SAP (Simple Aperture Photometry) data, but retains local features such as transits. The transit signal passed all the diagnostic tests conducted by Data Validation module [Twicken et al., 2018; Li et al., 2019], and the difference image centroiding test located TOI-2498 to within  $3.55 \pm 2.75$  arcsec of the location of the transit source.

In this work, the PDCSAP lightcurves are flattened by removing the transits and fitting a spline to the data. The resulting flattened lightcurves are used in the joint model outlined in section 3.3.2. We present the normalised lightcurves along with the generated best-fit model in Figure 3.1.

Figure 3.2 shows the *TESS* Target Pixel File (TPF) created with `tpfplotter`<sup>1</sup> [Aller et al., 2020], with TOI-2498 as the central object overlaid with nearby catalog sources. As can be seen in Figure 3.2, there are several sources of potential contamination around the target star, meaning it is likely that the *TESS* data is affected by blending of sources. To accurately measure the extent of this blending and correct for it, follow up ground based photometry was necessary; the details of these observations are described below.

### 3.2.2 LCOGT follow-up photometry

The *TESS* pixel scale is  $\sim 21'' \text{ pixel}^{-1}$  and photometric apertures typically extend out to roughly 1 arcminute, generally causing multiple stars to blend in the *TESS* aperture. To determine the true source of the TOI-2498b detection in the *TESS* data, improve the transit ephemeris, and check the SPOC pipeline transit depth after accounting for the crowding metric, we conducted ground-based lightcurve follow-up observations of the field around TOI-2498 as part of the *TESS* Follow-up Observing Program<sup>2</sup> Sub Group 1 [TFOP; Collins, 2019]. We used the *TESS* Transit Finder, which is a customized version of the *Tapir* software package [Jensen, 2013],

<sup>1</sup><https://github.com/jlillo/tpfplotter>

<sup>2</sup><https://tess.mit.edu/followup>

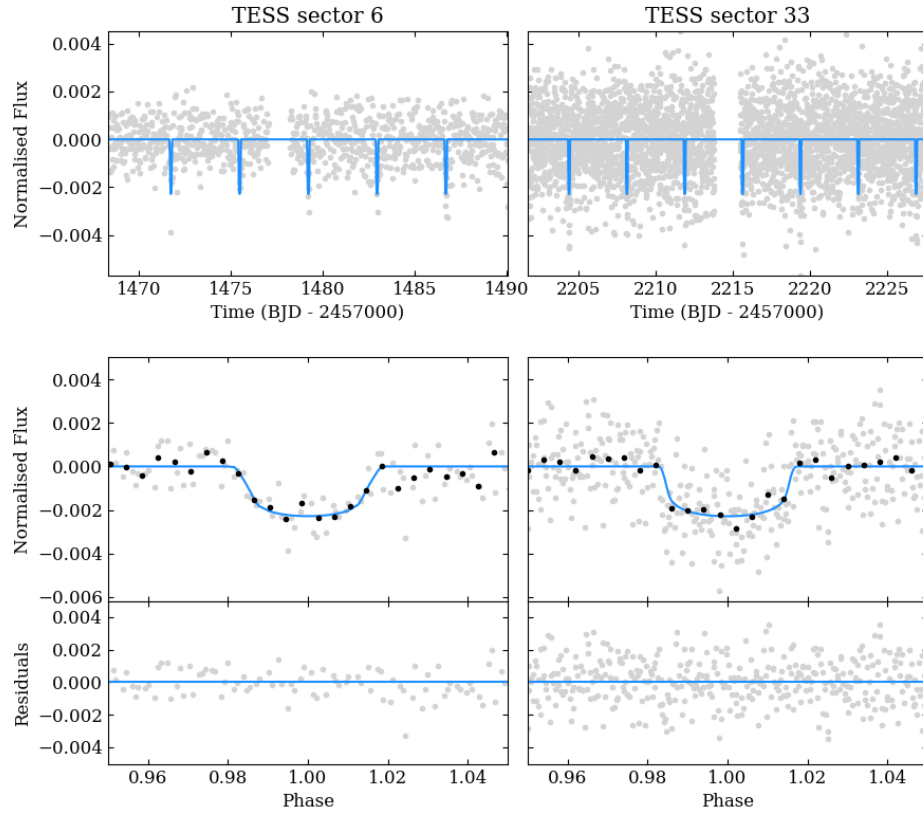


Figure 3.1: The top plots show the *TESS* PDCSAP lightcurves from sector 6 (30 minute cadence) and sector 33 (2 minute cadence), flattened via a spline fit. Overplotted in blue is the best fit model resulting from the analysis described in section 3.3.2. The middle plots show this same data phase folded, with the binned data shown in black. Residuals of this fit can be found in the bottom plots.

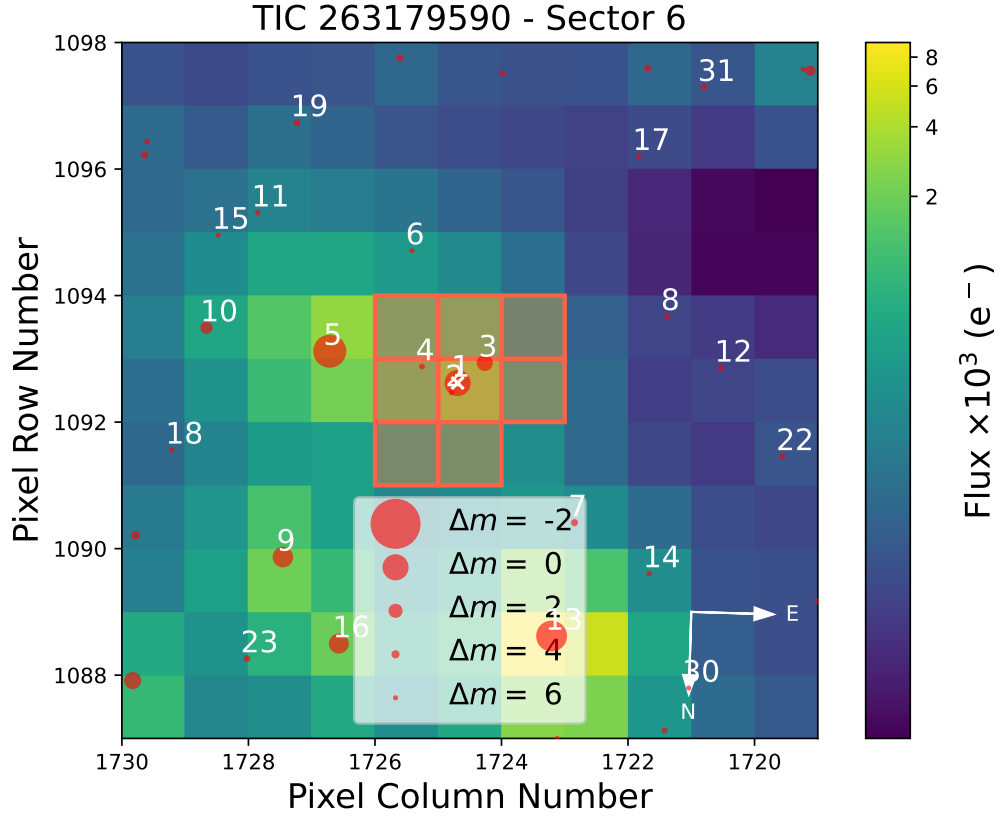


Figure 3.2: Target Pixel File (TPF) from *TESS* sector 6. The shaded red squares indicate the aperture mask used by the SPOC pipeline. The target system (TOI-2498) is marked by a white cross, and the red circles mark nearby sources from the *Gaia* DR3 catalogue, with sizes proportional to the difference in magnitude to the target.

to schedule our transit observations.

We observed a full predicted transit window of TOI-2498.01 on 2022 December 01 UT simultaneously using the Las Cumbres Observatory Global Telescope [LCOGT; Brown et al., 2013] 1.0 m network nodes at Teide Observatory and Cerro Tololo Inter-American Observatory. We also attempted a full transit observation on 2023 January 07 UT from the LCOGT 1.0 m network node at Siding Spring Observatory, but deteriorating weather limited the in-transit coverage to about 60% of the transit duration. The 1 m telescopes are equipped with  $4096 \times 4096$  SINISTRO cameras having an image scale of  $0.''389$  per pixel, resulting in a  $26' \times 26'$  field of view. The images were calibrated by the standard LCOGT BANZAI pipeline [McCully et al., 2018] and differential photometric data were extracted using *AstroImageJ* [Collins et al., 2017].

We conducted focused observations to improve the separation of TOI-2498 from its nearest Gaia DR3 neighbor, which is  $3.''8$  northwest and 5.7 magnitudes fainter in *TESS* band. Typical stellar point spread functions (PSFs) in the images had full-width half-maximum (FWHM) in the range of 2-3 arcseconds. The Teide light curve had the smallest FWHM of  $2.''16$  and the longest pre- and post-transit baseline of all three light curves, so resulted in the strongest constraints on transit model parameters. We first extracted differential light curves using circular photometric apertures with radius  $5.''8$ . In this case, the target star aperture included most of the flux of the nearest Gaia DR3 neighbor. A clear transit-like event was detected with a depth of  $\sim 2000$  ppm (deeper than predicted by the SPOC pipeline). We then extracted light curves using smaller  $3.''1$  apertures that exclude the majority of the flux from the  $3.''8$  neighbor. We again find a  $\sim 2000$  ppm event in the smaller target aperture, confirming that the event occurs on-target relative to known Gaia DR3 stars. Since the flux contamination in the larger target star aperture is less than 1%, we use the light curves from the the  $5.''8$  apertures in the joint modeling in Section 3.3.2. We present the normalised lightcurves and generated best-fit model in Figure 3.3.

### 3.2.3 ULMT photometry

We observed transit windows of TOI-2498 on 2021 February 26 and again on 2023 February 10 in the Sloan  $r'$  band from the 0.61 m University of Louisville Manner Telescope (ULMT) located at the Steward Observatory near Tucson, AZ. We

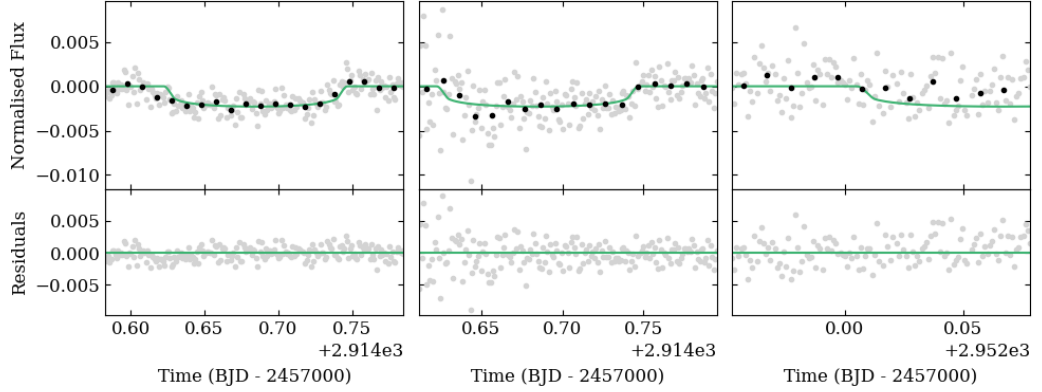


Figure 3.3: LCOGT lightcurves from Teide Observatory (left), Cerro Tololo Inter-American Observatory (middle) and Siding Spring Observatory (right). The data is shown as grey points, with binned values in black. Overplotted is the best fit model from the joint fit described in section 3.3.2. The bottom plots show the residuals of this fit for each lightcurve.

used the *TESS* Transit Finder to schedule these transit observations based on the ephemerides current at those times. The  $4096 \times 4096$  SBIG STX-16803 camera on ULMT has an image scale of  $0''.39$  per pixel, resulting in a  $26' \times 26'$  field of view. The images on both nights were slightly defocused and had typical stellar point-spread-functions with FWHM of  $3''.4$  and  $2''.9$  respectively. The images were calibrated and photometric data were extracted with *AstroImageJ* [Collins et al., 2017] using circular aperture with radii  $15''.9$  and  $5''.9$  respectively. In 2021, we tentatively detected a shallow event on-target and did not find any obvious evidence of a blended nearby eclipsing binary that could be the cause of the *TESS* detection. In 2023, the shallow ingress was detected in detrended fitting. Due to the relatively high amount of noise compared the rest of our photometry, we decide not to include this data in our analysis.

### 3.2.4 HARPS Radial Velocity observations

We acquired 16 spectra through the HARPS-NOMADS program (PI Armstrong, 1108.C-0697) using *HARPS* (the High Accuracy Radial velocity Planetary Searcher Mayor et al. [2003]). *HARPS* is an Echelle spectrograph mounted on the ESO 3.6-m telescope at the La Silla Observatory in Chile. The data were collected between 2022 September 30 to October 12 and 2022 November 15 to November 18. The *HARPS* High-Accuracy mode was utilised, with a fibre diameter of  $1''$ , a resolution

of  $R \approx 115,000$  and an exposure time of approximately 1800 seconds. This resulted in a signal to noise ratio (SNR) of between 30 and 35 per pixel at a wavelength of 550nm. The standard *HARPS* data reduction software outlined in Lovis & Pepe [2007] was used to reduce the raw *HARPS* data, in which a weighted cross correlation is applied with a G2 spectral mask. Measurements of the Radial Velocity (RV), FWHM, the line bisector span, the contrast of the Cross-Correlation Function (CCF) and the S-index are displayed in Table 3.2. The median photon noise per measurement for this dataset is  $3.45 \text{ m s}^{-1}$ . The last datapoint from the first set of observations is discarded due to anomalous results in RV error, FWHM, bisector span, contrast and S-index (see Table 3.2). This datapoint also has a lower SNR than the others, which we attribute to cloud coverage at the time of observation.

We present the *HARPS* radial velocity data along with the generated best-fit model (see Section 3.3.2 for details) in Figure 3.4.

### 3.2.5 SOAR imaging

High-angular resolution imaging is needed to search for nearby sources that can contaminate the *TESS* photometry, resulting in an underestimated planetary radius, or be the source of astrophysical false positives, such as background eclipsing binaries. We searched for stellar companions to TOI-2498 with speckle imaging on the 4.1-m Southern Astrophysical Research (SOAR) telescope [Tokovinin, 2018] on 27 February 2021 UT, observing in Cousins I-band, a similar visible bandpass as *TESS*. This observation was sensitive to a 5.1-magnitude fainter star at an angular distance of 1 arcsec from the target. More details of the observations within the SOAR *TESS* survey are available in Ziegler et al. [2020]. The  $5\sigma$  detection sensitivity and speckle auto-correlation functions from the observations are shown in Figure 3.5. No nearby stars were detected within  $3''$  of TOI-2498 in the SOAR observations.

### 3.2.6 Shane imaging

We observed TOI-2498 on 2021 March 4 using the ShARCS camera on the Shane 3-meter telescope at Lick Observatory [Kupke et al., 2012; Gavel et al., 2014; McGurk et al., 2014]. Observations were taken with the Shane adaptive optics system in natural guide star mode to search for nearby, unresolved stellar companions. We collected a single sequence of observations using a  $K_s$  filter ( $\lambda_0 = 2.150 \mu\text{m}$ ,  $\Delta\lambda = 0.320 \mu\text{m}$ ).

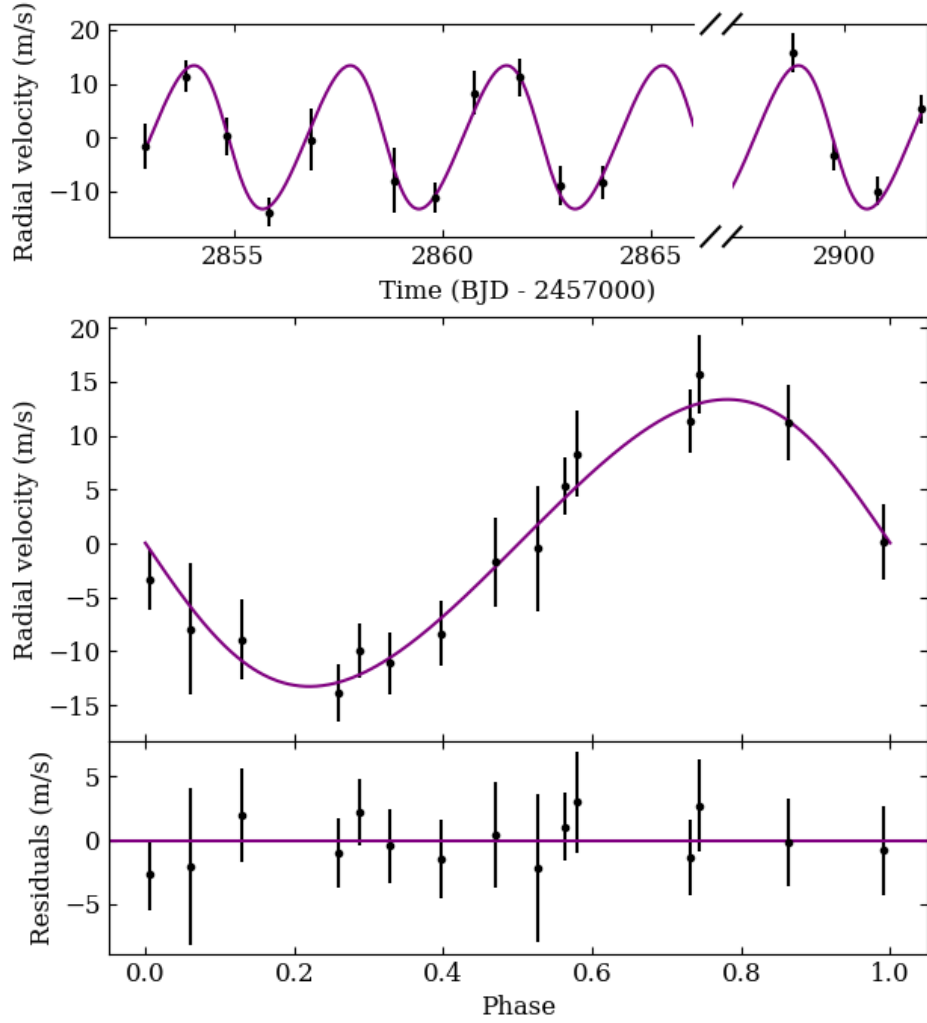


Figure 3.4: Top: *HARPS* radial velocity data for TOI-2498. Overplotted is the best fit model obtained from the joint fit described in section 3.2, corresponding to the orbital period of TOI-2498 b. Middle: The same data and model phase folded. Bottom: Residuals of the fit (observed RV - computed RV).

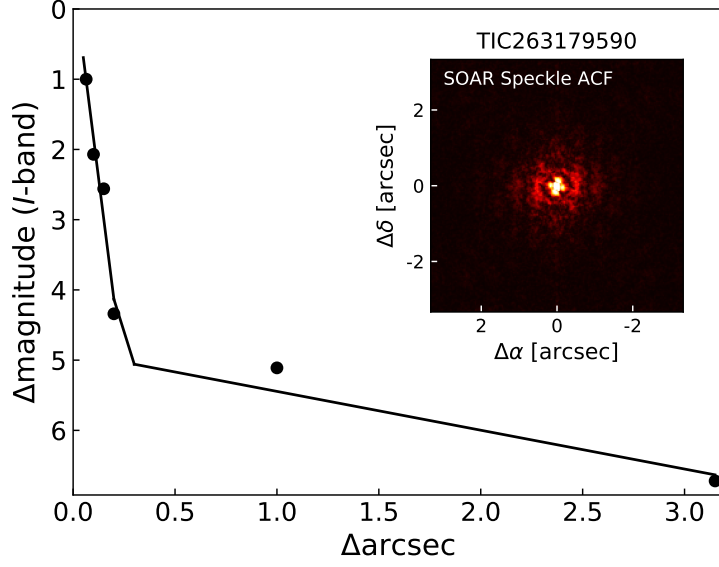


Figure 3.5: Contrast curve computed from the high-resolution speckle observations in Cousins I-band on the 4.1 m Southern Astrophysical Research telescope. Inset is the speckle autocorrelation function centered on the target star. No bright companions are detected within 3'' of TOI-2498 in this observation.

We reduced the data using the publicly available **SiMmER** pipeline [Savel et al., 2020, 2022].<sup>3</sup> Our reduced images and corresponding contrast curves are shown in Figure 3.6. Our observations achieve a contrast of 2.9 at 1'' and 4.8 at 2''. We detect the known star TIC 715328024 ( $\Delta T = 5.7$ , sep = 3.8'', PA = 328°), but find no other nearby stellar companions within our detection limits.

### 3.3 Analysis and Results

#### 3.3.1 Stellar Analysis

We used ARES+MOOG to derive the stellar atmospheric parameters  $T_{\text{eff}}$ ,  $\log g$ , microturbulence and  $[\text{Fe}/\text{H}]$ , and their respective uncertainties following the methodology described in Sousa [2014]; Santos et al. [2013]. We measured equivalent widths (EW) of iron lines on the combined *HARPS* spectrum of TOI-2498 using the ARES v2 code<sup>4</sup> [Sousa et al., 2015]. Then we used a minimization process where we assume ionization and excitation equilibrium to converge in the best set of spectroscopic pa-

<sup>3</sup><https://github.com/arjunsavel/SimMER>

<sup>4</sup>The last version of ARES code (ARES v2) can be downloaded at <http://www.astro.up.pt/~sousasag/ares>



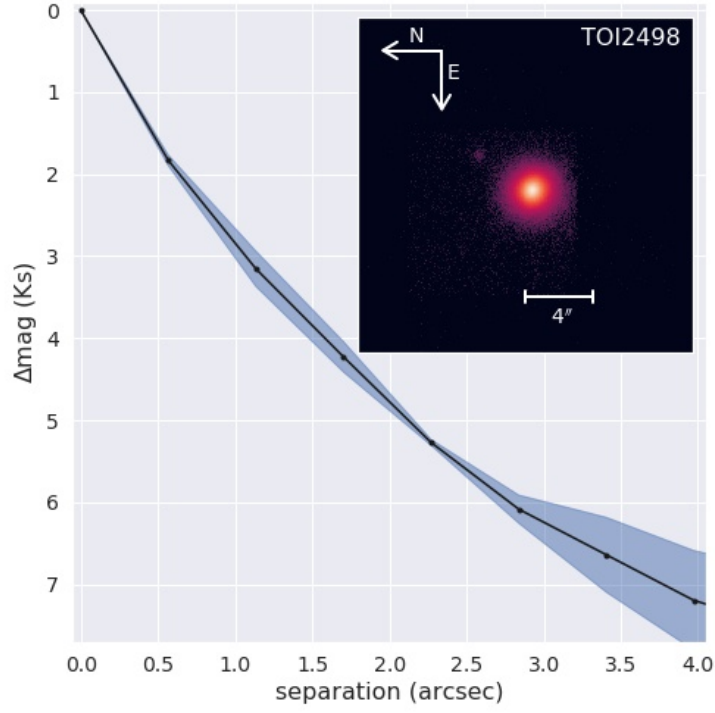


Figure 3.6: Adaptive optics images of TIC 263179590 taken with the ShARCS camera on the Shane 3-meter telescope at Lick Observatory. We also present a contrast curve generated by calculating the median values (solid lines) and root-mean-square errors (blue, shaded regions) in annuli centered on each target, where the bin width of each annulus is equal to the full width at half max of the point spread function. TIC 715328024 ( $\Delta T = 5.7$ ,  $\text{sep} = 3.8''$ ) is visible to the N NW of the target star.

Table 3.2: *HARPS* spectroscopy. The row in **bold** text represents the data point that has been discarded due to anomalous results.

| Time (BJD<br>-2457000) | RV<br>(m/s)   | RV error<br>(m/s) | FWHM<br>(m/s) | Bisector span<br>(m/s) | Contrast<br>(%) | S-index <sub>MW</sub> |
|------------------------|---------------|-------------------|---------------|------------------------|-----------------|-----------------------|
| 2852.89471             | 7441.0        | 4.2               | 7262.1        | 17.8                   | 46.57           | 0.13                  |
| 2853.86784             | 7454.1        | 2.9               | 7282.7        | -3.0                   | 46.93           | 0.14                  |
| 2854.83784             | 7443.0        | 3.5               | 7285.0        | 8.3                    | 46.87           | 0.13                  |
| 2855.84365             | 7429.0        | 2.7               | 7295.1        | 2.2                    | 46.90           | 0.13                  |
| 2856.84238             | 7442.3        | 5.8               | 7251.6        | 11.1                   | 46.90           | 0.11                  |
| 2858.83733             | 7434.8        | 6.1               | 7302.1        | 6.6                    | 46.72           | 0.14                  |
| 2859.83526             | 7431.7        | 2.9               | 7286.3        | -3.9                   | 46.86           | 0.13                  |
| 2860.77664             | 7451.0        | 4.0               | 7281.4        | -0.68                  | 46.45           | 0.11                  |
| 2861.83705             | 7453.9        | 3.4               | 7259.7        | 9.3                    | 46.65           | 0.14                  |
| 2862.83113             | 7433.9        | 3.7               | 7265.3        | 1.5                    | 46.46           | 0.12                  |
| 2863.83660             | 7434.4        | 3.0               | 7281.2        | 12.5                   | 46.64           | 0.13                  |
| <b>2864.86315</b>      | <b>7463.7</b> | <b>11.4</b>       | <b>7176.2</b> | <b>40.1</b>            | <b>44.29</b>    | <b>0.06</b>           |
| 2898.77390             | 7458.4        | 3.6               | 7285.9        | 8.1                    | 46.77           | 0.12                  |
| 2899.75712             | 7439.4        | 2.7               | 7276.7        | 1.1                    | 46.96           | 0.14                  |
| 2900.80942             | 7432.8        | 2.6               | 7287.5        | 11.6                   | 46.81           | 0.12                  |
| 2901.84129             | 7448.1        | 2.7               | 7289.8        | -2.3                   | 46.86           | 0.13                  |

rameters. This process makes use of a grid of Kurucz model atmospheres [Kurucz, 1993] and the radiative transfer code MOOG [Snedden, 1973].

Stellar abundances of the elements were derived using the classical curve-of-growth analysis method assuming local thermodynamic equilibrium and with the same codes and models that were used for the stellar parameters determinations. For the derivation of chemical abundances of refractory elements we closely followed the methods described in Adibekyan et al. [2012, 2015]; Delgado Mena et al. [2017]. Abundances of the volatile elements, C and O, were derived following the method of Delgado Mena et al. [2021]; Bertran de Lis et al. [2015]. We note that the oxygen lines are very weak and difficult to measure given the signal to noise ratio of the co-added spectrum and thus the final abundance has a large uncertainty. All the  $[X/H]$  ratios are obtained through a differential analysis with respect to a high S/N solar (Vesta) spectrum from HARPS. The stellar parameters and abundances of the elements are presented in Table 3.3.

We find that the  $[X/Fe]$  ratios of  2498 are typical for a thin disk star. Moreover, we used the chemical abundances of some elements to derive ages through the so-called chemical clocks (i.e. certain chemical abundance ratios which have a strong correlation for age). We applied the 3D formulas described in Table 10 of Delgado Mena et al. [2019], which also consider the variation in age produced by the effective temperature and iron abundance. The chemical clocks  $[Y/Mg]$ ,  $[Y/Zn]$ ,  $[Y/Ti]$ ,  $[Y/Si]$ ,  $[Y/Al]$ ,  $[Sr/Ti]$ ,  $[Sr/Mg]$  and  $[Sr/Si]$  were used from which we obtain a weighted average age of  $3.6 \pm 1.1$  Gyr.

### Spectral Energy Distribution Analysis

As an independent determination of the basic stellar parameters, we performed an analysis of the broadband spectral energy distribution (SED) of the star together with the *Gaia* DR3 parallax [with no systematic offset applied; see, e.g., Stassun & Torres, 2021], in order to determine an empirical measurement of the stellar radius, following the procedures described in Stassun & Torres [2016]; Stassun et al. [2017, 2018]. We pulled the  $B_T V_T$  magnitudes from *Tycho-2*, the  $JHK_S$  magnitudes from *2MASS*, the W1–W3 magnitudes from *WISE*, and the  $G_{BP}G_{RP}$  magnitudes from *Gaia*. Together, the available photometry spans the full stellar SED over the wavelength range 0.4–10  $\mu\text{m}$ .

We performed a fit using PHOENIX stellar atmosphere models [Husser et al., 2013a], with the effective temperature ( $T_{\text{eff}}$ ), surface gravity ( $\log g$ ), and metallicity ( $[\text{Fe}/\text{H}]$ ) initially set to the spectroscopically determined values. The remaining free parameter is the extinction  $A_V$ , which we limited to maximum line-of-sight value from the Galactic dust maps of Schlegel et al. [1998]. The resulting fit has a best-fit  $A_V = 0.05 \pm 0.05$ , with a reduced  $\chi^2$  of 1.3. Integrating the (unreddened) model SED gives the bolometric flux at Earth,  $F_{\text{bol}} = 7.62 \pm 0.18 \times 10^{-10} \text{ erg s}^{-1} \text{ cm}^{-2}$ . Taking the  $F_{\text{bol}}$  together with the *Gaia* parallax, gives the bolometric luminosity,  $L_{\text{bol}} = 1.823 \pm 0.044 L_{\odot}$ , which via the Stefan-Boltzmann relation gives the stellar radius,  $R_{\star} = 1.291 \pm 0.018 R_{\odot}$ . In addition, we can estimate the stellar mass from the empirical eclipsing-binary relations of Torres et al. [2010], giving  $M_{\star} = 1.17 \pm 0.07 M_{\odot}$ .

Finally, we performed a fit allowing the stellar parameters to vary, finding only the metallicity differed marginally from the spectroscopically determined value,  $[\text{Fe}/\text{H}] = 0.05 \pm 0.15$ , with an improved reduced  $\chi^2$  of 0.8. In that case, the resulting stellar properties are as follows:  $A_V = 0.05 \pm 0.05$ ,  $F_{\text{bol}} = 7.77 \pm 0.18 \times 10^{-10} \text{ erg s}^{-1} \text{ cm}^{-2}$ ,  $L_{\text{bol}} = 1.860 \pm 0.045 L_{\odot}$ ,  $R_{\star} = 1.305 \pm 0.018 R_{\odot}$ , and  $M_{\star} = 1.15 \pm 0.07 M_{\odot}$ .

As all determined stellar parameters were in agreement, we adopt the ARES+MOOG parameter set for consistency.

### 3.3.2 Joint modelling

The photometry from both *TESS* and LCO and spectroscopy from HARPS, described in Section 3.2, were combined in a joint fit using the **exoplanet** [Foreman-Mackey et al., 2021] code framework. This package also makes use of **starry** [Luger et al., 2019] and **PYMC3** [Salvatier et al., 2016b].

#### Photometry

We include the flattened photometric data from the two *TESS* sectors described in section 3.2.1 and the two full and one partial transit from LCOGT described in section 3.2.2.

Firstly, we normalise all photometry by dividing each lightcurve by the median of the out-of-transit flux and subtracting one. Each transit is then modelled through

`exoplanet` as a Keplerian orbit, with quadratic limb-darkening parameterisation from Kipping [2013]. The Keplerian orbit model is parameterised in terms of stellar mass ( $M_\star$ ) and radius ( $R_\star$ ) in solar units, the orbital period  $P$  in days, central transit ephemeris  $T_C$  in TBJD (BJD - 2457000), impact parameter  $b$ , eccentricity  $e$  and argument of periastron  $\omega$  in radians. Transit models are generated using `starry`, and include planetary radius ( $R_p/R_\star$ ) and the exposure time for the relevant instrument.

## Spectroscopy

We include the spectroscopic data from *HARPS* described in section 3.2.4. We find no need to fit a GP model as periodogram analysis through the DACE<sup>5</sup> platform shows no indication of stellar activity or signals from stellar rotation, suggesting that TOI-2498 is magnetically quiet. We fit for the semi-amplitude  $K$  of the RV signal, starting with a widely set uniform prior centered around the value found via analysis using DACE ( $13.37 \text{ m s}^{-1}$ ). We also fit for *HARPS* instrument offset, and implement a noise model which adds a white noise (jitter) term in quadrature with the nominal RV uncertainties.

## Joint fit results

We first maximise the log probability of the `PYMC3` model, and use the resulting parameters as our initial fit values. We then use a No U-Turn Sampler (NUTS) variant of the Hamiltonian Monte Carlo (HMC) algorithm to draw samples from the posterior chain, for which we use 20 chains with 20,000 steps. We treat the first 4000 samples drawn as burn-in and subsequently discard them.

Through the results of this analysis, we determine that TOI-2498 b is a Super-Neptune of radius  $6.06 \pm 0.29 R_\oplus$  and mass  $34.62 \pm 4.10 M_\oplus$ . From this we infer a bulk density of  $0.86 \pm 0.25 \text{ g cm}^{-3}$ . We present all parameter best-fit results in Table 3.5.

### 3.3.3 Transit timing variations

We perform an initial check for additional planets using the DACE platform. Using DACE, we generate a lomb-scargle periodogram of the *HARPS* data and search for

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<sup>5</sup>DACE can be accessed at <https://dace.unige.ch>

Table 3.3: Stellar parameters of TOI-2498 derived from this work

| Stellar Parameters                       | Value                     |
|------------------------------------------|---------------------------|
| Mass ( $M_{\odot}$ )                     | $1.12 \pm 0.02$           |
| Radius ( $R_{\odot}$ )                   | $1.26 \pm 0.04$           |
| Density ( $\text{g cm}^{-3}$ )           | $0.79^{+0.10}_{-0.08}$    |
| $\log g$                                 | $4.297 \pm 0.021$         |
| $T_{\text{eff}}$ (K)                     | $5905 \pm 12$             |
| $v_{\text{turb}}$ ( $\text{km s}^{-1}$ ) | $1.125 \pm 0.016$         |
| Age (Gyr)                                | $3.6 \pm 1.1$             |
| <b>Stellar abundances</b>                |                           |
| [Fe/H] (dex)                             | $0.167^{+0.010}_{-0.041}$ |
| [C/H] (dex)                              | $0.071 \pm 0.029$         |
| [O/H] (dex)                              | $0.028 \pm 0$             |
| [Mg/H] (dex)                             | $0.19 \pm 0.06$           |
| [Al/H] (dex)                             | $0.22 \pm 0.07$           |
| [Si/H] (dex)                             | $0.16 \pm 0.03$           |
| [Ti/H] (dex)                             | $0.18 \pm 0.03$           |
| [Ni/H] (dex)                             | $0.17 \pm 0.02$           |
| [Cu/H] (dex)                             | $0.213 \pm 0.025$         |
| [Zn/H] (dex)                             | $0.144 \pm 0.016$         |
| [Sr/H] (dex)                             | $0.146 \pm 0.077$         |
| [Y/H] (dex)                              | $0.171 \pm 0.056$         |
| [Zr/H] (dex)                             | $0.089 \pm 0.065$         |
| [Ba/H] (dex)                             | $0.29 \pm 0.028$          |
| [Ce/H] (dex)                             | $0.137 \pm 0.059$         |
| [Nd/H] (dex)                             | $0.135 \pm 0.033$         |

Table 3.4: Prior distributions of fitted parameters

| Parameter                                        | Prior distribution              | Fitted value            |
|--------------------------------------------------|---------------------------------|-------------------------|
| TESS Sector 6 mean                               | $\mathcal{N}(0, 1)$             | $0.00005 \pm 0.00002$   |
| TESS Sector 33 mean                              | $\mathcal{N}(0, 1)$             | $0.00002 \pm 0.00002$   |
| Contamination *                                  | $\mathcal{N}(0.66, 0.2)$        | $0.63 \pm 0.05$         |
| LCO Teide mean                                   | $\mathcal{N}(0, 1)$             | $-0.0001 \pm 0.00009$   |
| LCO CTIO mean                                    | $\mathcal{N}(0, 1)$             | $-0.0003 \pm 0.0001$    |
| LCO SSO mean                                     | $\mathcal{N}(0, 1)$             | $0.0004 \pm 0.0001$     |
| $\log(K)$ ( $\text{m s}^{-1}$ )                  | $\mathcal{U}(0.0, 4.0)$         | Table 3.5               |
| <i>HARPS</i> offset                              | $\mathcal{N}(7442.50, 10.0)$    | $7442.8 \pm 0.9$        |
| $\log(\textit{HARPS}$ jitter)                    | $\mathcal{N}(1.895, 5.0)$       | $-2.27^{+2.37}_{-3.43}$ |
| LD coefficient $u_1$                             | Kipping [0.0, 0.3] <sup>†</sup> | $0.34 \pm 0.30$         |
| LD coefficient $u_2$                             | Kipping [0.0, 0.3] <sup>†</sup> | $0.31 \pm 0.34$         |
| Orbital period (days)                            | $\mathcal{N}(3.737882, 0.001)$  | Table 3.5               |
| $T_C$ (TBJD)                                     | $\mathcal{N}(2204.4183, 0.01)$  | Table 3.5               |
| $\log(R_p)$ ( $R_\odot$ )                        | $\mathcal{N}(-3.05, 1.0)$       | Table 3.5               |
| $[\sqrt{e} \sin(\omega), \sqrt{e} \cos(\omega)]$ | unitdisk <sup>‡</sup>           | Table 3.5               |
| Impact parameter                                 | $\mathcal{U}(0.0, 1.0)$         | Table 3.5               |

\* Proportion of the measured flux from TESS that is due to TOI-2498.

<sup>†</sup> The distributions for limb darkening coefficients are built into the `exoplanet` framework and are based on Kipping [2013].

<sup>‡</sup> Eccentricity and the argument of periastron are sampled with a Uniform distribution on a unit disk in two dimensions using `pmx.unitdisk` from PYMC3 [Salvatier et al., 2016c].

$\mathcal{N}(\mu, \sigma)$ : Normal distribution with mean  $\mu$  and standard deviation  $\sigma$ .

$\mathcal{U}(a, b)$ : Uniform distribution with lower bound  $a$  and upper bound  $b$ .

Table 3.5: TOI-2498 b parameters

| <b>Fitted Parameters</b>              | <b>Value</b>            |
|---------------------------------------|-------------------------|
| Orbital period (days)                 | $3.738252 \pm 0.000004$ |
| Radius ( $R_{\oplus}$ )               | $6.06^{+0.29}_{-0.27}$  |
| $R_p/R_*$                             | $0.04 \pm 0.01$         |
| $T_C$ (TBJD)                          | $2204.4167 \pm 0.0001$  |
| Impact parameter                      | $0.42 \pm 0.13$         |
| $K$ ( $\text{m s}^{-1}$ )             | $13.25 \pm 1.36$        |
| Eccentricity                          | $0.089 \pm 0.075$       |
| Argument of periastron ( $^{\circ}$ ) | $89.99 \pm 99.14$       |
| <b>Derived Parameters</b>             | <b>Value</b>            |
| Mass ( $M_{\oplus}$ )                 | $34.62^{+4.10}_{-4.09}$ |
| Density ( $\text{g cm}^{-3}$ )        | $0.86^{+0.25}_{-0.20}$  |
| Inclination ( $^{\circ}$ )            | $87.12 \pm 1.70$        |
| Semi-major axis (AU)                  | $0.0491 \pm 0.003$      |
| Temperature $T_{\text{eq}}$ (K) *     | $1443^{+15}_{-28}$      |

\* Assuming Albedo = 0 and uniform surface temperature



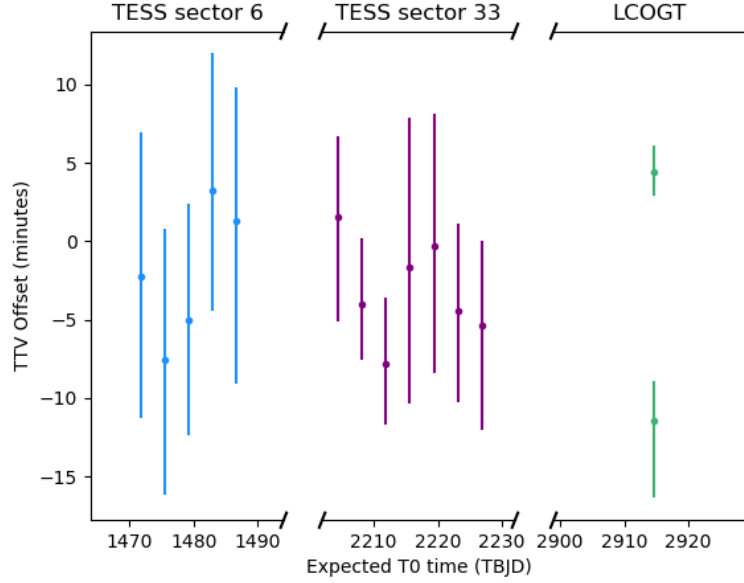


Figure 3.7: TTV offsets for all transits from *TESS* sector 6 and sector 33, and LCOGT transits from CTIO and Teide Observatory.

additional signals after removal of the radial velocity signal caused by TOI-2498 b. We find no evidence of additional signals above a False Alarm Probability (FAP) of 0.1, suggesting that TOI-2498 b is the only massive, short period planet orbiting TOI-2498.

To support this analysis, we examine each individual full transit from *TESS* and LCO and check for transit timing variations. We re-run the transit model described in section 3.3.2 for each individual transit. We fix all of the parameters to the best fit results in Table 3.5, other than the central transit time  $T_0$ , for which we set a uniform prior, centered around the expected value. The results of this fitting are subtracted from the expected value to find the TTV offset for each transit. We present this analysis in Figure 3.7. We again find no evidence of additional planets, although more transits would allow a more thorough check. It is worth noting the apparent discrepancy between the two LCOGT TTV offsets, as these points are different observations of the same transit and therefore should agree. We attribute this discrepancy to high airmass having a significant impact on the ingress of one of the transits (see Figure 3.3).

## 3.4 Discussion

### 3.4.1 Planet position in the Neptune Desert

We find that TOI-2498 b is situated just within the Neptune desert, close to the lower edge in the mass-period parameter space. The positioning is displayed in Figure 3.8 in both the mass-period and radius-period parameter spaces, with boundaries as given in Mazeh et al. [2016].

As explained in Owen & Lai [2018a], it is thought that the upper boundary is due to high-eccentricity migration, while the lower boundary is due to photoevaporation. Mazeh et al. [2016] also provides an alternative explanation for the lower boundary, suggesting that as the planet-star separation grows, the size of the Hill sphere of the forming planet, the orbital path and the dust-to-gas ratio all increase. This results in an increased core mass at the end of the first stage of planetary formation. Hence planets that are further from their host stars have an increased total mass.

As is apparent from Figure 3.8, the upper boundary of the Neptune desert is significantly more defined than the lower. There is an observational bias to take into account here, where larger, higher mass planets are substantially easier to detect and characterise. Consequently, as more planets close to the lower edge of the mass-period desert (such as TOI-2498 b) are added to the sample, the boundary becomes even more blurred. This raises the question of whether the lower boundary of the Neptune desert needs to be re-evaluated. However, it is worth pointing out that programs such as HARPS-NOMADS specifically target planets within the desert parameter space, creating a biased sample of planets and potentially providing some explanation for this blurring of the boundary.

### 3.4.2 Planet density

We plot the position of TOI-2498 b in mass-radius parameter space in Figure 3.9. When considering the general exoplanet population, it can be seen that TOI-2498 b sits in a relatively sparse area of this parameter space. This Figure also shows the planets proximity to composition models from Zeng et al. [2016, 2019], with the closest relation being the model for planets with a 5% H<sub>2</sub> envelope and a rocky core with a surface equilibrium temperature of 2000 K.

We also present the position of TOI-2498 b in a more mass-constrained mass-radius

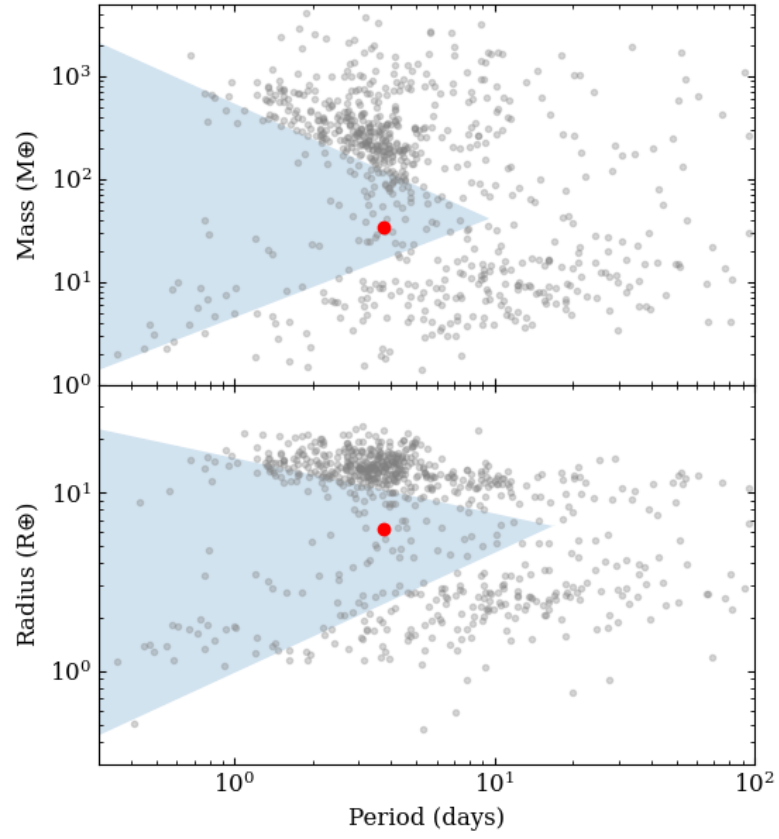


Figure 3.8: The Neptunean desert shown in both mass-period (top) and radius-period (bottom) parameter space. The shaded blue regions indicate the areas within the boundaries laid out by Mazeh et al. [2016]. The grey circles represent known exoplanets with mass uncertainties smaller than 30% and radius uncertainties smaller than 10%. The position of TOI-2498 b is depicted by a larger red circle.

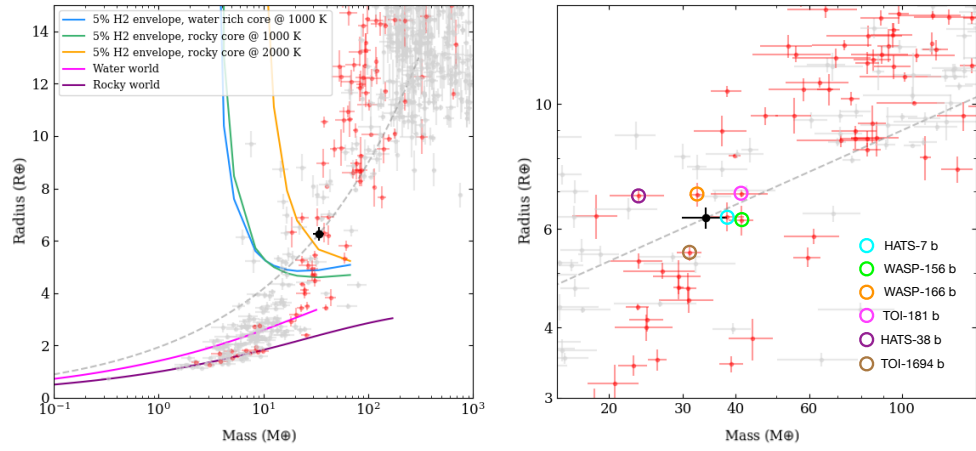


Figure 3.9: Position of TOI-2498 b in mass-radius parameter space. In both plots, TOI-2498 b is depicted as a black circle and the points in the background show the positions of all other confirmed planets with a radius uncertainty below 10% and a mass uncertainty below 25%. The points highlighted in red are planets that are located within the Neptunean desert as defined by Mazeh et al. [2016]. The grey dotted line is a line of constant density at  $0.758 \text{ g cm}^{-3}$  (the calculated density of TOI-2498). The left plot shows the positioning within a large parameter space and includes composition models from Zeng et al. [2016, 2019]. The right plot highlights planets within the Neptunean desert that are close to TOI-2498 b within mass-radius parameter space. Note that the right plot is shown in log-log scale.

space in the right-hand side of Figure 3.9. In this plot, planets that are located within the Neptune desert are highlighted in red. Note that for these planets, there is an apparent upper size bound that falls rapidly as mass decreases. This could be a reflection of planets’ on a closer orbit (shorter period) inability to maintain their envelopes due to irradiation from host stars.

We highlight 6 Neptune desert planets closest to TOI-2498 b in mass-radius parameter space in Figure 3.9. These planets are as follows: HATS-7 b [Bakos et al., 2015], WASP-156 b [Demangeon et al., 2018], WASP-166 b [Hellier et al., 2019], TOI-181 b [Mistry et al., 2023b], HATS-38 b [Jordán et al., 2020], TOI-1694 b [Mistry et al., 2023a].

Of particular interest here is WASP-166 b, as not only does it share a very similar mass and radius to TOI-2498 b, it also has a similar orbital period and equilibrium temperature. These similarities suggest that there is potential insight to be gained from a comparative study between atmospheres of TOI-2498 b and WASP-166 b. Several atmospheric studies have been performed on WASP-166 b, in particular searches for sodium [Seidel et al., 2022] and water [Lafarga et al., 2023]. We therefore suggest that TOI-2498 b is a potential candidate for searching for species such as water or sodium in the optical using high-resolution, and also perhaps for carbon based molecules in the infrared using JWST.

### 3.4.3 Composition and Internal structure

TOI-2498 b’s low density of  $0.86 \text{ g cm}^{-3}$  is indicative of the presence of a gaseous envelope. We estimate its internal structure by assuming it is comprised of a rocky core surrounded by an H/He-rich atmosphere, following Rogers & Owen [2021]. This model consists of four parameters: the rocky core radius  $R_{\text{core}}$  and mass  $M_{\text{core}}$ , and the envelope thickness  $R_{\text{env}}$  and mass fraction  $f_{\text{env}}$ . The envelope mass fraction is defined as the ratio of envelope mass to total planet mass  $f_{\text{env}} = M_{\text{env}}/M_{\text{p}} = (M_{\text{p}} - M_{\text{core}})/M_{\text{p}}$ .

To solve for these parameters, we adopted a system of four equations. These include (1) the definition of envelope mass fraction above, (2) the definition of envelope thickness as the difference between planet and core radii  $R_{\text{env}} = R_{\text{p}} - R_{\text{core}}$ , (3) the mass-radius relations for rocky cores by Otegi et al. [2020], and (4) the envelope structure model by Chen & Rogers [2016], which determines the thickness of the

Table 3.6: TOI-2498 b internal structure assuming a rocky core surrounded by a H/He-rich envelope.

| Property               | Symbol (Units)                 | Value            |
|------------------------|--------------------------------|------------------|
| Core radius            | $R_{\text{core}} (R_{\oplus})$ | $2.62 \pm 0.14$  |
| Core mass              | $M_{\text{core}} (M_{\oplus})$ | $25.12 \pm 3.41$ |
| Envelope thickness     | $R_{\text{env}} (R_{\oplus})$  | $3.43 \pm 0.36$  |
| Envelope mass fraction | $f_{\text{env}}$               | $0.27 \pm 0.04$  |

gaseous envelope from its mass. The resulting internal structure of TOI-2498 b, as shown in Table 3.6, indicates that the planet hosts a significant gaseous envelope which consists of  $27 \pm 4\%$  of its mass. However, this model assumes no water content or significant atmospheric metallicity. Whilst massive planets with high water content are thought to have a mixed interior with a moderate metallicity gradient [Stevenson et al., 2022], smaller dry sub-Neptunes are thought to settle into a structure with distinct core and envelope [Bodenheimer et al., 2018]. TOI-2498 b is intermediate in size and would likely fall somewhere between these two scenarios. Future spectroscopic observations could constrain the metallicity of its atmosphere and its H<sub>2</sub>O content.

### 3.4.4 Evaporation history

Atmospheric evaporation is thought to have a significant influence in sculpting exoplanet populations, giving rise to the Neptune desert [Owen & Lai, 2018b] as well as the period-radius valley [e.g. Lopez et al., 2012; Owen & Wu, 2013b; Jin et al., 2014; Owen & Wu, 2017]. The underlying mechanisms for evaporation, however, are still unclear. One of the proposed mechanisms is photoevaporation, where X-ray and extreme ultraviolet photons (together, XUV) emitted by stars are readily absorbed by the upper atmospheres of close-in planets, heating up the gas and driving a hydrodynamic wind that escapes the planet’s gravitational well [e.g. Lammer et al., 2003; Erkaev et al., 2007; Kislyakova et al., 2013]. Additional mechanisms have also been proposed, such as core-powered mass loss [Ginzburg et al., 2016; Gupta & Schlichting, 2020b], in which the energy for evaporation is provided by the core’s internal heat.

Moreover, the XUV emission history of a star can be estimated from its spin period history, as the two quantities are related via the rotation-activity relation [Wright et al., 2011], where a shorter stellar rotation period leads to a brighter X-ray emis-

sion. We adopted the stellar spin evolution models by Johnstone et al. [2021] to determine the X-ray emission past of TOI-2498. For a given stellar mass, they modelled a distribution of starting rotation periods which is then evolved in time through various angular momentum transfer mechanisms. The spin and X-ray evolution models for a  $1.1 M_{\odot}$  star are shown on Figure 3.10. Even though we did not measure a rotation period for TOI-2498, we were able to determine an age of  $3.6 \pm 1.1$  Gyr, from which these models predict a present-day spin period between 8 and 24 days.

We modelled the evaporation history of TOI-2498 b using the method by Fernández Fernández et al. (submitted). We utilise the `photoevolver` code <sup>6</sup> to simulate the evaporation history of the planet. This method combines three ingredients: (1) a description of the stellar XUV emission history from the models by Johnstone et al. [2021] as shown on Figure 3.10, (2) the evaporation model by Kubyshkina et al. [2018], which determines the mass loss rate from the incident XUV flux, and (3) the envelope structure model by Chen & Rogers [2016], which recalculates the envelope thickness after mass is removed from it. We evolved the planet under photoevaporation backwards in time to the age of 10 Myr and forwards to 7.5 Gyr.

Figure 3.11 shows the evaporation history of TOI-2498 b. Overall, we find TOI-2498 b to be a stable super-Neptune that has experienced little evaporation throughout its lifetime, relative to its mass. The planet, after formation, might have started out as a puffy Saturn-sized world of radius  $8\text{--}10 R_{\oplus}$  and envelope mass fraction 30–45 %. We also find its envelope is unlikely to be stripped prior to its host star evolving off the main sequence.

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<sup>6</sup>The code is available on GitHub through: <https://github.com/jorgefz/photoevolver>

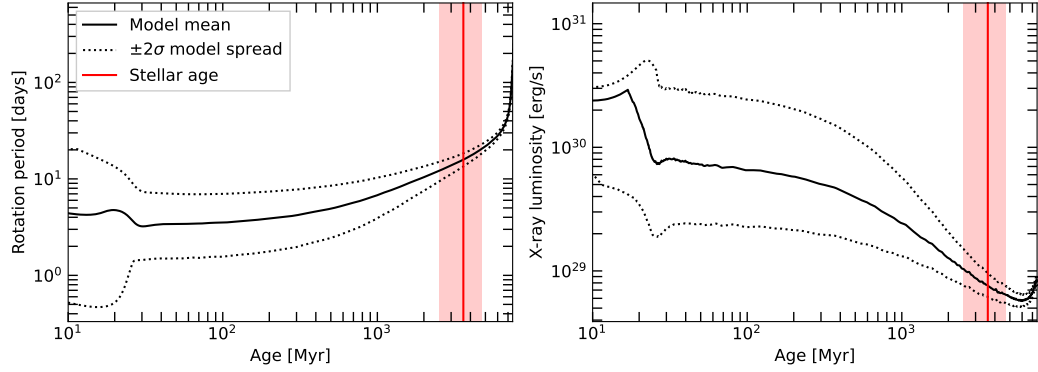


Figure 3.10: **Left panel:** spin evolution models for a  $1.1 M_{\odot}$  star following the models by Johnstone et al. [2021]. These include the mean and  $2\sigma$  spread in starting rotation periods. The current age of TOI-2498, and its uncertainty, are shown as a red line and shaded region, respectively. **Right panel:** models of the X-ray luminosity evolution for a  $1.1 M_{\odot}$  star, akin to the left panel.

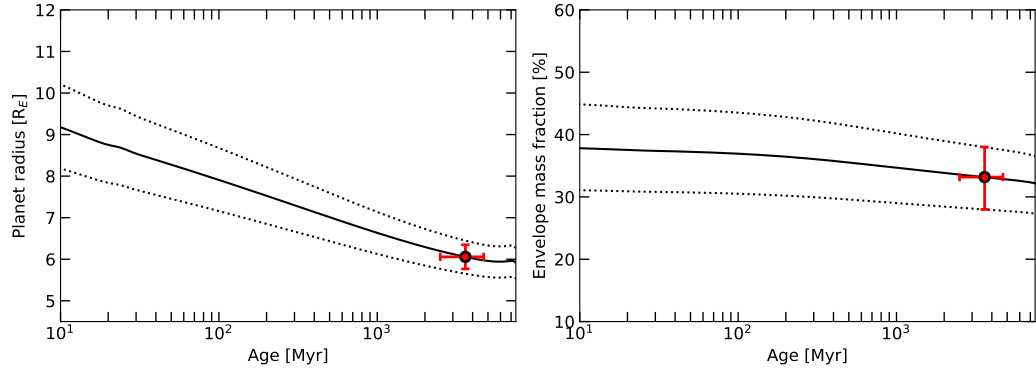


Figure 3.11: **Left panel:** plot of planet radius against age. The black lines represent the evolution of the radius of TOI-2498b under photoevaporation, both the mean (solid line) as well as  $1\sigma$  spread (dotted lines) based on the errors on the present-day mass, radius, and age, which are plotted as a red circle. **Right panel:** plot of the planet's envelope mass fraction against age, following the left-hand panel.



### 3.5 Chapter Conclusions

In this work, we have presented the discovery of a hot, bloated Super-Neptune transiting a G type star. Our analysis includes photometry from *TESS* sector 6 and sector 33, follow up ground based photometry from LCOGT and spectroscopy from HARPS. We combine this data in a joint model to discern a planet radius of  $6.1 \pm 0.3 R_{\oplus}$ , planet mass of  $35 \pm 4 M_{\oplus}$  and an orbital period of 3.7 days. We calculate a stellar mass of  $1.12 \pm 0.02 M_{\odot}$  and a stellar radius of  $1.26 \pm 0.04 R_{\odot}$ . We find no indication of additional planets through radial velocity periodograms and TTV analysis.

We estimate through internal structure models that  $27 \pm 4\%$  of the mass of TOI-2498 b constitutes a gaseous envelope. We present the evaporation history of the planet and find that it is likely a stable Super-Neptune, with little evaporation having taken place throughout its lifetime. We find that TOI-2498 b likely started its life as a puffy Saturn-sized world before shrinking to its current size over  $3.6 \pm 1.1$  Gyr.

We highlight similarities in mass, radius, period and temperature in TOI-2498 b and WASP-166 b and suggest that there is potential for comparative atmospheric studies between the two planets. We also point out that spectroscopic atmospheric observations would allow for constraints on water content and atmospheric metallicity. This would improve our abilities to study the composition and internal structure of TOI-2498 b.

## Part II

# Modelling the spectroscopic impact of granulation

## Chapter 4

# An Introduction to Stellar Variability in Solar-type Stars

*“Here, on the edge of what we know, in contact with the ocean of the unknown, shines the mystery and beauty of the world. And it’s breathtaking.”*

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*Carlo Rovelli, Seven Brief Lessons on Physics*

### 4.1 Motivations and scope

Solar-type stars exhibit intrinsic variability arising from surface convection, oscillations, rotation, and magnetic activity. These processes generate time-dependent brightness and velocity fields across the stellar surface, which imprint themselves on both photometric and spectroscopic observations. For exoplanet studies targeting solar-type hosts, such variability represents a fundamental astrophysical limitation: the signals produced by stellar surface phenomena can be comparable to, or larger than, those induced by low-mass planets.

As observational precision has improved, stellar variability has emerged as a dominant source of uncertainty in exoplanet detection and characterisation around Sun-like stars. In radial velocity measurements, convective motions and magnetic regions introduce apparent Doppler shifts and line-profile distortions that can obscure or mimic planetary signals at the metre-per-second and sub-metre-per-second level. In transit observations, surface inhomogeneities bias inferred planetary radii and can imprint stellar spectral features onto transmission spectra. An understanding of

Table 4.1: Summary of the dominant sources of stellar variability in solar-type stars.

| Phenomenon       | Spatial scale             | Timescale   | Origin                       |
|------------------|---------------------------|-------------|------------------------------|
| Granulation      | $\sim 1\text{--}2$ Mm     | minutes     | Convection                   |
| Supergranulation | $\sim 20\text{--}30$ Mm   | hours–days  | Large-scale convection       |
| p-modes          | global                    | minutes     | Acoustic oscillations        |
| Spots            | $\sim 10\text{--}100$ Mm  | days–months | Magnetic suppression         |
| Faculae          | $\sim 10\text{--}100$ Mm* | days–months | Magnetic flux concentrations |

\*composed of sub-Mm elements

variability in solar-type stars is therefore essential for interpreting high-precision exoplanet data.

The sources of variability in solar-type stars span a wide range of spatial and temporal scales. Small-scale convective flows produce granulation and excite acoustic oscillations known as pressure-modes (p-modes) on timescales of minutes. Larger-scale flows, such as supergranulation, evolve over hours to days, while magnetic features including starspots and faculae persist over days or months (often exceeding stellar rotational timescales). Although these phenomena arise from distinct physical mechanisms, they coexist on the stellar surface and contribute simultaneously to disc-integrated observables, complicating their separation from planetary signals. A brief overview of the dominant sources of variability in solar-type stars is given in Table 4.1. A summary of the impact on RV measurements from each source at different timescales is shown in Figure 4.1.

The aim of this chapter is to introduce the principal sources of stellar variability relevant to exoplanet detection and characterisation in solar-type stars. Particular attention is given to variability associated with surface convection, as this forms the foundation for the modelling framework developed in subsequent chapters. Note that whilst I comment on the observational impact of each source in respect to both detection and characterisation, the discussion of mitigation strategies is limited to the removal of contamination from RV times series for the purpose of exoplanet detection.

## 4.2 Pressure-mode oscillations (p-modes)

Globally occurring stellar oscillations are commonly classified according to their dominant restoring force. Pressure (p-) modes are acoustic oscillations for which

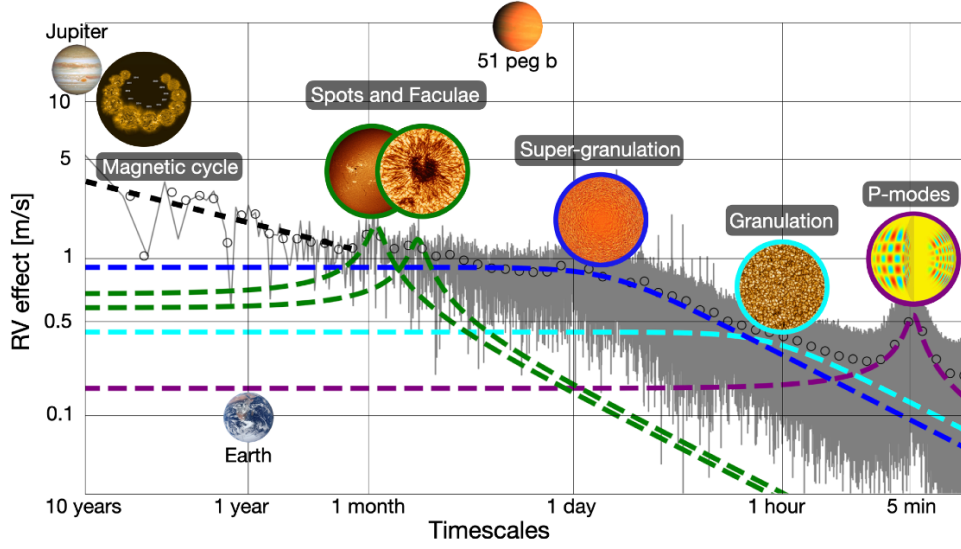


Figure 4.1: **Figure and caption from Burt et al. [2025]**. Summary of the approximate timescales and RV semi-amplitudes of the stellar phenomena that most directly impact EPRV science efforts for a Sun-like star, with the RV semi-amplitudes of Earth, Jupiter, and 51 Peg b for reference. These phenomena span timescales from minutes to decades and RV semi-amplitudes of  $\text{cm s}^{-1}$  to dozens of  $\text{m s}^{-1}$  which poses significant challenges for designing RV survey and analysis techniques that can accurately sample, model, and mitigate their impacts. The background grayscale image represents the solar power spectrum density from Al Moulla et al. [2023] with fitted contributions for the different stellar phenomena as colored dashed lines. Adapted from Al Moulla et al. [2023] and a figure concept from Ryan Rubenzahl.

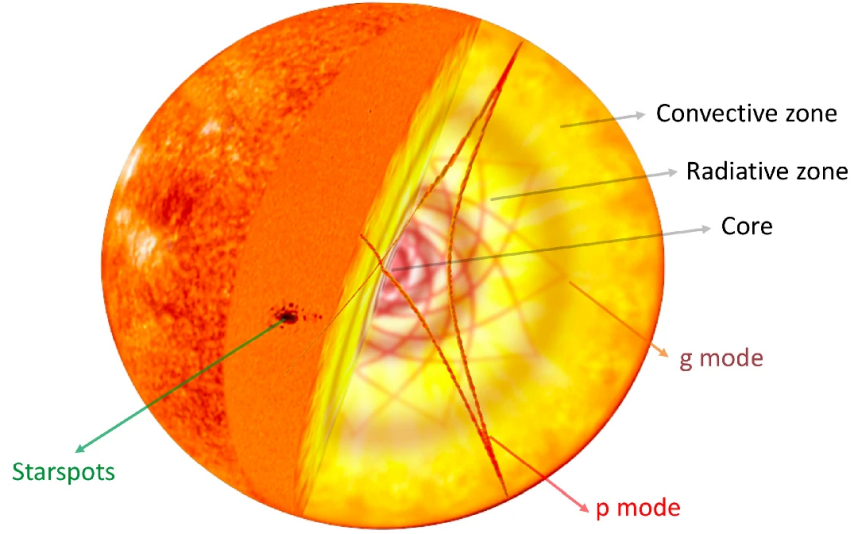


Figure 4.2: **Figure and caption from García & Ballot [2019]**. Artistic view of the structure of a typical cool main-sequence solar-like pulsating star where two modes are propagating, a low-degree p mode and a g mode. The structure of the star is divided in two main regions: the inner radiative zone (including the core where the nuclear reactions take place) and the external convective zone. In the Sun, the convective envelope extends inward from the surface 30% of its radius

pressure provides the restoring force, while gravity (g-) modes are buoyancy-driven oscillations, restored by gravity acting on density perturbations. The two mode types probe different regions of the stellar interior and occupy distinct frequency regimes [Aerts et al., 2010].

In solar-type stars, p-modes dominate observationally. These modes have their largest amplitudes in the outer layers of the star and are efficiently excited by turbulent convection in the near-surface convective envelope. In contrast, g-modes are confined primarily to the radiative interior, where convective driving is inefficient, and their amplitudes at the stellar surface are expected to be extremely small (See Figure 4.2). As a result, g-modes have not been robustly detected in disc-integrated observations of main-sequence Sun-like stars, whereas p-modes are readily observed in both photometric and spectroscopic data [Chaplin & Miglio, 2013; Appourchaux et al., 2010].

The oscillations considered in this work are therefore pressure modes. These p-modes arise from stochastic excitation by near-surface convection, producing a spectrum of damped, global standing waves with characteristic periods of  $\sim 5$  minutes in the Sun,

and ranging from a few minutes to tens of minutes in solar-type stars depending on their stellar properties [Ulrich, 1970; Goldreich & Keeley, 1977].

#### 4.2.1 Physical origin

In solar-type stars, the convective envelope extends close to the stellar surface. The vigorous, turbulent nature of convection in these layers produces broadband acoustic noise, which continuously excites and damps oscillation modes. As a result, p-modes have finite lifetimes (typically a few days in the Sun) and appear as Lorentzian peaks in the frequency domain rather than as coherent, long-lived oscillations [Chaplin & Miglio, 2013].

Each p-mode is characterised by three quantum numbers: the radial order  $n$ , the angular degree  $\ell$ , and the azimuthal order  $m$ . Low-degree modes ( $\ell \lesssim 3$ ) dominate disc-integrated observations because higher-degree modes undergo strong cancellation across the stellar disc. For Sun-like stars, the strongest p-mode power is concentrated around a characteristic frequency,  $\nu_{\max}$ , which scales approximately with the acoustic cut-off frequency and hence with surface gravity and effective temperature [Brown et al., 1991; Kjeldsen & Bedding, 1995].

#### 4.2.2 Observational impact

P-modes produce quasi-periodic variations in both stellar brightness and apparent radial velocity on timescales of a few minutes (for solar-type stars,  $\sim 5$  min). In integrated sunlight, the rms radial velocity amplitude of the dominant modes is of order  $0.5\text{--}1\text{ m s}^{-1}$  [Kjeldsen & Bedding, 1995; Chaplin et al., 2019]. Photometric amplitudes are typically a few parts-per-million (ppm) in the Sun, increasing for more evolved stars [Huber et al., 2011]. Because the modes are stochastically excited and damped, the signal is not strictly periodic but instead appears as a comb of Lorentzian peaks modulated by a Gaussian-like power envelope centred on  $\nu_{\max}$  (see Figure 4.3).

In radial velocity data, p-modes manifest as rapid Doppler shifts that increase short-timescale scatter. They do not mimic planetary signals in frequency space, as their characteristic periods (minutes) are far shorter than typical orbital timescales (days to years). However, they can significantly degrade instantaneous RV precision if

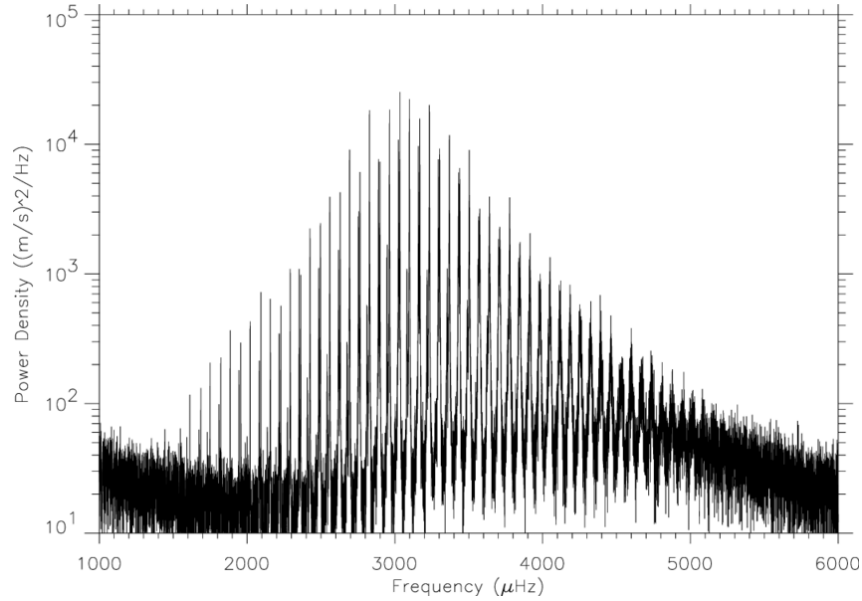


Figure 4.3: **Figure from Lazrek et al. [1997].** Example power spectrum of solar acoustic (p-mode) oscillations. Turbulent convection in the outer layers of the Sun continuously excites and damps these modes, giving them finite lifetimes. As a result, each mode appears as a Lorentzian-shaped peak in the frequency domain rather than a sharp, discrete line.

exposure times are short compared to the oscillation period. In disc-integrated spectra, p-modes behave predominantly as global, coherent velocity shifts of the stellar surface and therefore do not introduce variations in shapes of absorption lines comparable to those produced by granulation or starspots.

In high-precision photometry, p-modes contribute a high-frequency component to stellar variability. For transit observations, the oscillation signal is largely averaged out over the several-hour duration of a typical transit. However, p-modes are astrophysically valuable in this context: asteroseismic analysis of the oscillation spectrum yields precise stellar masses and radii, which directly propagate into improved planetary parameters [Huber et al., 2013; Chaplin & Miglio, 2013]. In this sense, while p-modes constitute a source of stellar “noise” for exoplanet detection on minute timescales, they simultaneously provide one of the most powerful diagnostics of stellar structure and age.



### 4.2.3 Mitigation strategies

The most effective mitigation strategy for p-mode variability in radial velocity observations is temporal averaging. P-modes in solar-type stars have characteristic periods of approximately 3–15 minutes, with amplitudes that can reach several  $\text{m s}^{-1}$  for evolved stars [Kjeldsen & Bedding, 1995; Chaplin et al., 2011]. By using exposure times that are long compared to these dominant oscillation periods, the stochastic p-mode signals can be efficiently averaged out, significantly reducing their contribution to the overall RV scatter [Dumusque et al., 2011; Meunier et al., 2015; Chaplin et al., 2019]. When longer exposures are impractical due to telescope scheduling constraints or photon-limited observations of faint targets, multiple short exposures can be combined to achieve similar mitigation effects [Chaplin et al., 2019].

The residual p-mode amplitude after temporal averaging depends critically on stellar parameters and can be predicted with reasonable accuracy. Chaplin et al. [2019] provides guidelines for selecting exposure durations tailored to stellar properties (mass, luminosity, and effective temperature), with the goal of suppressing oscillation-induced RV variations to levels of either  $0.1 \text{ m s}^{-1}$  or the Earth-analog reflex amplitude for the target star. Their framework accounts for the intrinsic stochastic nature of solar-like oscillations and recommends choosing exposure times at the telescope that can later be binned as needed, rather than committing to fixed long exposures that cannot be subdivided for analysis. As instrumental precision approaches the  $0.1 \text{ m s}^{-1}$  level with next-generation spectrographs, such tailored observing strategies become essential for maximizing planet detection sensitivity.

In addition to temporal averaging, p-mode variability can be modeled statistically when sufficient data quality and temporal coverage are available. Gaussian process (GP) frameworks have proven particularly effective for modeling correlated stellar noise, including the contribution from oscillations [Rajpaul et al., 2015]. When the observing cadence is not optimized for temporal averaging (e.g., sparse or irregularly sampled data), p-modes can be treated as an additional white-noise or correlated-noise term in RV analyses. The appropriate treatment depends on the exposure time relative to the oscillation periods and the overall sampling pattern of the observations [Dumusque et al., 2011].

For stars with extensive, high-cadence time series, particularly from dedicated asteroseismic surveys or intensive RV monitoring campaigns, it is in principle possible to perform detailed asteroseismic modeling to characterize the oscillation spectrum

explicitly and subtract the p-mode signal from the RV measurements [Chaplin & Miglio, 2013]. This approach requires detecting individual oscillation modes with sufficient signal-to-noise to measure their frequencies, amplitudes, and linewidths. However, such detailed characterization is rarely feasible for typical planet-search observations, which are generally optimized for long-term stability and wide target coverage rather than the high-cadence, continuous monitoring required for asteroseismology. As a result, temporal averaging remains the most practical and widely implemented mitigation strategy for p-mode noise in exoplanet RV surveys.

Overall, while p-modes are an unavoidable consequence of stochastic excitation by convection in solar-type stars, their short timescales (minutes), well-understood statistical properties, and predictable dependence on fundamental stellar parameters make them one of the more tractable sources of stellar variability in high-precision exoplanet observations. When combined with appropriate observing strategies and, where necessary, statistical modeling frameworks, p-mode noise can be reduced to levels that do not significantly impair the detection of low-mass planets, even in the habitable zones of nearby Sun-like stars.

### 4.3 Granulation

Stars are not static objects with homogeneous surfaces. The stellar “surface”, typically identified with the photosphere, is structured by convection into a continuously evolving granulation pattern. This pattern consists of bright, hot, up-flowing regions of plasma known as granules, separated by narrow, darker intergranular lanes where cooler material descends back into the stellar interior (see Figure 4.4). In the Sun, individual granules typically have characteristic horizontal scales of  $\sim 1\text{--}2$  Mm and lifetimes of a few minutes, after which they fragment, merge, or are replaced by newly emerging granules [Nordlund et al., 2009; Gray, 2005].

The granulation pattern is inherently time-dependent. Individual granules continuously evolve as rising flows fragment, merge, or are disrupted by radiative cooling and shear, while new granules emerge to replace them. The resulting surface velocity field is highly structured and asymmetric, with upflows occupying a larger area but downflows reaching higher velocities. Although individual granules are short-lived, their collective behaviour sustains persistent fluctuations in intensity and Doppler velocity that contribute to stellar variability in disc-integrated observations.

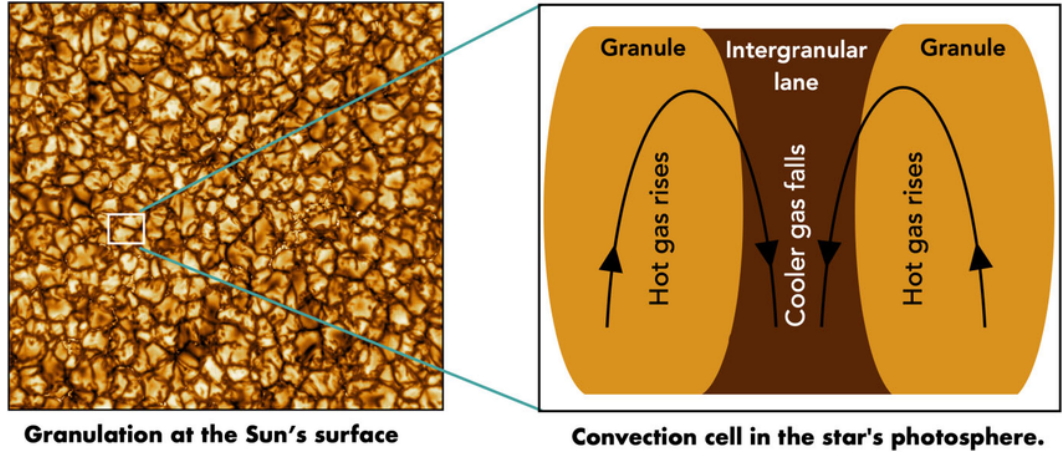


Figure 4.4: **Figure from Dalal et al. [2023]**. Left-hand panel: A  $36,500 \times 36,500$   $\text{km}^2$  region of the solar surface, with a clearly visible granulation pattern. Right-hand panel: Illustration of the cross-section of a granular cell, spanning approximately 30-1500 km in length, where hot gas rises in the granules (orange region) and falls in the intergranular lane (dark brown region).

#### 4.3.1 Physical origin

Granulation arises from convective energy transport in the outer layers of solar-type stars. Energy generated in the stellar interior is carried outward by convection in the near-surface layers, where hot, buoyant plasma rises toward the photosphere. As this material reaches regions of low density and optical depth, it cools rapidly through radiative losses, reducing its buoyancy and causing it to overturn and sink back into the stellar interior through narrow intergranular lanes. This process establishes a pattern of broad, slow upflows surrounded by fast, concentrated downflows, producing the characteristic brightness and velocity contrast observed in granulation [Nordlund et al., 2009].

#### 4.3.2 Observational Impact

Granulation is intrinsically asymmetric in both its brightness and velocity fields (see Figure 4.5). Bright, hot granules correspond to broad regions of rising plasma that occupy a larger fraction of the stellar surface, while the cooler intergranular lanes are narrower, darker, and host concentrated downflows. The lanes' reduced surface coverage and lower intensity mean that their spectroscopic contribution is compar-

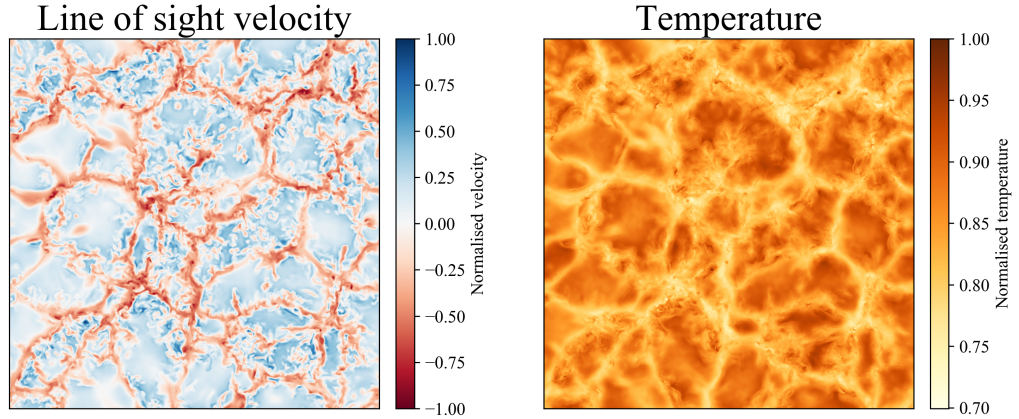


Figure 4.5: Line of sight velocity and temperate values from MURaM [Vögler et al., 2005] on the “optical surface” of the sun for a  $9 \times 9 \text{ Mm}^2$  region at disc center. The optical surface in this instance is defined as the height where the optical depth  $\tau = 1$  for  $\lambda = 500 \text{ nm}$ .

atively weak. As a result, the disc-integrated spectrum is dominated by the signal from blueshifted granules, resulting in a net convective blueshift in spectroscopic observations [Dravins et al., 1981; Gray, 2009].

The formation of spectral lines is strongly modulated by this convective structure. Absorption lines formed in granules experience a higher local continuum intensity and sample rising, blueshifted material, leading to deeper and blueshifted line cores relative to those formed in intergranular lanes, where the continuum is weaker and the plasma is redshifted. Because granules contribute disproportionately to the emergent flux, their line profiles dominate the disc-integrated signal. When the contributions from granules and lanes are combined, the resulting line profile is asymmetric, with the line wings and core sampling different velocity regimes across the stellar surface [Dravins, 1982; Asplund et al., 2000].

This asymmetry is commonly characterised using the line bisector, which traces the midpoint of the line profile as a function of depth. In solar-type stars, the bisector typically exhibits a characteristic C-shape. The shape and velocity of this bisector is sensitive to the underlying convective dynamics and evolves in time as the granulation pattern changes, making granulation a key contributor to both line-profile variability and RV variability in high-precision spectroscopic observations [Cegla, 2019].

The RV variability arises from inconsistencies in the net convective blueshift due to changes in granulation patterns. Current estimates of the solar RV rms caused by granulation range from  $\sim 0.3 \text{ m s}^{-1}$  [Elsworth et al., 1994; Dalal et al., 2023; Lakeland et al., 2024] to  $\sim 0.4 \text{ m s}^{-1}$  [Collier Cameron et al., 2019] to  $\sim 0.8 \text{ m s}^{-1}$  [Meunier et al., 2015]. All of these values place granulation as an important contributor to the contamination of the RV signal on a solar-like star imprinted by an Earth analogue ( $\sim 0.1 \text{ m s}^{-1}$ ).

In addition to its impact on RV measurements, granulation also affects exoplanet characterisation through transmission spectroscopy. During a transit, the planet occults different regions of the stellar disc whose spectral properties vary systematically with limb angle due to centre-to-limb variations (CLV) in both intensity and line shape. Granulation contributes to this CLV because the contrast between bright granules and dark intergranular lanes, as well as their projected velocities, changes towards the limb. Near disc centre, vertical convective motions dominate; towards the limb, horizontal flows contribute more significantly and the apparent line asymmetries and equivalent widths are altered [Dravins, 1982; Asplund et al., 2000]. As a result, the stellar spectrum blocked by the planet is not uniform across the transit chord.

If unaccounted for, these spatially dependent line-profile variations can imprint spurious signals in the residual transmission spectrum [Czesla et al., 2015; Yan et al., 2017]. The problem is compounded by the intrinsic temporal variability of granulation, which introduces stochastic fluctuations in the stellar line shapes during transit observations [Chiavassa et al., 2017]. Consequently, accurate planet characterisation requires forward modelling of spatially resolved stellar spectra that incorporate realistic granulation patterns. The use of 3D atmospheric models is of high importance due to horizontal flow contributions [Dravins & Nordlund, 1990]. This topic is further discussed in Chapter 5.

### 4.3.3 Mitigation strategies

Granulation-driven variability is challenging to mitigate because it arises from a continuously evolving surface velocity field spanning a broad range of spatial and temporal scales. Unlike p-mode oscillations, which have well-defined characteristic frequencies and can be efficiently suppressed through temporal averaging, granulation exhibits power across a wide range of frequencies with a characteristic timescale

of approximately 5–10 minutes for solar-type stars [Meunier et al., 2015; Dalal et al., 2023]. Mitigation strategies have evolved along two complementary paths: statistical characterisation of granulation in the time and frequency domains, and physically motivated diagnostics that link spectroscopic variability directly to convective flows.

**Statistical and frequency-domain approaches** One class of approaches treats granulation as a stochastic noise source whose statistical properties can be characterised in the frequency domain. Studies of solar and stellar RV power spectra have shown that granulation contributes significant low-frequency power, typically modeled using Harvey functions (power-law profiles with characteristic timescales) in the RV power spectral density [Lefebvre et al., 2008; Meunier et al., 2015]. Characterising the power spectrum provides direct insight into the dominant variability timescales and amplitude of granulation, allowing observing strategies to be tailored accordingly. In particular, knowledge of the characteristic turnover frequency informs the choice of exposure time and cadence; if observations are integrated over timescales comparable to or longer than the dominant granulation timescale, some stochastic fluctuations can be averaged down.

Dumusque et al. [2011] used stellar simulations to demonstrate that carefully optimised observing strategies could significantly reduce the impact of short-timescale stellar noise sources, including granulation and oscillations, on long-period planet searches. They found that three ten minute exposure measurements per night, spaced by 2 hours provided the most efficient averaging of granulation and oscillations, and were optimistic that structured cadence and exposure choices could lower the effective stellar noise floor enough to detect Earth analogues. However, Meunier et al. [2015], using Sun-as-a-star observations, found that although temporal averaging over  $\sim 10$ – $15$  minutes partially mitigates granulation signals, a substantial fraction of the power extends to longer timescales and therefore cannot be efficiently suppressed through simple averaging alone. This highlights an important limitation: while characterising the power spectrum allows optimisation of cadence and integration time, granulation variability is distributed across a continuum of timescales rather than concentrated at a single dominant frequency, limiting the effectiveness of simple temporal averaging.

Such power-spectrum-based methods therefore provide valuable guidance for survey design, noise budgeting, and setting realistic detection limits, but they do not by

themselves disentangle convective signals from planetary Doppler shifts in individual observations. More recent work has refined predictions for the intrinsic granulation noise floor as a function of stellar parameters. Dalal et al. [2023] developed a simple analytical model for convective blueshift and RV dispersion due to granulation across a wide range of FGK stars, finding that stars with higher metallicities exhibit lower RV dispersion for a given mass range, a prediction corroborated by magnetohydrodynamic (MHD) simulations. Their formulae enable targeted selection of optimal stellar hosts for extreme precision radial velocity (EPRV) surveys by identifying stars where granulation noise is intrinsically minimized.

**Physically motivated diagnostics and line-by-line techniques** A complementary and increasingly powerful line of work uses forward modelling of stellar surface convection to predict the imprint of granulation on spectroscopic observables, particularly spectral line shapes and bisector asymmetries. Using three-dimensional magnetohydrodynamic simulations of solar photospheres, Cegla et al. [2013, 2018, 2019] demonstrated that granulation-induced RV shifts correlate strongly with diagnostic measures of line profile asymmetry, such as the bisector inverse slope (BIS). A schematic of the BIS and other bisector diagnostics is shown in Figure 4.6. The physical basis for these correlations lies in the differential velocities of granular upflows and intergranular downflows, which distort line profiles in a characteristic manner. Applied to Sun-as-a-star simulations, these physically motivated diagnostics were shown to reduce granulation-driven radial velocity scatter by several tens of percent, highlighting their promise for  $\text{cm s}^{-1}$  precision radial velocity surveys.

A different approach involves the development of empirical models that use spatially and temporally resolved solar observations to simulate realistic granulation-driven spectral variability. Palumbo et al. [2022] introduced the GRanulation And Spectrum Simulator (GRASS), a tool designed to create time-series synthetic spectra with granulation-driven variability from disc-resolved observations of solar absorption lines. Unlike computationally expensive MHD simulations, GRASS leverages actual solar data to efficiently generate synthetic stellar spectra with known barycentric velocity, providing a controlled testbed for evaluating mitigation techniques. In follow-up work, Palumbo et al. [2024] extended GRASS to an expanded library of 22 solar lines and systematically tested the efficacy of bisector-based mitigation strategies under realistic observational conditions. They confirmed that summary statistics of bisector shape (e.g., bisector inverse slope) are strongly correlated with

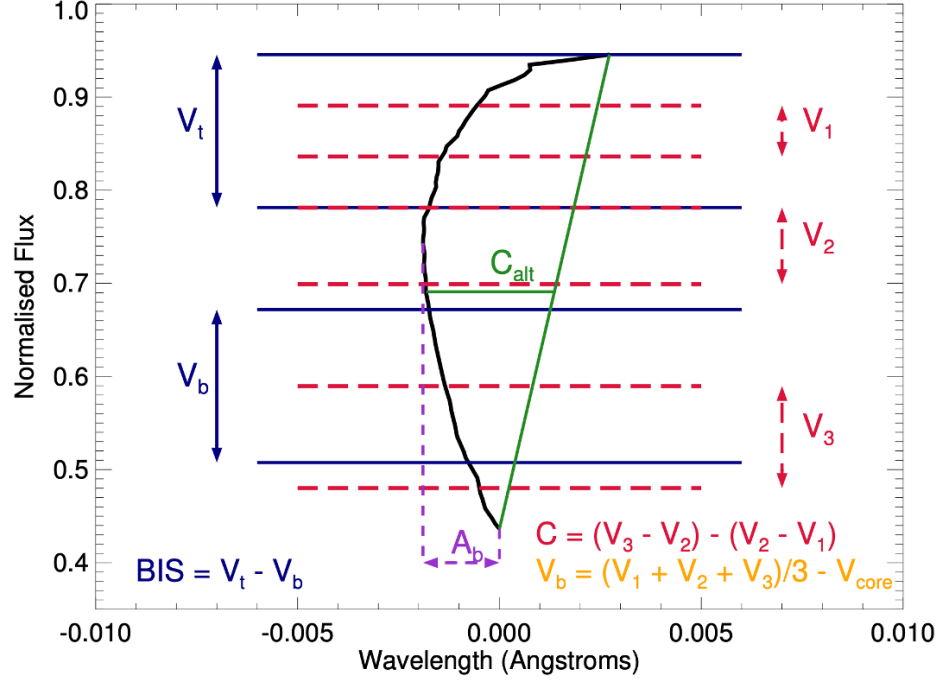


Figure 4.6: **Figure and caption from Cegla et al. [2019]**. Schematic to illustrate the various bisector diagnostics, with an example bisector (from Kurucz et al. [1984]) shown in black. BIS is defined as the difference between an average region near the top and bottom of the bisector (shown in blue).  $C$  is the difference between three average regions (shown in red), and the  $V_b$  is average of those relative to the line core (defined in orange).  $A_b$  is the difference between the line core and the most blue-shifted region of the bisector (shown in purple), and  $C_{alt}$  is the perpendicular distance between the bisector and the midpoint of a line connecting the top and bottom of the bisector (shown in green).



granulation-induced RV variations at high spectral resolution ( $R \gtrsim 200,000$ ) and high signal-to-noise ratio. However, they also demonstrated that these correlations weaken or disappear at the typical spectral resolutions and SNRs of current EPRV instruments when considering individual lines. Crucially, Palumbo et al. [2024] suggests that with the information content of a full spectrum, it is possible in principle to achieve a  $\gtrsim 30\%$  reduction in granulation-induced RMS RV variability. They demonstrated this by constructing artificially expanded spectra by repeating multiple instances of individual lines, thereby averaging out uncorrelated noise while preserving the coherent granulation signal. The achievable reduction is most strongly limited by the spectral resolution of the observing instrument, with ultra-high-resolution spectrographs like ESPRESSO [Pepe et al., 2013] offering the best prospects for resolving and mitigating convective variability in bright stars.

However, there are two key limitations for empirical approaches such as GRASS. The first being the potential for contamination via tellurics, residual p-modes, supergranulation or meridonal flows; the true isolation of the granulation signal in observed spectra cannot be demonstrated unambiguously and therefore cannot be rigorously verified. The second being a lack of adaptability for different stellar conditions; the method is reliant on extremely precise measurements and is therefore currently restricted to the solar case.

The key limitation of physically motivated line-by-line approaches in general is the critical dependence on the spectral resolution and signal-to-noise ratio of the observations. Ultra-high-resolution spectrographs such as ESPRESSO ( $R \sim 190,000$ ) and PEPSI ( $R \sim 270,000$ ) offer resolving power with potential to detect subtle line-shape variations and bisector asymmetries induced by granulation. Nevertheless, even with these capabilities, the challenge remains formidable for individual spectral lines at typical EPRV data quality, prompting the development of approaches that combine information across many lines [Al Moulla et al., 2022].

Moreover, correlations between granulation-induced radial velocity shifts and line-shape diagnostics are not uniform across spectral lines, as evident in Palumbo et al. [2024]. Because different lines form at different heights in the stellar atmosphere, they sample distinct velocity and temperature structures within the convective flow [Dravins, 1982; Asplund et al., 2000]. Consequently, the strength and form of these correlations depend on line formation depth and intrinsic line properties, underscoring the importance of modelling individual spectral lines in order to characterise

and understand this depth-dependent behaviour (e.g: Sowmya et al. 2025).

It is clear that granulation mitigation requires not only high-quality data but also sophisticated analysis techniques that can extract correlated information from across the spectrum while avoiding overfitting or inadvertently removing genuine planetary signals. The creation of synthetic time-varying spectral lines with known barycentric velocities, either through simulations or empirical methods, provide a valuable validation tool for proposed mitigation methods. They also provide a means of establishing realistic expectations for the degree to which granulation noise can be suppressed in practise. This is the focus of Chapters 7 and 8.

**Current observational implementation and prospects** Despite the advances outlined above, granulation mitigation remains largely aspirational in most current EPRV surveys. While statistical characterisation can incorporate granulation as part of a broader correlated-noise model, the line-by-line and bisector-based techniques that offer the most promise for physical mitigation require data quality (in terms of both resolution and SNR) that is only potentially achievable for the brightest targets with state-of-the-art instruments. As extreme precision spectrographs become more widely deployed and observing strategies are optimised to balance temporal coverage with per-observation SNR, the integration of granulation-specific diagnostics into standard RV pipelines is expected to become increasingly feasible.

Overall, while granulation represents a significantly more challenging noise source than p-mode oscillations, ongoing efforts are steadily advancing our ability to characterise, model, and ultimately mitigate its impact on high-precision exoplanet detection and characterisation.

## 4.4 Supergranulation

In addition to granulation, stellar photospheres exhibit larger scale flow patterns known as supergranulation, whose physical origin remains an open question. Supergranulation refers to a pattern of predominantly horizontal flows on scales of  $\sim 20\text{--}35$  Mm, an order of magnitude larger than granules, with characteristic lifetimes of  $\sim 1\text{--}2$  days [Leighton et al., 1962; Rieutord & Rincon, 2010]. The phenomenon is detectable through Doppler measurements of solar surface flows, as shown in Figure

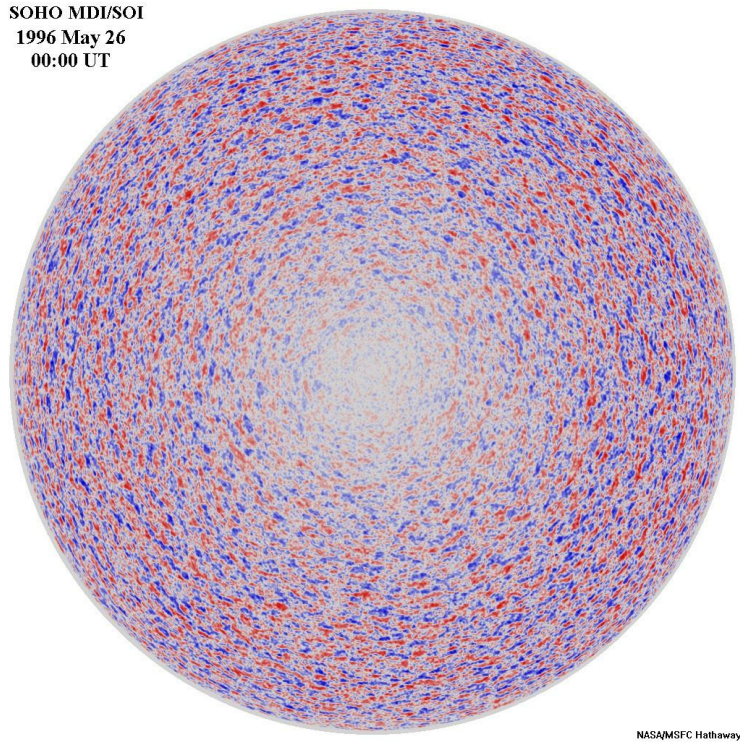


Figure 4.7: Image taken from [solarscience.msfc.nasa.gov](http://solarscience.msfc.nasa.gov). Doppler shift measurements on the Sun from the Michelson Doppler Imager (MDI) on board the Solar and Heliospheric Observatory (SOHO) spacecraft. Red sections indicate movement away from the observer, whereas blue sections indicate movement towards the observer. Darker colouring indicates higher magnitude velocity flows. The velocity magnitude being low at disc center and increasing towards the limb is highly suggestive of horizontal flows, an artefact of supergranulation.

#### 4.7.

Supergranular cells are characterised by broad horizontal outflows from cell centres, with velocities of a few hundred  $\text{m,s}^{-1}$ , and converging downflows at cell boundaries. These flows are observed in the photosphere, while their boundaries coincide with the chromospheric network, where magnetic flux is swept and concentrated by the horizontal motions [Simon & Leighton, 1964; Rieutord & Rincon, 2010]. While the vertical velocity component associated with supergranulation is weak compared to that of granulation, its large spatial scale and long coherence time allow it to contribute significantly to disc-integrated velocity variability.

#### 4.4.1 Physical origin

The physical origin of supergranulation remains an active area of research. Unlike granulation, which is well understood as the direct manifestation of near-surface convective overturning, the driving mechanism of supergranulation is less clear. Proposed explanations include the collective interaction of granules leading to large-scale flow organisation and the role of rotational or magnetic constraints on convection [Rincon & Rieutord, 2018]. Numerical simulations have reproduced supergranular-like flow patterns under certain conditions (e.g: Ustyugov 2006), but no single mechanism has yet achieved consensus. An in-depth review of the competing theoretical frameworks proposed to explain supergranulation is beyond the scope of this thesis. Please see [Rincon & Rieutord, 2018] for a detailed discussion.

#### 4.4.2 Observational impact

Supergranulation contributes to stellar variability primarily through its associated velocity field rather than intensity fluctuations. The dominant contribution arises from large-scale horizontal flows, which are largely perpendicular to the line of sight at disc centre but become projected along the line of sight toward the stellar limb, producing low-frequency Doppler shifts on timescales of hours to days.

The vertical velocity component is comparatively weak ( $\sim 20\text{--}30\text{ m s}^{-1}$ ) and is further suppressed by limb projection effects. While incomplete cancellation of these vertical motions across the stellar disc can produce a residual radial velocity signal, this contribution is secondary to that arising from the horizontal flow field [Meunier et al., 2015].

Sun-as-a-star observations have demonstrated that supergranulation contributes power at very low frequencies in radial velocity time series, often dominating over granulation on timescales longer than several hours [Meunier et al., 2015]. Despite slower velocities than granulation, the large spatial scale of supergranulation ( $\sim 30\text{--}35\text{ Mm}$ ) compared to granulation ( $\sim 1\text{ Mm}$ ) leads to larger disc-integrated RV variations. Various studies have estimated the amplitude of supergranulation-induced RV signals in the Sun to be in the range  $0.5\text{--}1.0\text{ m s}^{-1}$  using both simulations [Meunier et al., 2015; Meunier & Lagrange, 2019, 2020] and Sun-as-a-star observations [Al Moulla et al., 2023; Lakeland et al., 2024; O’Sullivan et al., 2025]. This makes supergranulation the second-largest stellar variability signal after magnetic activity in

the Sun and a significant limiting factor in the RV detection of Earth-like exoplanets [Meunier & Lagrange, 2019, 2020]. Because of its long coherence time ( $\sim 24\text{--}48$  h), supergranulation-induced variability cannot be efficiently averaged down with short exposures, making it a fundamental noise source for Doppler planet searches targeting  $\text{cm s}^{-1}$  precision.

In photometry, the intensity signature of supergranulation is substantially weaker and more ambiguous than that of granulation. This weak thermal signature has historically been one of the main challenges in identifying the physical origin of supergranulation [Rincon & Rieutord, 2018]. Nevertheless, for extremely high-precision photometric surveys such as transit observations with PLATO, supergranulation may in principle contribute detectable signatures, though these are expected to be swamped by temporal stellar variability from other sources [Morris et al., 2020].

#### 4.4.3 Mitigation strategies

Mitigation of supergranulation-driven radial velocity variability is particularly challenging. Its long timescale ( $\sim 24\text{--}48$  h) renders high-cadence averaging ineffective, and its weak photometric signature limits the utility of simultaneous photometry as a correction tool. As a result, mitigation efforts have largely focused on statistical characterisation rather than direct removal.

Observational strategies based on optimising the temporal sampling have been explored but face fundamental limitations. Meunier et al. [2015] demonstrated through simulations that the supergranulation signal is highly resistant to temporal averaging. Unlike shorter-timescale signals that can be averaged down with multiple exposures per night, supergranulation’s long coherence time means that averaging between 30 min and 2 h does not affect detection limits [Meunier et al., 2015]. This resistance to brute-force averaging makes supergranulation particularly problematic for exoplanet detection, as detection limits above  $1 M_{\oplus}$  can easily be reached for long-period planets even with extended total observing time [Meunier et al., 2015].

Stochastic modelling approaches have become the most widely adopted mitigation strategy. Power-spectrum-based methods model supergranulation as a low-frequency stochastic process, typically using a Harvey-like power spectral density similar to what is used for granulation. These models enable the supergranulation contribution to be incorporated into noise models for RV surveys [Meunier

et al., 2015; Al Moulla et al., 2023]. More sophisticated implementations use Gaussian process (GP) regression to model supergranulation directly in the time domain. O’Sullivan & Aigrain [2024]; O’Sullivan et al. [2025] developed scalable two-component GP models using overdamped harmonic oscillator kernels to model supergranulation simultaneously with other stellar variability sources in Sun-as-a-star observations. The GP kernel employed typically takes the form of a stochastically-driven damped harmonic oscillator, which produces a power spectral density similar to the Harvey law but with a steeper asymptotic power-law slope (index 4 rather than 2) at high frequencies [O’Sullivan et al., 2025]. These methods allow direct measurement of the variance and characteristic timescale of supergranulation from RV time series.

However, a critical limitation of GP-based approaches is that supergranulation cannot be treated as stationary over long observational baselines. Recent Sun-as-a-star observations have shown that the characteristic time-scale of the supergranulation component varies significantly over the solar magnetic cycle, being longest at activity minimum and strongly anti-correlated with sunspot number [O’Sullivan et al., 2025]. This implies that GP models trained on short baselines may not accurately represent supergranulation behaviour over multi-year campaigns, and that a single set of hyperparameters for the supergranulation amplitude and time-scale may be insufficient over an activity cycle.

Moreover, it is important to note that these stochastic models are fundamentally phenomenological. While they can reproduce the statistical properties of low-frequency variability and provide estimates of characteristic timescales and amplitudes, they do not uniquely identify the underlying physical origin of the signal. In particular, similar power spectral signatures may arise from different physical processes, meaning that a fitted “supergranulation” component in a GP or power spectrum model does not constitute direct evidence that the variability is driven by supergranulation.

Currently, no direct method exists to remove supergranulation signatures from individual RV measurements. Unlike other variability sources, supergranulation lacks robust observational proxies due to its predominantly horizontal flow pattern and negligible intensity contrast [Langfellner et al., 2016; Rincon & Rieutord, 2018]. Consequently, supergranulation remains one of the most difficult stellar variability sources to mitigate and represents a key limitation for the detection of long-period,



low-mass exoplanets around Sun-like stars [Meunier & Lagrange, 2020; Lakeland et al., 2024].

## 4.5 Spots and Faculae

In addition to convection-driven surface variability, magnetic activity produces long-lived surface features that significantly modulate both the brightness and spectral appearance of Sun-like stars. The most prominent of these are spots and faculae: regions that are cooler or hotter than the surrounding photosphere, respectively. These features are observed across a range of spectral types and magnetic activity levels. Individual spots and faculae evolve on timescales of days to weeks, while their overall coverage, distribution, and emergence rates are modulated by stellar rotation and longer-term magnetic activity cycles (e.g: Saar & Donahue 1997; Boisse et al. 2011).

Sunspots are dark, relatively cool regions in the photosphere where intense magnetic fields (1–3 kG) inhibit convective heat transport, leading to temperature deficits of several hundred to a few thousand kelvin relative to the quiet photosphere [Solanki, 2003]. They consist of a central dark umbra and a surrounding penumbra with filamentary structure (see Figure 4.8). On other stars, analogous starspots are inferred from rotational modulation of photometric light curves and Doppler imaging, often covering a much larger fraction of the stellar surface than solar spots (e.g: Boisse et al. 2011). Recent work has also resolved starspots using high-resolution transit spectroscopy, through line profile changes during spot occultations [Kunovac et al., 2025].

Faculae are bright magnetic regions associated with concentrations of magnetic flux that enhance local intensity relative to the quiet photosphere, particularly near the stellar limb where the geometric contrast is greatest [Shapiro et al., 2016]. See Figure 4.9 for an image of spot and faculae coverage on the sun.

The term “plage” is often used to refer to the chromospheric counterpart of photospheric faculae, that is, the same magnetic structures observed in chromospheric emission lines (such as Ca II K or H $\alpha$ ) rather than in continuum wavelengths. Since faculae and plage represent the same underlying physical phenomenon observed at different atmospheric heights, the term “faculae” is used throughout this chapter

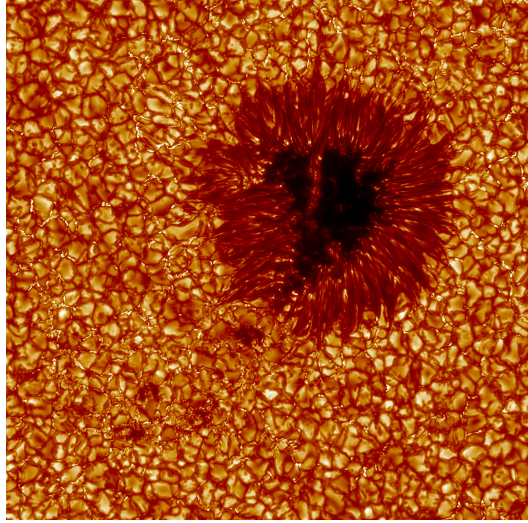


Figure 4.8: **Image credit: The Royal Swedish Academy of Sciences, V.M.J. Henriques.** A sunspot surrounded by granulation imaged by the Swedish 1-m Solar Telescope. The central dark umbra and bordering penumbra is clearly visible here. The horizontal scale of this image is 47,000km.

to refer to bright magnetic features in general, noting that observational signatures will differ depending on the wavelength regime.

#### 4.5.1 Physical origin

Spots and faculae are visible surface manifestations of magnetic fields emerging from within a star. In the Sun, they are ultimately the product of a magnetic activity cycle, in which magnetic fields are continuously generated, amplified, transported and reorganised inside the convection zone. Understanding their physical origin therefore requires first outlining how large-scale magnetic fields are produced.

**Magnetic field generation: the solar dynamo.** The Sun’s magnetic field is thought to be maintained by a dynamo process operating in its convection zone. A dynamo converts kinetic energy from plasma motions into magnetic energy. Two ingredients are essential: differential rotation (the fact that the Sun rotates at different angular speeds depending on latitude and depth) and turbulent convection in a rotating, stratified plasma. The magnetic field is often described as having two components:



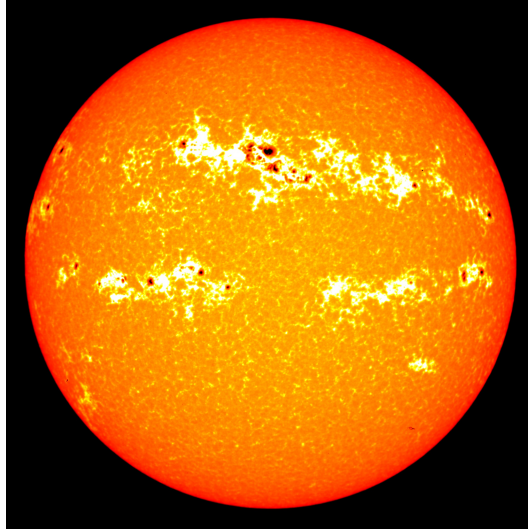


Figure 4.9: **Image from NASA/Goddard Space Flight Center Scientific Visualization Studio.** An image from the Solar Dynamics Observatory (SDO) of the sun at a time of high magnetic activity (March 28, 2001). The small black/red regions are sunspots, the larger white speckled regions are faculae.

- a **poloidal field**, which lies in meridional planes (running roughly north–south),
- a **toroidal field**, which wraps around the Sun in the east–west direction.

The  $\Omega$  effect refers to the stretching of the poloidal field into a toroidal field by differential rotation. Because the equator rotates faster than the poles, magnetic field lines are gradually wound up in the azimuthal direction. Over time, this shearing motion amplifies the toroidal magnetic component. This process is particularly efficient at the interface between the convection zone and the radiative interior known as the tachocline line, where strong radial shear is present [Parker, 1955; Charbonneau, 2010].

However, to sustain a magnetic cycle, the toroidal field must somehow be converted back into a poloidal field. This regeneration is often described in terms of the  $\alpha$  effect. In its simplest form, the  $\alpha$  effect arises because convection in a rotating star is not symmetric: rising and sinking plasma motions are twisted by the Coriolis force. These twisted motions can bend and reconnect magnetic field lines, producing a net large-scale poloidal field from an existing toroidal one [Parker, 1955; Charbonneau, 2010]. See Figure 4.10 for a schematic of a classical mean-field  $\alpha - \Omega$  dynamo.

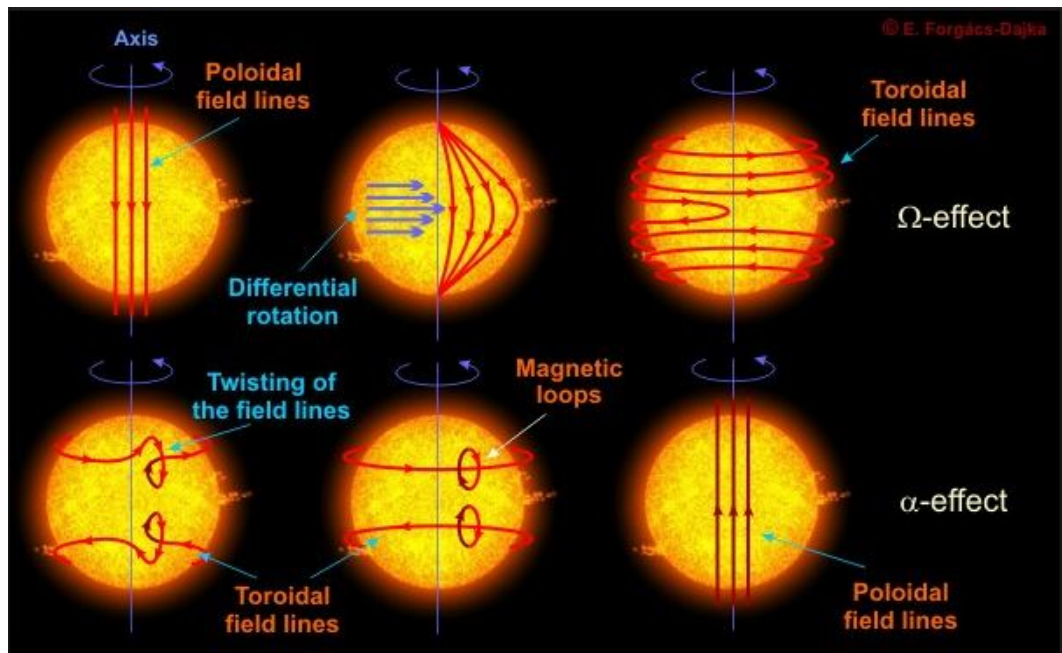


Figure 4.10: **Figure produced by Emese Forgacs-Dajka.** Schematic illustration of the classical  $\alpha$ – $\Omega$  dynamo cycle. A pre-existing poloidal magnetic field (top left) is stretched by differential rotation, generating a toroidal field through the  $\Omega$ -effect (top right). Helical convective motions in the rotating convection zone then twist and lift toroidal field lines (bottom left), producing magnetic loops that regenerate a large-scale poloidal component via the  $\alpha$ -effect (bottom right).

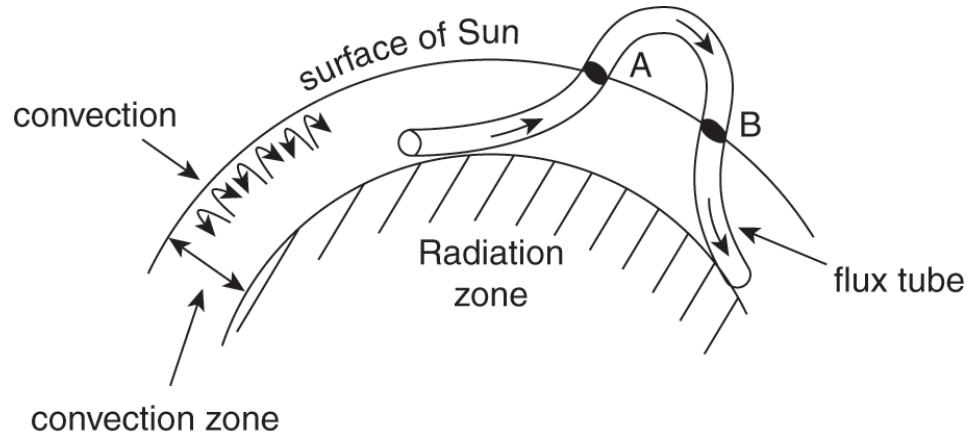


Figure 4.11: **Figure and caption from Davidson [2001].** A buoyant flux tube rises up through the convection zone and erupts through the surface of the sun. Sunspots form at A and B where the magnetic field suppresses the turbulence.

In the solar case, an important additional contribution comes from the Babcock–Leighton mechanism [Babcock, 1961; Leighton, 1969]. When strong toroidal flux rises to the surface, it emerges in the form of bipolar magnetic regions (two regions of opposite polarity). These regions are systematically tilted with respect to the equator. As they decay and their magnetic flux is transported by surface flows, they produce a net contribution to the global poloidal field, completing the magnetic cycle. For detailed reviews of the Babcock–Leighton mechanism and its role in solar cycle dynamos, see [Charbonneau, 2007] and more recent reviews such as Hazra [2021].

**Sunspots: strong magnetic flux concentrations.** Sunspots form when concentrated bundles of toroidal magnetic field rise through the convection zone and emerge at the surface. See Figure 4.11 for a schematic. If the magnetic field strength is sufficiently large (of order kilogauss in the solar case), it can locally suppress convective heat transport.

In the photosphere, magnetic pressure inside a flux concentration partially evacuates the plasma to maintain pressure balance with its surroundings. Because energy transport by convection is inhibited, less heat reaches the surface in that region. The result is a lower temperature compared to the quiet photosphere, and therefore reduced intensity. This produces the dark appearance of the sunspot umbra. The surrounding penumbra contains somewhat weaker and more inclined magnetic

fields, allowing partial convective transport and producing a filamentary structure [Solanki, 2003; Rempel & Schlichenmaier, 2011].

**Faculae: small-scale magnetic brightening.** Faculae are also associated with magnetic flux emergence, but correspond to smaller-scale, fragmented magnetic elements typically located in intergranular lanes. These magnetic flux concentrations are partially evacuated, meaning that magnetic pressure contributes to the local pressure balance and reduces the gas density within the structure. This reduction in density lowers the local opacity and depresses the optical depth unity surface, allowing radiation to escape from deeper, hotter layers of the atmosphere.

At disc centre, this effect leads to the appearance of magnetic bright points, as the observer looks directly down into the flux concentration. Toward the stellar limb, the viewing geometry changes such that the side walls of the depressed optical surface become visible. This so-called “hot-wall” effect enhances the visibility of deeper, hotter material, producing the bright facular contrast observed near the limb [Spruit, 1976; Steiner, 2005]. Radiative magnetohydrodynamic simulations confirm that these geometric and radiative transfer effects are sufficient to reproduce observed facular contrasts [Keller et al., 2004].

#### 4.5.2 Observational impact

Spots and faculae imprint characteristic signatures on both photometric and spectroscopic observations. As active regions rotate across the visible stellar disc, the flux imbalance between magnetically active and quiet regions produces quasi-periodic brightness variations at the stellar rotation period and its harmonics. The amplitude of this variability depends on the filling factor, temperature contrast, and spatial distribution of active regions, as well as the inclination of the stellar rotation axis. In optical bandpasses, spot-induced dimming often dominates short-term photometric variability because the reduced temperature of spot umbrae and penumbrae leads to a significant local deficit in emergent flux. Faculae, by contrast, exhibit a more complex centre-to-limb contrast behaviour and can contribute substantially to variability on longer timescales, particularly over magnetic activity cycles where changes in facular coverage modulate the star’s total irradiance [Shapiro et al., 2016; Yeo et al., 2020]. In solar-like stars, the relative contribution of spots and faculae depends on activity level. More active stars tend to be spot-dominated, while less active stars often exhibit faculae-dominated variability. The Sun itself

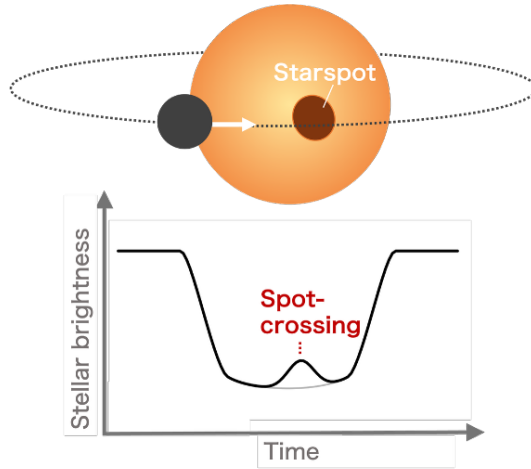


Figure 4.12: **Image credit: Mayuko Mori, Astrobiology Center.** A depiction of a light curve from a star with a transiting planet, with a visible bump upon starspot occultation.

is a well-studied example of this behaviour: despite the increased number of dark sunspots at activity maximum, the net solar irradiance is higher due to the enhanced contribution from faculae and the magnetic network, demonstrating that the Sun is faculae-dominated on activity-cycle timescales [Shapiro et al., 2016; Yeo et al., 2020].

In exoplanet detection via transit, if unocculted spots are present, the out-of-transit flux is reduced relative to that of a uniform stellar disc, causing the measured transit depth, and hence the inferred planetary radius, to be overestimated. Conversely, when a planet crosses a spot, localised anomalies appear in the transit light curve [Oshagh et al., 2013]. See Figure 4.12 for a schematic of this effect.

Beyond broadband photometry, stellar surface inhomogeneities introduce wavelength-dependent (chromatic) effects. This has an impact on transmission spectroscopy, where the transit depth is measured as a function of wavelength to infer planetary atmospheric properties. Because the contrast between active regions and the quiet photosphere is itself wavelength dependent, unocculted spots or faculae can imprint spurious slopes or spectral features in the derived transmission spectrum (e.g: Sing et al. 2011; Oshagh et al. 2014). Such stellar contamination is a major hurdle for high-precision atmospheric characterisation of small exoplanets. A common method of correcting for the wavelength-dependent activity contamination in atmospheric retrieval algorithms has been to represent spectra of magnetic features using spectra of quiet stars with differing effective temperatures [Husser et al.,

2013b]. However, work from Witzke et al. [2022] has shown this 1D approach to be inadequate compared to more detailed 3D modeling of magnetic features with magnetohydrodynamics simulations. This result has been corroborated by numerous works (e.g: Norris et al. 2023; Kostogryz et al. 2024; Smitha et al. 2025), highlighting the importance of 3D atmospheric models (further discussed in Chapter 5).

In spectroscopic observations, magnetic active regions introduce RV variability through multiple mechanisms. The suppression of convective blueshift within magnetised regions leads to a net redshifted contribution relative to the quiet photosphere, since granular upflows are inhibited and the balance between bright rising plasma and darker sinking plasma is altered. The magnitude of this effect scales approximately with the surface coverage of active regions and is often the dominant contributor to activity-driven RV signals in solar-type stars [Saar & Donahue, 1997; Haywood et al., 2016].

In addition, as spots or faculae traverse the visible hemisphere due to stellar rotation, they alter the contribution of light from different projected velocities. A dark spot on the approaching limb suppresses blueshifted light, biasing the integrated line profile toward redder velocities; when it moves to the receding limb the opposite occurs (see Figure 4.13). Analogous but contrast-dependent effects arise for faculae. These distortions of line shape generate apparent Doppler shifts that vary over the rotation period and can mimic or obscure exoplanetary signals [Saar & Donahue, 1997; Boisse et al., 2011; Lanza et al., 2011; Dumusque et al., 2014; Huélamo et al., 2008]. Line bisector shapes can also be altered due to active regions through Zeeman broadening and temperature inhomogeneities (e.g: Kunovac et al. 2025).

### 4.5.3 Mitigation strategies

Mitigating spot- and faculae-driven variability is challenging due to the non-linear, multi-timescale, and evolving nature of stellar magnetic activity. Active regions grow, decay, migrate under differential rotation, and are continuously regenerated over magnetic cycles. As a result, activity signals are neither strictly periodic nor stationary, complicating their separation from Keplerian Doppler signatures.

One class of approaches exploits simultaneous photometric monitoring. Because rotating spots produce characteristic brightness modulation, the photometric time

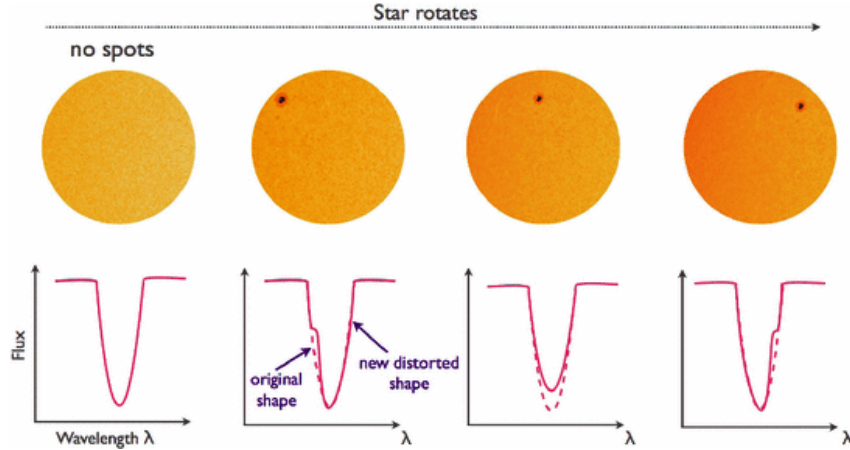


Figure 4.13: **Figure and caption from Haywood [2016]**. Diagram illustrating how flux blocked by starspots on the rotating stellar disc induces asymmetries in the spectral lines, leading to variations in RV

series can be used to constrain the distribution and evolution of active regions and predict their impact on RVs [Aigrain et al., 2012; Lanza et al., 2011]. Such methods are particularly effective when the dominant RV signal arises from rotational flux imbalance, in which asymmetric surface brightness modifies the relative contribution of Doppler-shifted regions across the stellar disc. However, photometry is less predictive when RV variability is dominated by suppression of convective blueshift within magnetised facular regions. In this regime, inhibition of granular upflows produces significant velocity shifts with comparatively small brightness contrast, leading to substantial RV variability that is only weakly correlated with the light curve [Meunier et al., 2010; Haywood et al., 2016].

A complementary strategy relies on spectroscopic activity diagnostics. Chromospheric emission indices (e.g. Ca II H&K, H $\alpha$ ), line-bisector span, full width at half maximum (FWHM), and other line-shape indicators can correlate with activity-induced RV variations [Boisse et al., 2011; Haywood et al., 2016; Lanza et al., 2018]. Empirical decorrelation techniques model the RV signal as a function of one or more such tracers, removing components attributable to magnetic variability. More flexible statistical frameworks, such as GP regression with quasi-periodic kernels, have proven particularly powerful in modelling rotationally modulated and evolving signals without requiring explicit spot maps [Rajpaul et al., 2015; Haywood et al., 2014; Barragán et al., 2022]. While GP models can successfully capture the covariance structure of stellar activity, care must be taken to avoid absorbing genuine planetary signals, especially when orbital and rotation periods are comparable.

Physically motivated forward models provide a more explicit approach. These models construct parameterised representations of stellar surfaces, in which spots and faculae are placed on an idealised rotating star, and compute the resulting disc-integrated observables. In doing so, they account for brightness contrast, centre-to-limb variation, rotational Doppler shifts, and convective blueshift suppression. Solar-calibrated models demonstrate that both flux contrast and magnetically suppressed convection must be included to reproduce observed RV variability [Lanza et al., 2011; Shapiro et al., 2016].

Tools such as **SOAP** [Boisse et al., 2012] and **SOAP 2.0** [Dumusque et al., 2014] enable detailed simulation of line profile distortions and photometric modulation induced by active regions by generating synthetic observations of such model stars. These frameworks have been extended to incorporate solar observations as realistic inputs, improving predictive capability for Sun-like stars. More recent tools, such as **SOAP-GPU** [Zhao & Dumusque, 2023], employ stellar atmosphere models (e.g. **PHOENIX**) to extend these approaches beyond solar-like conditions and enable modelling across a wider range of spectral types. Synthetic data produced by these tools can be used to train machine learning models to remove stellar activity signals (e.g. de Beurs et al. 2022).

However, these models remain inherently simplified representations of stellar surfaces. They rely on parameterised descriptions of active regions, often assuming fixed contrasts, simple geometries, and solar-like behaviour. As a result, degeneracies between parameters such as spot size, temperature contrast, and spatial distribution can limit the uniqueness of inferred solutions. Consequently, while forward models provide valuable physical insight and controlled test environments, their ability to fully capture the complexity of stellar magnetic activity is limited.

Additional mitigation strategies exploit wavelength dependence. The flux contrast between cool spots and the surrounding photosphere decreases toward the near-infrared, so spot-driven line-profile distortions and the associated RV “jitter” are often reduced at longer wavelengths [Reiners et al., 2010; Huélamo et al., 2008]. By contrast, RV variability associated with magnetically suppressed convective blueshift in facular/plage regions is not expected to diminish as strongly with wavelength because it arises from changes in the photospheric velocity field and line formation rather than purely from continuum brightness contrast [Dumusque et al., 2014].



Consequently, comparing RVs extracted from different wavelength ranges (or obtained simultaneously in the optical and NIR) provides a useful diagnostic to separate activity-induced signals from genuine Doppler motion, and has been demonstrated in practice with combined optical–NIR datasets [Jeffers et al., 2022; Baroch et al., 2020; Larue et al., 2025]. Simultaneous optical and near-infrared observations therefore offer a promising avenue for reducing activity contamination, particularly in active or low-mass stars.

Despite these advances, magnetic activity remains a dominant limitation for  $\text{cm s}^{-1}$  precision radial velocity surveys targeting Earth analogues around Sun-like stars. The degeneracy between activity-driven signals and low-amplitude planetary signatures, especially when periods coincide with stellar rotation or its harmonics, continues to motivate the development of physically informed, multi-diagnostic mitigation frameworks.

## Chapter 5

# Spectral Line Formation in Stellar Atmospheres

*“Science is made up of so many things that appear obvious after they are explained”*

---

*Frank Herbert, Dune*

### 5.1 Fundamentals of Spectral Line Formation

Absorption lines in stellar spectra arise from bound–bound transitions in atoms and ions located within the stellar atmosphere. When radiation emerging from deeper layers passes through cooler material capable of absorbing photons at specific energies, light at those wavelengths is selectively removed from the beam. The spectrum we observe is therefore not formed at a single physical depth, but is shaped by radiation travelling through a stratified atmosphere in which temperature, density, and opacity vary continuously with height.

The continuum radiation originates predominantly in the deeper, hotter regions of the photosphere, where the optical depth at continuum wavelengths becomes of order unity. Here, the optical depth can be understood as a measure of how opaque the material is along the line of sight, with a value of order unity corresponding roughly to the depth from which photons can escape. At wavelengths corresponding to an atomic transition, however, the opacity increases due to the additional contribution from line absorption. This enhanced opacity means that photons at line centre reach optical depth unity higher in the atmosphere than continuum pho-

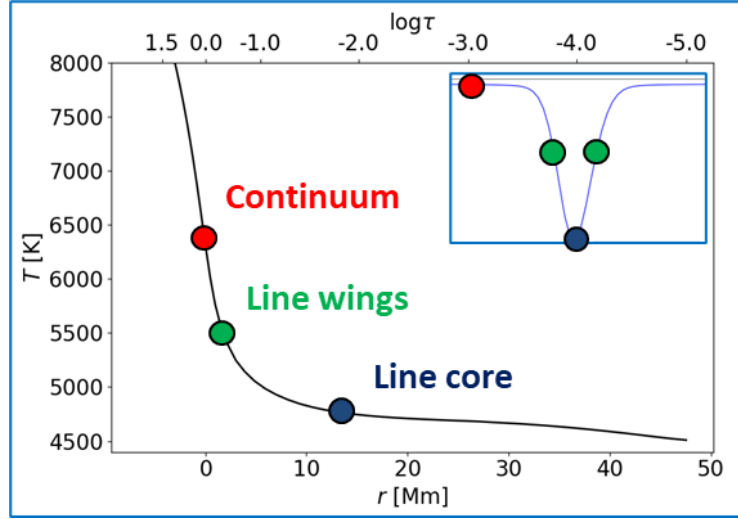


Figure 5.1: **Figure produced by Cis Lagae.** Schematic showing varying formation heights, temperatures and opacities of different wavelength points in a stellar absorption line.

tons do. Since temperature generally decreases with height in the photosphere, the radiation emerging at line centre comes from cooler layers and therefore has lower intensity than the continuum. The result is the characteristic absorption feature superimposed on the stellar spectrum.

It is therefore useful to think of each wavelength as probing the atmosphere at a slightly different depth, demonstrated in Figure 5.1. The wings of a line typically form deeper than the core, and the detailed shape of the profile reflects the physical conditions in the layers from which the radiation escapes. Spectral lines thus provide a depth-dependent diagnostic of the stellar atmosphere, linking the observed profile directly to the underlying thermal and dynamical structure. [Gray, 2005; Rutten, 2003].

The propagation of radiation through the atmosphere is described by the radiative transfer equation,

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu, \quad (5.1)$$

where  $I_\nu$  is the specific intensity at frequency  $\nu$ ,  $\alpha_\nu$  is the monochromatic extinction coefficient, and  $j_\nu$  is the emissivity. Introducing optical depth through  $d\tau_\nu = -\alpha_\nu ds$  and the source function  $S_\nu = j_\nu/\alpha_\nu$ , the equation can be rewritten as

$$\frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu. \quad (5.2)$$

In local thermodynamic equilibrium (LTE), the source function is given by the Planck function,  $S_\nu = B_\nu(T)$ , where  $B_\nu(T)$  is the spectral radiance at frequency  $\nu$  and temperature  $T$ . The emergent intensity at each frequency is therefore determined by the temperature structure of the atmosphere, with the dominant contribution arising from layers where photons can escape most efficiently (i.e. where the optical depth is of order unity) [Rutten, 2003; Hubeny & Mihalas, 2015].

For a plane-parallel atmosphere, the formal solution for the outward emergent intensity at optical depth  $\tau_\nu$  is

$$I_\nu(\tau_\nu, \mu) = \int_{\tau_\nu}^{\infty} S_\nu(t_\nu) \exp\left(-\frac{t_\nu - \tau_\nu}{\mu}\right) \frac{dt_\nu}{\mu}, \quad (5.3)$$

where  $\mu = \cos \theta$  specifies the line-of-sight angle relative to the surface normal, and  $t_\nu$  is the optical depth used as an integration variable (see Rutten 2003, page 17). Evaluated at the surface ( $\tau_\nu = 0$ ), this reduces to

$$I_\nu(0, \mu) = \int_0^{\infty} S_\nu(t_\nu) \exp\left(-\frac{t_\nu}{\mu}\right) \frac{dt_\nu}{\mu}. \quad (5.4)$$

This expression shows that the intensity at a given frequency is a weighted integral over optical depth, and is not determined at a single geometrical layer. The main contribution arises from regions where  $\tau_\nu \sim \mu$ , leading to the commonly used Eddington–Barbier approximation,  $I_\nu(0, \mu) \approx S_\nu(\tau_\nu = \mu)$  [Gray, 2005; Rutten, 2003].

This angular dependence has an immediate physical consequence. For rays emerging at different viewing angles, the effective formation depth varies as  $\tau_\nu \sim \mu$ . At disc centre ( $\mu \approx 1$ ), the line of sight penetrates deeper into the atmosphere, sampling hotter layers and yielding higher emergent intensities. Toward the limb ( $\mu \ll 1$ ), the line of sight becomes increasingly oblique and probes higher, cooler layers, resulting in a systematic decrease in intensity. This effect is known as limb darkening and arises naturally from radiative transfer in a stratified atmosphere (see Figure 5.2).

The integrand of the formal solution (Equation 5.3) defines the contribution function  $C_\nu$ , which quantifies the relative contribution of each layer to the emergent intensity at a given frequency. The peak and width of  $C_\nu$  provide a quantitative definition of the effective formation region at each wavelength [Edmonds, 1969; Amarsi, 2015].

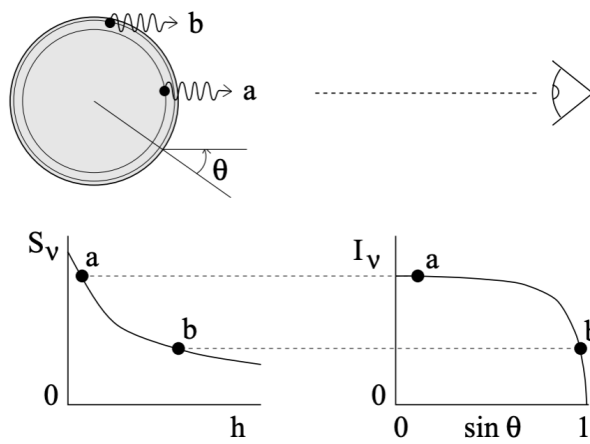


Figure 5.2: **Figure from Gray [2005]**. Rays emerging at different viewing angles probe different depths in the stellar atmosphere. At disc centre (point a,  $\mu \approx 1$ ), the line of sight penetrates deeper layers where the temperature, and hence the source function  $S_\nu$ , is higher. Toward the limb (point b,  $\mu \ll 1$ ), the line of sight becomes increasingly oblique and samples higher, cooler layers with lower  $S_\nu$ . The resulting decrease in emergent intensity  $I_\nu$  with decreasing  $\mu$  produces the observed limb darkening. The lower panels illustrate the monotonic decrease of the source function with height and the corresponding angular dependence of the emergent intensity.

Because opacity varies strongly across a spectral line, the peak of the contribution function moves to different geometric heights between the continuum, line wings, and line core. As mentioned previously, spectral lines therefore form over a range of depths, and their profiles encode the vertical structure of temperature, density, ionisation, and velocity through their influence on the source function and extinction coefficient [Gray, 2005; Amarsi, 2015].

In addition to this wavelength dependence, the formation height also varies spatially across the stellar surface due to inhomogeneous atmospheric structure. In convective photospheres, granules are characterised by hotter, rising plasma, while intergranular lanes are cooler, denser, and host downflows. These differences modify the local temperature and opacity stratification, shifting the contribution function to different geometric heights in each component. As a result, the same spectral line can form at systematically different depths in granules and lanes, contributing to the observed line asymmetries in disc-integrated spectra [Dravins et al., 1981; Asplund et al., 2000].

Aside from the depth-dependent nature of line formation, the detailed shape of a spectral line is also further modified by a range of physical broadening processes. These broadening mechanisms are summarised in the following subsection.

### 5.1.1 Line Broadening mechanisms

Even in an idealised stellar atmosphere, several physical processes act to broaden and shape spectral lines around their central frequency. These mechanisms originate from fundamental atomic physics as well as bulk motions of the emitting or absorbing material. In realistic stellar atmospheres, multiple broadening processes operate simultaneously, and their combined effect determines the observed line profile.

**Natural Broadening:** Natural broadening, also referred to as radiative broadening, arises because atomic energy levels have finite radiative lifetimes. According to the time-energy uncertainty principle, a finite upper-level lifetime  $\Delta t$  implies an intrinsic energy uncertainty  $\Delta E \sim \hbar/\Delta t$ , leading to a spread in transition frequency. The resulting profile is Lorentzian:

$$\phi(\nu) \propto \frac{\gamma}{(\nu - \nu_0)^2 + \gamma^2}, \quad (5.5)$$

where  $\nu$  is the frequency,  $\nu_0$  is the central transition frequency, and  $\gamma$  is the damping constant (the half-width at half-maximum of the profile), which is related to the finite lifetime of the atomic energy levels. Natural broadening is typically small in stellar photospheres but contributes to the extended wings of strong lines [Gray, 2005].

**Collisional (Pressure) Broadening:** In dense environments, perturbations from nearby particles modify atomic energy levels. These interactions shorten the effective level lifetimes and therefore increase the damping constant. In stellar atmospheres, the dominant contributors are:

- **Van der Waals Broadening**, due to collision with neutral hydrogen atoms.
- **Stark Broadening**, due to electric fields from charged particles.

Collisional broadening also produces Lorentzian wings [Gray, 2005; Hubeny & Mihalas, 2015].

**Thermal (Doppler) Broadening:** Atoms in the photosphere possess a Maxwellian velocity distribution. Their motion along the line of sight produces Doppler shifts that broaden the absorption profile. The resulting line profile is Gaussian:

$$\phi(\nu) \propto \frac{1}{\Delta\nu_D} \exp\left[-\frac{(\nu - \nu_0)^2}{\Delta\nu_D^2}\right], \quad (5.6)$$

where  $\nu_0$  is the central transition frequency and  $\Delta\nu_D$  is the Doppler width. The Doppler width is given by:

$$\Delta\nu_D = \frac{\nu_0}{c} \sqrt{\frac{2kT}{m}}, \quad (5.7)$$

where  $T$  is the local temperature,  $m$  is the atomic mass,  $k$  is Boltzmann's constant, and  $c$  is the speed of light.

Thermal broadening therefore increases with temperature and is larger for lighter atomic species. In realistic cases, both Doppler and damping effects operate simultaneously. The resulting profile is the convolution of a Gaussian and Lorentzian function, known as the Voigt profile. Weak lines are typically Doppler-dominated, whereas strong lines exhibit Doppler cores and pressure-broadened wings [Jefferies, 1968].

**Rotational Broadening:** If the star rotates, surface elements exhibit different line-of-sight velocities across the disc. The observed line profile is therefore the convolution of the intrinsic local profile with a rotational broadening kernel that depends on  $v \sin i$  and limb darkening. Rotational broadening increases overall line width in a symmetric manner, and the equivalent width of the line is preserved. In slow rotators such as the Sun, its effect is modest; in rapidly rotating stars, it can dominate the line shape.

## 5.2 Modelling Spectral Absorption Lines

In practice, modelling spectral absorption lines involves coupling an atmospheric structure model with radiative transfer calculations to predict the emergent intensity as a function of wavelength. The resulting line profile encodes information about temperature stratification, velocity fields, pressure, and chemical composition. However, isolating these physical contributions requires careful consideration of the processes that modify the intrinsic transition profile.

Real stellar atmospheres are not static or horizontally uniform. Convective flows, oscillations, and magnetic structures introduce velocity fields and temperature fluctuations on a range of spatial and temporal scales. As discussed in Chapter 4, these processes imprint asymmetries and line shifts on observed spectra. From a modelling perspective, however, the central question is how such effects are represented in theoretical atmospheres and spectral synthesis calculations.

### 5.2.1 One-Dimensional Atmosphere Models

One-dimensional (1D) stellar atmosphere models provide a computationally efficient framework for interpreting stellar spectra. In these models, all physical quantities



are assumed to vary only with depth, neglecting horizontal inhomogeneities and time-dependent dynamics. Radiative transfer is solved through a stratified atmosphere under the assumptions of hydrostatic equilibrium and either plane-parallel or spherical symmetry.

Examples of 1D stellar atmosphere models include **ATLAS** [Kurucz, 1970; Castelli & Hubrig, 2004], **MARCS** [Gustafsson et al., 1975, 2008], **PHOENIX** [Hauschildt et al., 1999] and **MAFAGS** [Grupp, 2004]. In these models, convective energy transport is treated using mixing-length theory, a simplified prescription in which convection is represented by buoyant fluid elements that travel a characteristic distance before exchanging heat with their surroundings. This distance, known as the mixing length, is treated as a free parameter and is typically expressed as a multiple of the local pressure scale height. Consequently, convective transport is parameterised rather than derived from first-principles hydrodynamics. Because the underlying velocity field is not solved self-consistently, their effects on spectral line formation must be incorporated through parameterised prescriptions. This leads to the introduction of microturbulent and macroturbulent velocities (discussed below), which are designed to mimic the impact of unresolved motions on spectral line profiles.

Despite their simplifications, 1D stellar atmosphere models have played a transformative role in stellar astrophysics. Their computational efficiency has enabled the construction of extensive, publicly available grids spanning wide ranges in effective temperature, surface gravity, and metallicity (e.g. Kurucz 1970; Gustafsson et al. 2008; Husser et al. 2013b; Coelho et al. 2005). These grids underpin systematic spectroscopic analyses by providing forward models for parameter and abundance inference, and they remain practical for iterative fitting and automated pipelines in large surveys (e.g. García Pérez et al. 2016).

**Microturbulence:** In classical one-dimensional (1D) stellar atmosphere models, convective velocity fields are not explicitly included. Instead, small-scale motions are parameterised through a quantity known as the microturbulent velocity,  $\xi_{\text{micro}}$ . Microturbulence represents unresolved small-scale velocity fields whose characteristic spatial scale is assumed to be smaller than the photon mean free path. A photon therefore traverses many turbulent eddies before escaping, sampling a statistical distribution of velocities rather than a coherent flow structure. Under this assumption, the turbulent motions modify the local absorption coefficient in the same manner

as thermal motions, effectively increasing the Doppler width of the line profile. The resulting broadening is symmetric about the line centre and may be incorporated by replacing the thermal Doppler width  $\Delta\nu_D$  with an effective width that includes both thermal and microturbulent contributions:

$$\Delta\nu_{\text{eff}}^2 = \Delta\nu_D^2 + \xi_{\text{micro}}^2. \quad (5.8)$$

Microturbulence therefore increases the width of the local absorption profile without altering its symmetry. It is introduced primarily to reproduce observed equivalent widths within the framework of 1D LTE modelling. However, it is not derived from first principles, but instead serves as an empirical correction that compensates for unresolved velocity fields.

Because microturbulence alters the effective Doppler width, it modifies the strength of lines and therefore impacts abundance determinations. The inferred stellar abundances can depend sensitively on the adopted value for  $\xi_{\text{micro}}$ , thus considerable effort has been devoted to constraining this parameter empirically in 1D analyses (e.g: Nissen & Gustafsson 1978; Nissen 1981; Steffen et al. 2013; Takeda 2022).

**Macroturbulence:** Larger-scale velocity fields are represented in 1D models through macroturbulence,  $\xi_{\text{macro}}$ . In contrast to microturbulence, macroturbulence is assumed to act on spatial scales larger than the photon mean free path. It therefore does not alter the local absorption coefficient, but instead broadens the emergent line profile through a convolution with a prescribed velocity distribution function.

Macroturbulence broadens spectral lines while leaving their equivalent width unchanged. It is commonly modelled using Gaussian or radial-tangential velocity fields [Gray, 2005]. As with microturbulence, it is an empirical construct introduced to mimic the integrated effect of unresolved convective motions in 1D atmospheres.

**Limitations of 1D Models:** The simplifying assumptions underlying 1D models introduce well-known physical limitations. The assumption of plane-parallel or spherical symmetry neglects horizontal inhomogeneities, despite the fact that stellar photospheres are intrinsically structured by convection. Observations of the solar surface reveal granulation patterns with strong temperature and velocity contrasts (e.g: Dravins 1982; Nordlund et al. 2009), demonstrating that real atmospheres are neither homogeneous nor static. In 1D models, these fluctuations are not properly

accounted for, thereby discarding correlations between temperature, density and velocity that influence spectral line formation. In Chapter 4, the asymmetry imprinted on spectral lines by granular patterns was discussed, in particular the characteristic C-shaped bisector [Dravins et al., 1981; Asplund et al., 2000]. Because 1D models are symmetric by construction, they cannot reproduce these effects.

A further consequence of this simplification is that 1D models do not accurately capture the centre-to-limb variation (CLV) of stellar spectral lines. In real stellar atmospheres, the emergent spectrum depends strongly on viewing angle. Radiation observed near the centre of the stellar disc originates from deeper atmospheric layers, where temperatures are higher and vertical convective flows dominate. Toward the limb, the line of sight samples higher layers and increasingly probes horizontal velocity fields. As a result, line depths, equivalent widths, convective blueshifts and line asymmetries vary systematically with limb angle [Dravins, 1982; Asplund et al., 2000]. These CLVs arise from the three-dimensional structure of the photosphere and cannot be accurately captured in models that assume horizontal homogeneity.

The neglect of realistic CLV has important implications for exoplanet transmission spectroscopy. During a transit, the observed stellar spectrum evolves as different regions of the stellar disc are occulted. Because spectral line profiles depend on limb angle, the local stellar spectrum behind the planet differs from the disc-integrated spectrum used as a reference. As a result, the ratio of in-transit to out-of-transit spectra can exhibit apparent variations in line depth or shape that are not of planetary origin, but instead arise from the intrinsic CLV of the stellar lines.

These effects are primarily driven by the wavelength-dependent limb darkening of spectral lines, which causes line depths and profiles to vary across the stellar disc. For example, Czesla et al. [2015] showed that CLV across strong Fraunhofer lines in HD 189733 can produce signals in transmission spectra comparable in amplitude to those attributed to hot-Jupiter atmospheres. Similarly, Yan et al. [2017] demonstrated that CLV effects alone can generate apparent Na I absorption signatures if not properly accounted for. More recently, Casasayas-Barris et al. [2020] showed that CLV, when combined with other stellar effects, can significantly modify the observed Na I transmission signal in HD 209458.

Although related to the Rossiter–McLaughlin effect, which arises from the occultation of regions with different projected rotational velocities, CLV-induced signals

are present even in the absence of stellar rotation [Cegla et al., 2016]. They instead reflect intrinsic spatial variations in the stellar line profile across the disc. Accurate modelling of CLV is therefore essential for interpreting high-resolution transmission spectra, particularly for strong lines such as Na I and H $\alpha$ , where limb-dependent variations are most pronounced [Czesla et al., 2015; Yan et al., 2017].

The limitations of 1D models motivate the development of more physically realistic models that explicitly resolve convective dynamics and atmospheric inhomogeneities. Three-dimensional radiative–hydrodynamic simulations address these shortcomings by modelling the coupled evolution of fluid motions and radiation from first principles.

### 5.2.2 Three-Dimensional Hydrodynamic Models

To overcome the limitations of 1D atmospheres, three-dimensional (3D) hydrodynamic (HD) simulations have been developed to model stellar surface convection from first principles. These simulations solve the time-dependent equations of compressible hydrodynamics together with radiative energy transport and a realistic equation of state. In doing so, they self-consistently reproduce the interaction between buoyant upflows, radiative cooling, and downflowing plasma, without recourse to mixing-length theory or micro- and macroturbulent broadening parameters. A full description of the numerical methods employed by these models is beyond the scope of this thesis; comprehensive reviews are given by Nordlund et al. [2009].

Several widely used numerical frameworks implement this approach, including the STAGGER code [Nordlund & Galsgaard, 1995; Magic et al., 2013a; Stein et al., 2024], CO5BOLD [Freytag et al., 2012], and MURaM [Vögler et al., 2005; Rempel, 2014]. For solar-type stars, these simulations are commonly performed in a box-in-a-star configuration, in which a small Cartesian domain is used to model a statistically representative patch of the stellar surface. Such models therefore resolve only a minute fraction of the full stellar surface, but do so at sufficiently high spatial and temporal resolution to capture realistic granulation and the associated correlations between temperature, density, and velocity.

These 3D simulations naturally produce the granular intensity pattern observed on stellar surfaces: hot, bright, rising plasma in granules surrounded by cooler, darker, descending material in intergranular lanes. Because the thermodynamic and veloc-

ity fields are computed self-consistently, they are able to reproduce key spectroscopic signatures that cannot emerge from symmetric 1D atmospheres, including convective blueshifts, asymmetric line bisectors, and centre-to-limb variations in line shape [Asplund et al., 2000; Pereira et al., 2013; Nordlund et al., 2009]. Figure 5.3 illustrates the appearance of granulation across the solar disc in synthetic and observed G-band images, highlighting the level of spatial realism achieved by modern 3D models. Figure 5.4 shows the side-on temperature structure within a solar simulation box from **STAGGER**, demonstrating how the visible granulation pattern is the surface manifestation of deeper convective motions. Fig. 5.5 presents a top-down view of the emergent continuum intensity from a **C05BOLD** simulation, with the network of granules and intergranular lanes clearly resolved.

An important extension of HD modelling is to include magnetic fields, giving rise to magnetohydrodynamic (MHD) simulations. These are essential when the aim is to model magnetically active photospheres, since magnetic fields modify the thermal and velocity structure of the atmosphere, suppress convective blueshifts in active regions, and introduce direct spectroscopic signatures through Zeeman broadening and splitting [Gray, 1984]. Magnetic fields can also substantially modify CLV of spectral intensity [Beeck et al., 2015]. Pure HD models remain extremely valuable when the goal is to isolate the effects of convection alone, but MHD simulations provide a more complete description of real stellar photospheres, particularly in the presence of spots, faculae, and plage [Cameron et al., 2007; Rempel et al., 2009].

While HD and MHD simulations provide the 3D atmospheric structure, synthetic spectra are usually generated in a separate step using dedicated radiative transfer codes. Examples include **NICOLE** [Socas-Navarro, 2015a] and **MPS-ATLAS** [Witzke et al., 2021]. These calculations adopt a so-called 1.5D approach, in which the radiative transfer is solved independently along many vertical columns or rays through the 3D snapshot. This retains the realistic thermal and velocity structure of the simulation, but neglects horizontal radiative coupling during the line-synthesis step. By computing emergent intensities for multiple viewing angles, these tools make it possible to construct spatially resolved line profiles that include realistic convective Doppler shifts. Disc-integrated spectra may then be obtained by integrating these local profiles across the stellar disc, enabling direct comparison with high-resolution observations (e.g: Cegla et al. 2013, 2018, 2019; Frame et al. 2025, 2026). Building on this principle, this thesis develops a framework for modelling disc-integrated spectra, described in detail in Chapters 7 and 8.

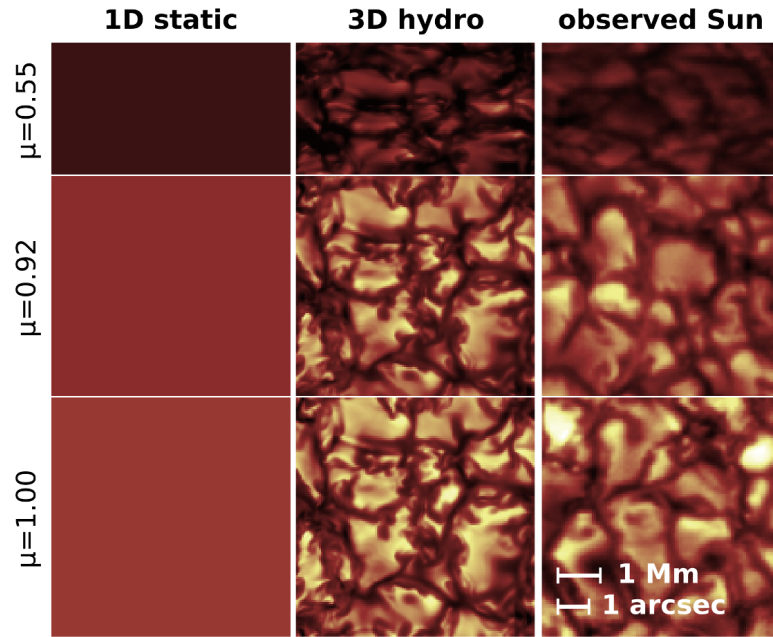


Figure 5.3: **Figure and caption from Hoppe et al. [2026]**. Comparison of synthetic and observed solar G-band intensity at wavelength  $4306.8 \pm 15 \text{Å}$  at different positions across the solar disc (different rows).

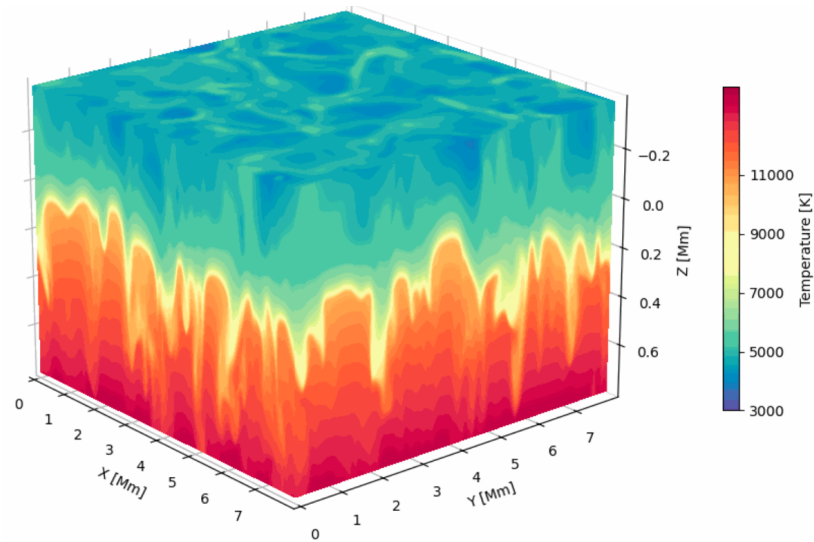


Figure 5.4: **Figure produced by Cis Lagae**. Side-on view of the temperature structure within a 3D STAGGER simulation. The figure shows how the surface granulation pattern arises from deeper convective upflows and cooler downflow lanes beneath the visible photosphere.

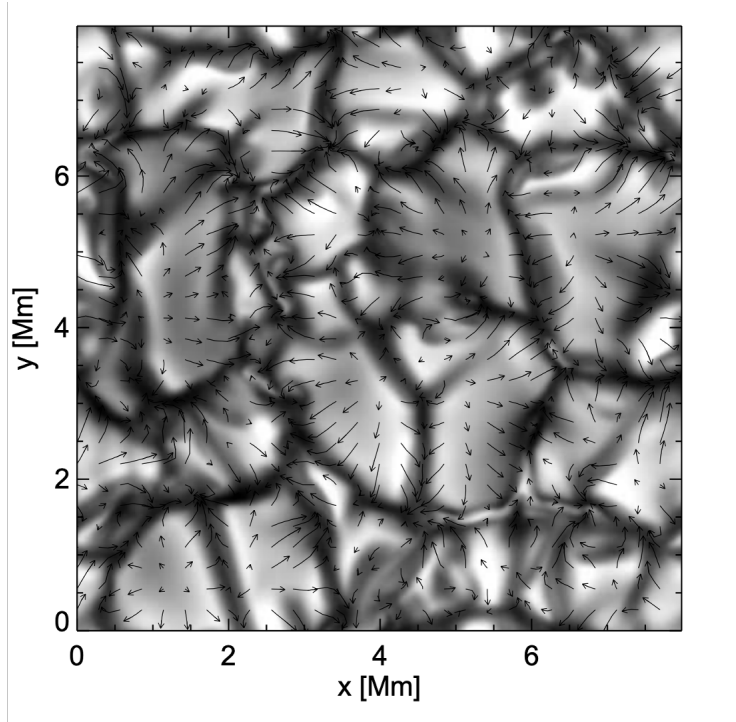


Figure 5.5: **Figure from Freytag et al. [2012].** Emergent continuum intensity at a wavelength of 500nm, synthesised using a CO5BOLD simulation. The arrows depict streamlines following the horizontal velocity on the surface (defined as optical depth unity).

# Interlude: Professional Development and Skills for Machine Learning

S2DS (Science to Data Science) is an intensive five week programme designed to simulate an industry style data science environment. It aims to provide academics with real-world experience in data science, and teach best practices in techniques and workflows. I completed this programme in August 2025 for the purpose of professional development and to learn machine learning skills I could carry over into my research. This interlude provides brief context for the methodological training gained through this programme and its influence on the analytical approach adopted in subsequent chapters. It does not itself form part of the scientific contribution of the thesis.

The S2DS programme focuses on core data science principles, including reproducible data analysis, model validation, and critical evaluation of machine learning methods. Training covered a range of applied techniques and best practices commonly used in non-academic data science settings, with particular emphasis on problem formulation, appropriate model selection, and transparent assessment of model performance. These principles are increasingly relevant to modern astronomical data analysis, where complex models are often applied to high-dimensional and noisy datasets.

A central element of the programme was a team-based project undertaken in collaboration with an external partner. This project involved translating an open-ended problem into a well-defined analytical task, implementing and validating machine learning models, and communicating results to a non-specialist audience. Although the subject matter of this project lay outside astrophysics, the experience reinforced



general methodological skills that are transferable across scientific domains.

The data science training provided by S2DS informed the methodological choices described in the following chapter, particularly with respect to model evaluation, validation strategies, and the avoidance of common pitfalls such as data leakage and overfitting. The specific techniques and implementations presented in this thesis, however, were developed independently and are tailored to the astrophysical context and scientific objectives of the work.

This interlude is included to situate the methodological discussion that follows within the broader context of doctoral training and professional development. The subsequent methodology and results chapters focus exclusively on original research in stellar variability and related astrophysical applications.

## Chapter 6

# Methodology II

*“Cooper, this is no time for caution”*

---

*CASE, Interstellar*

### 6.1 Overview of the Modelling Framework

The work presented in this thesis combines numerical simulations, statistical modelling, and machine learning techniques to investigate variability in stellar absorption line profiles. The overall methodology follows a multi-stage framework designed to transform simulation outputs into large ensembles of synthetic disc-integrated spectra that can be analysed statistically.

First, spectral line profiles are extracted from 3D hydrodynamic simulations of stellar surface convection. These simulations provide spatially resolved snapshots of the stellar photosphere that capture the physical structure of granulation and its influence on spectral line formation (as discussed in Section 5.2.2).

Second, a parameterisation framework is used to describe the statistical properties of the simulation-derived spectra in a compact form. Classification methods are employed to identify distinct surface components within the simulations, enabling the statistical behaviour of the stellar photosphere to be characterised without requiring the full simulation data. This parametrisation allows new disc-resolved spectral profiles to be constructed by reproducing the statistical distributions of the underlying surface components.

Third, dimensionality reduction techniques are applied to represent the spectra in a reduced basis, enabling efficient interpolation of line profiles across the stellar disc. The parameterised model is used to generate large ensembles of synthetic spectral line profiles. By sampling the distributions of the underlying parameters, many independent realisations of disc-integrated spectra can be produced. These synthetic datasets provide a controlled environment for studying spectral variability.

Finally, statistical and machine learning techniques are applied to analyse the resulting spectra. These methods are used to characterise spectral line properties, quantify variability between realisations, and explore relationships between different spectral diagnostics.

The following sections describe in detail the machine learning and statistical techniques employed throughout this framework.

## **6.2 Machine Learning Methods**

Several machine learning techniques are used throughout this thesis for both the construction and analysis of synthetic spectral datasets. This section provides a brief overview of the algorithms employed and outlines their general principles. Detailed applications of these methods are described in the relevant chapters.

### **6.2.1 Supervised Learning**

Supervised learning refers to a class of machine learning methods in which a model is trained using labelled data consisting of input features and corresponding target values. The objective is to learn a mapping between the inputs and outputs that can be used to make predictions on new data. In regression problems the target variable is continuous, while in classification problems the target variable corresponds to discrete classes. A range of algorithms exist for supervised learning, including linear regression, logistic regression, decision trees, and neural networks. Supervised learning techniques employed throughout this thesis are primarily linear and logistic regression. The algorithms are outlined below.

#### **Linear Regression**

Linear regression is a supervised learning technique used to model the relationship between a set of input features and a continuous target variable. The method

assumes that the target variable can be expressed as a linear combination of the input features,

$$y = \beta_0 + \sum_{i=1}^p \beta_i x_i + \epsilon, \quad (6.1)$$

where  $y$  is the predicted value,  $x_i$  are the input features,  $\beta_i$  are model coefficients,  $\beta_0$  is the intercept term, and  $\epsilon$  represents residual errors. The coefficients are typically estimated by minimising the sum of squared residuals between the predicted and observed values, a procedure known as ordinary least squares (OLS).

Linear regression is widely used due to its simplicity, computational efficiency, and interpretability. The fitted coefficients provide a direct measure of how variations in each input feature influence the predicted variable. This makes linear models particularly useful in situations where understanding relationships between variables is as important as making accurate predictions. These properties make linear regression especially well-suited to astrophysical research. Unlike many applied domains where predictive accuracy is the primary goal, astrophysics is fundamentally concerned with uncovering the physical mechanisms that govern observed phenomena. Furthermore, astrophysical datasets are frequently characterised by significant observational noise arising from instrumental limitations and atmospheric interference. In this high-noise regime, the relative simplicity of linear models acts as a form of regularisation, reducing the risk of overfitting that would otherwise cause more flexible models (such as neural networks) to mistake noise for signal, a particularly costly error when the goal is to draw physically meaningful conclusions rather than merely optimise a loss function.

## Logistic Regression

Logistic regression is a supervised machine learning algorithm commonly used for classification problems. Unlike linear regression, which predicts a continuous variable, logistic regression models the probability that an observation belongs to a particular class.

The method assumes that the log-odds of the class probability can be expressed as a linear combination of input features,

$$\log\left(\frac{p}{1-p}\right) = \beta_0 + \sum_i \beta_i x_i, \quad (6.2)$$

where  $p$  is the probability of belonging to the target class and  $x_i$  are the input features. The parameters  $\beta_i$  are determined by maximising the likelihood of the training data. In this context, the likelihood represents the probability of observing the class labels in the training dataset given a particular set of model parameters. The optimisation procedure therefore seeks parameter values that make the observed training labels most probable under the model.

Solving the log-odds relation for  $p$  yields the logistic, or sigmoid, function

$$p = \frac{1}{1 + e^{-(\beta_0 + \sum_i \beta_i x_i)}}, \quad (6.3)$$

which maps the linear predictor to the interval  $[0, 1]$ . The sigmoid function ensures that the model outputs a valid probability while retaining a linear dependence on the input features in log-odds space. Predictions are typically converted to class labels by applying a probability threshold, commonly  $p = 0.5$  for binary classification.

While logistic regression is naturally formulated for binary classification, it can be extended to multi-class problems. In this case, a softmax (also referred to as multinomial logistic) regression model is used. Given an input feature vector  $\mathbf{x}$  with label  $y$ , the softmax regression model will output a vector of probabilities, where the probability that the sample input belongs to class  $k$  is given by  $p_k = P(y = k | \mathbf{x})$ . Importantly, the probabilities for each class will sum to unity.

This is commonly implemented through the softmax function, which generalises the sigmoid to multiple classes by normalising the exponentiated linear predictors:

$$P(y = k | \mathbf{x}) = \frac{\exp(\beta_{0,k} + \beta_k \cdot \mathbf{x})}{\sum_{j=1}^K \exp(\beta_{0,j} + \beta_j \cdot \mathbf{x})}. \quad (6.4)$$

This formulation ensures that the predicted probabilities for all  $K$  classes are positive and sum to unity. The model parameters for each class are again determined by maximising the likelihood of the observed training labels. Multinomial logistic regression therefore allows the classification boundary between multiple classes to be learned directly from the feature space.

### 6.2.2 Principal Component Analysis

Principal Component Analysis (PCA) is an unsupervised machine learning technique commonly used for dimensionality reduction [Jolliffe & Cadima, 2016]. The goal of PCA is to transform a dataset with potentially correlated variables into a new set of orthogonal variables, referred to as principal components, that capture the dominant directions of variance in the data. By projecting the data onto a smaller number of these components, it is possible to represent the essential structure of the dataset while reducing its dimensionality.

Consider a dataset consisting of  $n$  observations and  $d$  features, represented by a matrix  $\mathbf{X}$ . Prior to applying PCA, the data are typically mean-centred so that each feature has zero mean. The covariance matrix of the dataset can then be written as

$$\mathbf{C} = \frac{1}{n-1} \mathbf{X}^\top \mathbf{X}. \quad (6.5)$$

The covariance matrix describes how the variables in the dataset vary with respect to one another. PCA seeks directions in feature space along which the variance of the projected data is maximised. These directions are obtained by solving the eigenvalue problem

$$\mathbf{C} \mathbf{v}_i = \lambda_i \mathbf{v}_i, \quad (6.6)$$

where  $\mathbf{v}_i$  are the eigenvectors of the covariance matrix and  $\lambda_i$  are the corresponding eigenvalues. Each eigenvector defines a principal component direction, while the associated eigenvalue quantifies the variance of the data along that direction.

The principal components are ordered according to decreasing eigenvalue, such that the first principal component captures the largest possible variance in the dataset, the second captures the largest remaining variance orthogonal to the first, and so on. Because the eigenvectors are orthogonal, the resulting components are uncorrelated.

Once the principal components have been determined, the original data can be projected onto this new basis. The transformed representation of the data is given by

$$\mathbf{Z} = \mathbf{X} \mathbf{V}, \quad (6.7)$$

where  $\mathbf{V}$  is the matrix whose columns are the eigenvectors of the covariance matrix.

Each column of  $\mathbf{Z}$  therefore represents the projection of the data onto a principal component.

Dimensionality reduction is achieved by retaining only the first  $k$  principal components, which correspond to the largest eigenvalues and therefore capture the majority of the variance in the dataset. In equation 6.7,  $\mathbf{V}$  is therefore truncated to  $k$  columns ( $\mathbf{V}_k$ ). The resulting  $\mathbf{Z}$  will have dimensions  $n \times k$  and is thus a lower-dimensional representation of the original dataset  $\mathbf{X}$ , while preserving the most significant patterns present in the original feature space.

### 6.2.3 Model Training and Validation Best Practices

The reliability of machine learning models depends not only on the choice of algorithm, but also on the procedures used for training and evaluation. Careful validation is essential to ensure that model performance reflects genuine predictive capability rather than artefacts of the training data.

A key challenge in machine learning is overfitting, whereby a model learns noise or spurious patterns in the training data rather than the underlying signal. Overfitting is particularly problematic in astrophysical applications, where datasets are often noisy and limited in size. Throughout this work, model simplicity is prioritised, as constraining model flexibility effectively acts as a form of regularisation, mitigating the risk of overfitting.

A fundamental principle, also to prevent overfitting, is the separation of data into distinct training and testing sets. The model is fitted using only the training data, while the test set is reserved for evaluating performance on unseen examples. This approach is employed throughout all evaluation in Chapter 8, and provides an unbiased estimate of generalisation performance. Model performance should always be evaluated on data not used during training to ensure that learned relationships are physically meaningful and not artefacts of noise.

Another critical consideration is the avoidance of data leakage. Data leakage occurs when information from the test set, or from future observations, is inadvertently used during training. This can arise, for example, when preprocessing steps such as normalisation or feature construction are performed using the full dataset rather than being restricted to the training subset. Leakage leads to overly optimistic performance estimates and undermines the validity of the model. In this work, all

preprocessing steps are applied within the training data and then consistently extended to validation or test sets, ensuring a fair evaluation.

Together, these practices help to ensure that machine learning models provide reliable and interpretable results, which is essential when they are used to draw physical conclusions about stellar variability and spectral line behaviour.

## 6.3 Statistical Techniques

### 6.3.1 Cross-Correlation Functions

Cross-correlation functions (CCFs) are widely used in spectroscopy to measure relative shifts between two signals [Tonry & Davis, 1979]. In stellar spectroscopy, they are commonly applied to determine radial velocity variations by comparing an observed spectrum with a reference template [Baranne et al., 1996; Pepe et al., 2002b]. The basic idea is to quantify the similarity between two spectra as a function of their relative displacement in wavelength or velocity space. All velocity calculations throughout the remainder of this thesis use this approach, which is detailed below.

Given two functions  $f(\lambda)$  and  $g(\lambda)$ , the cross-correlation function is defined as

$$C(\Delta\lambda) = \int f(\lambda) g(\lambda + \Delta\lambda) d\lambda, \quad (6.8)$$

where  $\Delta\lambda$  represents a shift applied to one of the signals. The cross-correlation therefore measures how well the two functions align for a given displacement. When the spectral features of the two functions coincide, the value of the cross-correlation function reaches a maximum. The location of this maximum provides an estimate of the relative shift between the spectra.

In practice, spectroscopic measurements are performed on discrete data. For a spectrum sampled at  $N$  wavelength points, the discrete cross-correlation can be written as

$$C(k) = \sum_{i=1}^N f_i g_{i+k}, \quad (6.9)$$

where  $k$  represents the discrete shift between the two signals. Directly evaluating



this expression for all possible shifts scales as  $\mathcal{O}(N^2)$  operations, which becomes computationally expensive for high-resolution spectra.

A more efficient approach makes use of the convolution theorem, which states that convolution or correlation in real space corresponds to multiplication in Fourier space [Bracewell, 2000]. The cross-correlation can therefore be computed using the Fourier transforms of the two signals,

$$C = \mathcal{F}^{-1} [\mathcal{F}(f)^* \mathcal{F}(g)], \quad (6.10)$$

where  $\mathcal{F}$  denotes the Fourier transform,  $\mathcal{F}^{-1}$  its inverse, and the superscript  $*$  represents the complex conjugate. In practice, the Fourier transforms are computed using the Fast Fourier Transform (FFT) algorithm [Duhamel, 1990], which reduces the computational complexity to  $\mathcal{O}(N \log N)$ .

The resulting cross-correlation function is then evaluated over a range of wavelength shifts. The peak of the correlation profile corresponds to the displacement that best aligns the spectral features of the two signals, providing an estimate of the wavelength shift between the spectra.

In radial velocity studies, the shift  $\Delta\lambda$  is typically converted to velocity using the Doppler relation

$$v = c \frac{\Delta\lambda}{\lambda_0}, \quad (6.11)$$

where  $c$  is the speed of light and  $\lambda_0$  is the reference wavelength. The resulting cross-correlation profile can be interpreted as an average spectral line constructed from the combined information of many absorption lines. By fitting a model function, such as a polynomial, to the peak of the cross-correlation function, the centroid of the profile can be determined with high precision, yielding an estimate of the stellar radial velocity.

The cross-correlation technique provides several advantages for spectroscopic analysis. By combining information from many spectral lines simultaneously, it increases the signal-to-noise ratio of the velocity measurement and reduces the sensitivity to noise in individual lines. For this reason, cross-correlation methods form the basis of many high-precision radial velocity pipelines (e.g: Baranne et al. 1996; Pepe et al. 2002b).

### 6.3.2 The Kolmogorov-Smirnov Test

A key desired outcome of the following chapters is the reconstruction of uncovered underlying distributions within simulated data. I therefore required a robust method for comparing distributions to one another. The Kolmogorov-Smirnov (KS) test [Kolmogorov, 1933; Smirnov, 1948] was a valuable tool for this due to its non-parametric nature (meaning it does not make assumptions about distribution type), its capability in handling small sample sizes, and its ease of interpretation.

There are two common formulations of the KS test. The one-sample KS test compares an observed sample against a reference theoretical distribution, while the two-sample KS test compares two observed samples against one another. Both formulations are based on the same underlying quantity: the empirical cumulative distribution function (ECDF).

#### The Empirical Cumulative Distribution Function

Given a sample of  $n$  observations  $\{x_1, x_2, \dots, x_n\}$ , the empirical cumulative distribution function is defined as

$$F_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}(x_i \leq x), \quad (6.12)$$

where  $\mathbf{1}(x_i \leq x)$  is the indicator function, equal to 1 if  $x_i \leq x$  and 0 otherwise. The ECDF therefore gives, at each value  $x$ , the fraction of observations in the sample that are less than or equal to  $x$ . As  $n \rightarrow \infty$ , the ECDF converges to the true underlying cumulative distribution function (CDF).

#### The One-Sample KS Test

In the one-sample case, the goal is to assess whether a sample of  $n$  observations is consistent with a reference CDF  $F_0(x)$ . The null hypothesis in this case is that the sample follows the specified distribution. The KS test statistic is defined as the maximum absolute deviation between the ECDF and the reference distribution,

$$D_n = \sup_x |F_n(x) - F_0(x)|, \quad (6.13)$$

where  $\sup$  denotes the supremum over all values of  $x$ . The statistic  $D_n$  therefore

captures the largest discrepancy between the observed data and the hypothesised distribution at any point.

A  $p$ -value is computed from the observed value of  $D_n$ , which quantifies the probability of obtaining a test statistic at least as large as that observed, assuming the null hypothesis is true. The null hypothesis is typically rejected when  $p < 0.05$ , indicating that the data are unlikely to be consistent with the reference distribution  $F_0$ .

### The Two-Sample KS Test

In the two-sample case, the goal is to determine whether two independent samples, of sizes  $n$  and  $m$  respectively, are drawn from the same underlying distribution. The test statistic is generalised to

$$D_{n,m} = \sup_x |F_n(x) - G_m(x)|, \quad (6.14)$$

where  $F_n$  and  $G_m$  are the ECDFs of the two samples. Again, a large value of  $D_{n,m}$  indicates that the two samples differ substantially in their distributions. Similarly to the one-sample test, the null hypothesis is accepted or rejected based on a calculated  $p$ -value. The null hypothesis in this case being that  $F_n$  and  $G_m$  come from the same underlying distribution.

## Chapter 7

# The Isolation of Granulation in *Disc-Resolved* Spectral Lines

*“When stupid ideas work, they become genius ideas”*

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*Andy Weir, Project Hail Mary*

### Note

This chapter is a reproduction of Frame et al. [2025], titled “Towards understanding stellar variability at the sub m/s level: isolating granulation signals in synthetic spectral lines”, originally published in May 2025 in Monthly Notices of the Royal Astronomical Society (MNRAS). All of the analysis and writing in this chapter was conducted by myself, with input and advice from co-authors.

### 7.1 Introduction

The aim of this chapter is to characterise the impact of granulation in solar-like stars on four individual spectral absorption lines (Fe I 617 nm, Fe I 525 nm, Fe I 627 nm, and Fe I 615 nm). We begin by focusing on disc-resolved regions of the stellar surface, allowing us to quantify the centre-to-limb variation (CLV) induced by granulation. To achieve this, we generate synthetic, time-varying absorption line profiles and introduce a novel framework for isolating granulation signatures.

A key advantage of this simulation-based approach, compared to studies relying on empirically constructed datasets (e.g. Palumbo et al. 2022), is the absence of

uncontrolled contamination from additional stellar or instrumental effects, as well as the flexibility to eventually extend the methodology to a broader range of stellar types. The techniques developed here therefore provide a controlled foundation for investigating granulation-driven variability, and are later extended to disc-integrated observations to assess mitigation strategies (see Chapter 8).

We conduct our study with lines synthesized through 3D Hydrodynamic (HD) simulations. This builds upon the work of Cegla et al. [2013, 2018, 2019], hereafter the Cegla Series (CS), who synthesized disc-integrated line profiles of the Fe I 6302 Å line for a solar type star with a 200 G magnetic field. CS used box-in-a-star MHD simulations of the stellar surface from MURaM [Vögler et al., 2005], paired with NICOLE [Socas-Navarro, 2015b; Socas-Navarro et al., 2015] for line synthesis. Since CS was published, improvements have been made to the MURaM code: Rempel [2014] modified the diffusion scheme to reduce the diffusive terms as much as possible, while ensuring numerical stability. To achieve a better agreement with solar observations, the new MURaM setup uses the equation of state look-up-table generated by the FreeEOS code [Irwin, 2012], together with an updated and consistent opacity table using the element composition by Asplund et al. [2009]. Furthermore, the radiative treatment was upgraded to consider 12 multi-group bins with similar thresholds as in Magic et al. [2013b]. For details on how these changes affect the accuracy of the simulations, see Appendix A.3 and B in Witzke et al. 2024.

The goal of this work is to expand the CS studies by using a wider range of atomic absorption lines whilst utilising the improved MURaM model atmospheres. To isolate the granulation effects from the pressure-modes present in MURaM MHD cubes and also to enable the reconstruction of lines with a lower computation cost, CS uses a method of parameterisation (see Cegla et al. [2013] for details). In this paper, where we focus on the HD case, we find that parts of this method are insufficient to properly remove the effects of p-modes whilst maintaining the granulation signature in our data. We attribute this to a combination of updates to MURaM and the much stronger p-modes present in the HD case compared to a 200G magnetic field.

We introduce a more rigorous parameterisation approach to model the impact of granulation on stellar line profiles. This method leverages information from 3D HD simulations to generate line profiles without requiring the computationally expensive step of rerunning the full simulations. By doing so, it significantly reduces computation time while retaining the critical details provided by the simulations.

As discussed in Chapter 5, traditional approaches to modelling spectral lines with 1D hydrostatic stellar atmosphere models rely on approximate methods to account for the missing large- and small-scale velocity fields. These methods rely on free parameters such as micro- and macro-turbulence, which act as simplified 1D approximations of complex 3D turbulent flow structures present in stellar atmospheres, despite their known inaccuracies [Takeda & UeNo, 2017; Uitenbroek & Criscuoli, 2011]. In contrast, the parameterisation approach incorporates the complex convection processes directly encoded in the parameters derived from the HD simulations, providing a simpler and more accurate way to account for the full range of stellar atmosphere information whilst reducing computation time. We also preserve granulation time-variability with our approach, allowing us to retain information on the evolution of granulation.

A description of the data used in this work is given in Section 7.2. An outline of our parameterisation method and a demonstration of its applicability at different positions on the stellar disc is provided in Section 7.3. A description of how the time series is reconstructed and comparison to observed power spectra are presented in Section 7.4. Section 7.5 provides an analysis of center-to-limb effects for the different lines. Finally, Section 7.6 contains a summary and conclusions from the study.

## 7.2 Data

We use a time series of 3D HD models generated using MURaM (Vögler et al. 2005) for a solar-like star ( $T_{\text{eff}} = 5787$  K). Each simulation box has a horizontal extent of  $9 \times 9$  Mm<sup>2</sup> containing  $512 \times 512$  pixels, and a vertical extent of 5 Mm containing 500 pixels. In the vertical direction, the model covers approximately 1 Mm of atmosphere above the photosphere and 4 Mm of sub-photosphere and convection zone, and is set on a uniform mesh with a spacing of 10 km. Our time series consists of 129 snapshots with a cadence of 30 seconds, spanning a total time of just over 1 hour.

As an artifact of the model initialisation and due to periodic side boundaries, the HD cubes show a horizontal drift through their periodic boundary conditions. To diminish the impact of this artificial velocity field on our results, we subtract the average horizontal root mean square (rms) velocity of the cube at each timestep. We observed no change in our parameterisation results after this, due to the relative

pixel-to-pixel velocity shifts being untouched.

For each of the  $512 \times 512$  vertical columns in each snapshot, we synthesise line profiles using **MPS-ATLAS** [Witzke et al., 2021], a 1D radiative transfer code that assumes local thermodynamic equilibrium (LTE). Line profiles are synthesised in the so-called 1.5D approach, meaning that the velocity fields of the 1D columns are inherited from the 3D cube. As such, no microturbulence is required for these calculations. Our line profiles have a resolution of  $R = 2,000,000$ . We choose to synthesise four lines at nine different limb angles ranging from  $\mu = 0.2$  to  $\mu = 1.0$  in steps of 0.1, and only one azimuthal angle. Note that  $\mu$  in this context refers to the cosine of the heliocentric angle, with  $\mu = 1.0$  corresponding to the disc centre. Before each line synthesis calculation, the hydrodynamic quantities of the 3D cubes are tilted and interpolated onto rays parallel to the viewing angle. The resulting vertical resolution of the new tilted cubes is kept similar to the original cube. For a more detailed description of how the **MURaM** boxes are generated and how **MPS-ATLAS** line synthesis works, refer to Section 2 in Witzke et al. [2024] and references therein.

Figure 7.1 presents an example of a single snapshot in time observed at three different heliocentric angles. The continuum intensity values displayed in this plot have been normalised by the maximum intensity at disc centre. Continuum intensity decreases towards the limb due to limb darkening. A consequence of inclining the cubes is a change in which pixels remain visible to the observer. The optical surface is located at higher altitudes in granules and lower in lanes, creating a 3D corrugated surface structure. By viewing the cube at an inclined angle, some pixels become obscured behind others. See Dravins [2008] for further discussion.

The four lines we synthesise are Fe I 617 nm, Fe I 525 nm, Fe I 627 nm and Fe I 615 nm. The focus on Fe I lines for this work is due to their sensitivity to photospheric conditions and largely well-established atomic properties. These four lines span a range of different line strengths, Landé factors and excitation potentials. Their atomic properties can be found in Table 7.1. Note that the Landé factors will have no effect on the results of this work, since we are not including a magnetic field in our model atmosphere. However these values will become important in future comparative studies including magnetic fields.

Figure 7.2 shows the spatially and temporally averaged **MPS-ATLAS** output for each spectral line at three limb angles. As before, the intensity values have been nor-

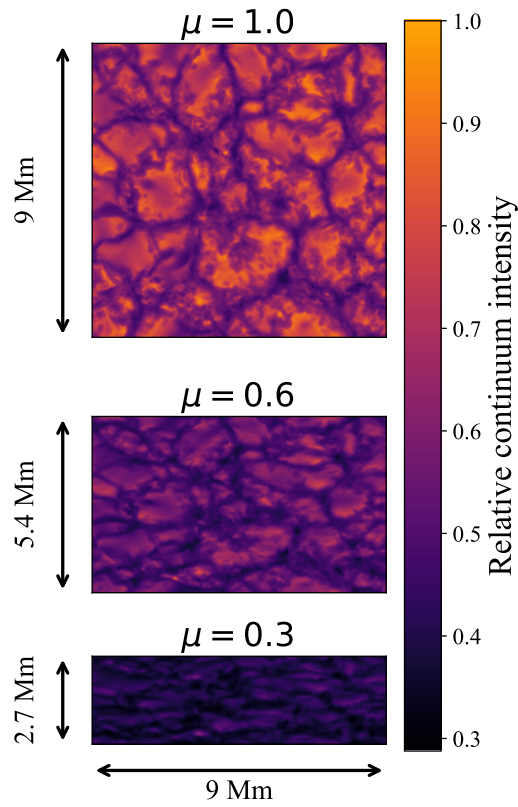


Figure 7.1: The continuum intensity at 617 nm plotted for each pixel at three limb angles. The units of intensity are arbitrary and scaled relative to the maximum intensity at disc center. Projected spatial dimensions of the cube at each limb angle are indicated with double arrows.



| Element + ionisation | Air wavelength (nm) | $\log(gf)$          | Landé factor | $\gamma_{\text{rad}}$ | $\gamma_{\text{Stark}}$ | $\gamma_{\text{vdW}}$ | Excitation potential (eV) |
|----------------------|---------------------|---------------------|--------------|-----------------------|-------------------------|-----------------------|---------------------------|
| Fe I                 | 525.021             | -4.938 <sup>†</sup> | 3.00         | 3.32                  | -6.28                   | -7.82*                | 0.121                     |
| Fe I                 | 615.162             | -3.299 <sup>†</sup> | 1.84         | 8.29                  | -6.16                   | -7.70*                | 2.176                     |
| Fe I                 | 617.333             | -2.880 <sup>†</sup> | 2.50         | 8.31                  | -6.16                   | -7.69*                | 2.223                     |
| Fe I                 | 627.128             | -2.701 <sup>‡</sup> | 1.49         | 8.23                  | -5.41                   | -7.28*                | 3.332                     |

Table 7.1: Atomic parameters for the lines selected for this work.  $\gamma_{\text{rad}}$ ,  $\gamma_{\text{Stark}}$  and  $\gamma_{\text{vdW}}$  refer to the radiative, Stark and Van der Waals damping parameters. All data is sourced from Kurucz [2014], unless marked otherwise.

**Key:** <sup>†</sup> Source: Fuhr et al. [1988]; <sup>‡</sup> Source: Bard & Kock [1994]; \* Source: Barklem et al. [2000].

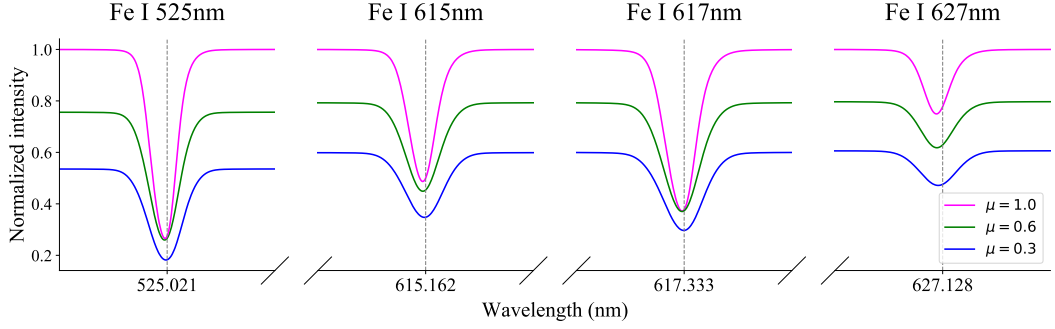


Figure 7.2: Spatially and temporally averaged line profiles calculated using the MURaM cubes with MPS-ATLAS at three limb angles  $\mu = 1.0$ ,  $0.6$  and  $0.3$ . The intensity of each profile has been normalised relative to the continuum intensity of the relevant disc-centre profile. The gray dotted lines are the rest wavelengths in air of the lines. Each section separated by the double diagonal lines covers the wavelength interval of  $0.04$  nm centered at the rest wavelength.

malised relative to the continuum intensity at disc centre. The gray dotted lines indicate the rest wavelength of each line. Note that due to the averaging, these lines contain no p-mode information and the evident convective blueshift seen in Figure 7.2 is a direct result of stellar surface granulation, where hot up-flowing granules occupy a larger surface area fraction compared to intergranular lanes [Dravins et al., 1981]. A more in-depth discussion on line shape changes across different limb angles for the different lines is given in Section 7.5.

In Figure 7.3, we compare the bisectors of the averaged line profiles from Figure 7.2 with disc-resolved observations from the Laser-based Absolute Reference Spectrograph (LARS) [Löhner-Böttcher et al., 2018] and from the Institut für Astrophysik, Göttingen (IAG) solar atlas [Ellwarth et al., 2023]. The intensity is normalized relative to the continuum intensity at each  $\mu$ . Doppler shifts are computed using the rest wavelengths listed in Table 7.1. However, a direct comparison of the simulated and observed mean bisector Doppler shift is not meaningful due to potential large-scale flows in the observed data (e.g., supergranulation, meridional flows). Instead, we focus on comparing the bisector shapes and align the observed profiles by shifting them to match the mean bisector velocity of our results. In Figure 7.3, the dotted lines are the shifted LARS bisectors (if available) and the dashed lines are the shifted IAG bisectors. We find a sufficient match in all cases, any differences can be attributed to the exclusion of magnetic effects in our simulations and the assumption of LTE in our line synthesis. It is also important to note that LARS and the IAG FTS do not match the spectral resolution of our synthetic spectra,

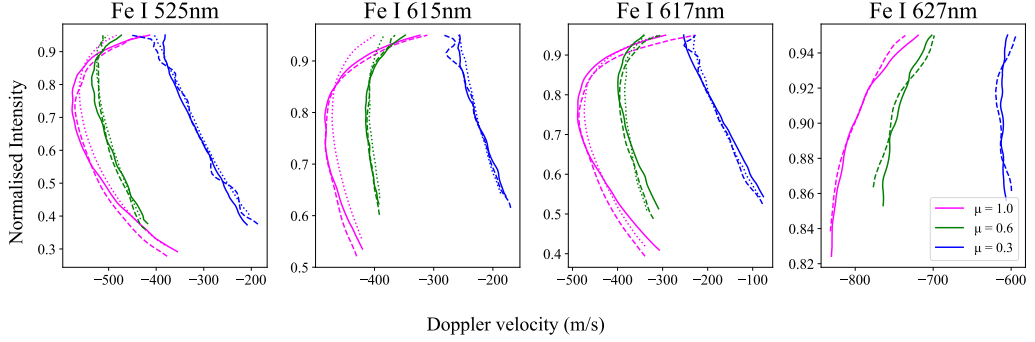


Figure 7.3: Bisectors of the profiles displayed in Figure 7.2. Intensity has been normalised relative to the relevant continuum intensity at each inclination. Note that each subplot has an independent y-axis scale to better visualize variations. Solid lines are results from this work, dotted lines are bisectors from LARS and dashed lines are bisectors from IAG. Both the LARS and IAG bisectors have been shifted in velocity space to match the mean bisector Doppler shift of the synthesised profiles.

and both are affected by an instrument-specific line spread function (LSF), which remains uncharacterised in this analysis.

### 7.3 The Parameterisation method

Generating line profile time series from HD cubes, as described in Section 7.2, is computationally demanding. Constructing disc-integrated profiles requires tiling a stellar grid (see Cegla et al. 2019), but covering a solar-sized star with unique  $9 \text{ Mm}^2$  HD cubes is infeasible due to computational costs. While repeating cubes across multiple tiles is possible, it may introduce biases in the resulting disc-integrated profile. Instead, we propose a new parameterisation method that leverages a single time series of HD cubes to construct unique, accurate line profiles, eliminating the need for separate HD simulations for each tile.

As well as computational efficiency, parameterisation allows us to disentangle the line changes driven by p-modes and granulation. This offers us a valuable opportunity to study the impact of granulation completely uncontaminated by other variability processes.

The idea of separating line profiles into distinct surface components was pioneered by Dravins [1990]. In our approach, the HD cube is separated into components such

as granules and intergranular lanes. We assume that each component has a distinct line-profile contribution, and solve for this contribution by averaging profiles from ‘granule’ and ‘lane’ pixels both spatially and temporally. We then assume that granulation-induced line shape changes can all be attributed to changes in component filling factor, which refers to the changing proportion of pixels belonging to each component in each snapshot. For an example of this method in practice, see Cegla et al. [2013] and the figures therein. For a simplified example of profile reconstruction via parameterisation see Figure 7.4.

The difficulty of this process lies in defining components and classifying pixels in each snapshot. In Cegla et al. [2013], cutoff values are defined in both continuum intensity and magnetic field strength. These cutoffs are applied uniformly to every snapshot to separate pixels into four components. However, in our non-magnetic dataset, we find that the average continuum intensity of each snapshot is heavily influenced by p-mode phase. Using a universally applied continuum cutoff value results in filling factors contaminated by the periodic effects of p-modes. We therefore present an updated technique for parameterisation that is more careful to ensure the elimination of p-mode effects whilst maintaining granulation signatures. This technique is applied independently to each of the four lines from Table 7.1. However, for the purpose of demonstrating this method, we will use the Fe I 617 nm line for the entirety of this section.

### 7.3.1 Pixel classification

It is vital to ensure that the parameters we use to assign pixels to specific components are not influenced by p-modes, so that the averaged components we end up with are free from contamination. This is challenging because both granulation and p-modes have overlapping effects on all available parameters. However, a key distinction is that granulation primarily influences the spatial characteristics of the cube, while p-modes mainly affect the temporal aspects: at any given moment, the pressure mode amplitude in the cube is mostly constant across pixels, while granulation causes spatial variability between the pixels. By examining a single snapshot, we can observe this spatial variation in granulation effects without the interference of time-dependent p-mode fluctuations. Therefore, when classifying pixels, we compare them only to other pixels within the same snapshot to determine their component.

We separate the pixels in each snapshot into three distinct groups, partially mo-

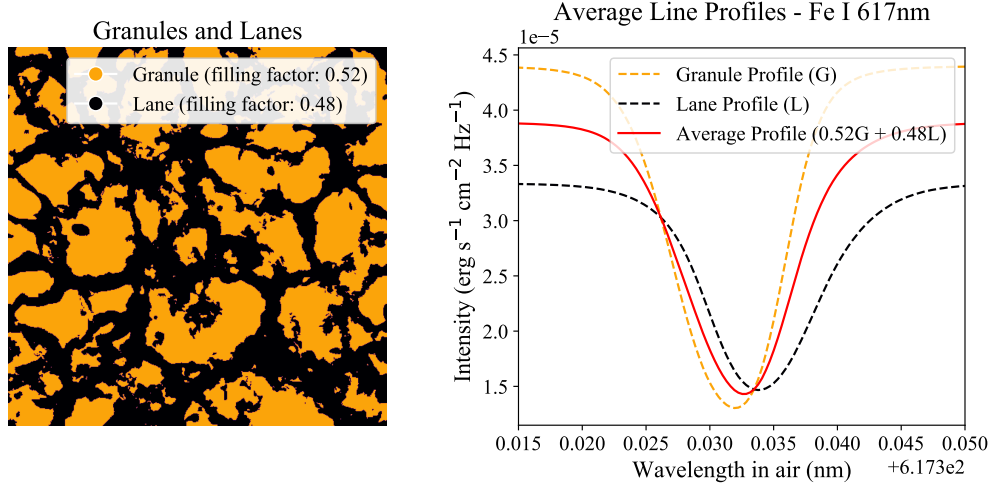


Figure 7.4: An example of reconstruction via parameterisation for demonstrative purposes. The granule profile is the average profile over all the “Granule” pixels and the lane profile is the average over the “Lane” pixels. The total average profile is simply the sum of the components weighted by their respective filling factor.

tivated by Dravins [1990], who also chose to treat granules separately from their centers.

- Granular Tops (GTs): the brightest, hottest points on a granule in which velocity up-flows are strongest.
- Outer Granular Regions (OGRs): The area of the granule surrounding the GT. These are a mixture of up-flows and down-flows as these regions contain plasma both rising to the GT and falling into the lanes.
- Intergranular Lanes (IgLs): The cooler regions that the plasma sinks into, consisting of mostly down-flows.

Each pixel in every snapshot is assigned to one of these groups. We base this decision on three key spectral parameters: the continuum intensity, the measured radial velocity, and the line depth. These chosen parameters capture essential aspects that track variability in the line and surrounding spectral region whilst minimizing potential biases from parameter correlations. All radial velocities in this work are calculated by cross-correlating the line profiles with the total time averaged profile as the template. We fit a parabola to the peak of the cross-correlation function (CCF) to determine the RV.

However, each of these parameters is contaminated snapshot-to-snapshot by p-mode oscillations. We therefore need to produce template parameters that evolve with the snapshots, thus capturing what each group should look like at a particular phase in the p-mode cycle.

We begin with a simple assumption that the very brightest points in a snapshot are GTs and the very darkest points are IgLs. We therefore use parameters from the brightest 2% of pixels as an initial GT template and the darkest 2% as an initial IgL template. Figure 7.5 shows how the average of these template parameters evolves with time. Note the instances of periodic behavior caused by p-mode oscillations. See the top leftmost plot in Figure 7.6 for locations of the template pixels.

A logistic regression model is trained on the template parameters for the two groups. This was done using scikit-learn’s LogisticRegression class [Pedregosa et al., 2011]. This model takes into account the full spread of parameters given and inherently assigns feature importance values for each parameter based on how strongly it correlates with the grouping. For each of the  $512 \times 512$  pixels, the probability of belonging to the GT group ( $P(\text{GT})$ ) or the IgL group ( $P(\text{IgL})$ ) is estimated by the model based on the pixel parameters compared to the template values. The classification value is then determined as follows, resulting in a range from -1 (definitely a GT) to +1 (definitely an IgL).

$$\text{Initial classification} = \begin{cases} \frac{P(\text{GT})-0.5}{0.5} & \text{if } P(\text{GT}) > P(\text{IgL}) \\ -\frac{P(\text{IgL})-0.5}{0.5} & \text{otherwise} \end{cases}$$

The initial classification results can be found in the first row of Figure 7.6. Note that at this stage we are only considering GTs and IgLs and are yet to introduce template parameters for the OGR group. We do this now by considering the 2% of pixels that have a classification value closest to zero (see the top rightmost plot in Figure 7.6). These pixels have been determined by the trained model to have an equal probability of being GTs or IgLs. By using these pixels as our templates for the OGR region group, we ensure that our three groups are as distinct as possible. We retrain the logistic regression model with the inclusion of this third template group and calculate again  $P(\text{GT})$  and  $P(\text{IgL})$ . This time we also calculate the probability that the pixel is an OGR ( $P(\text{OGR})$ ). Note that the sum of these three values for each pixel will sum to 1. We can therefore define our final classification value as

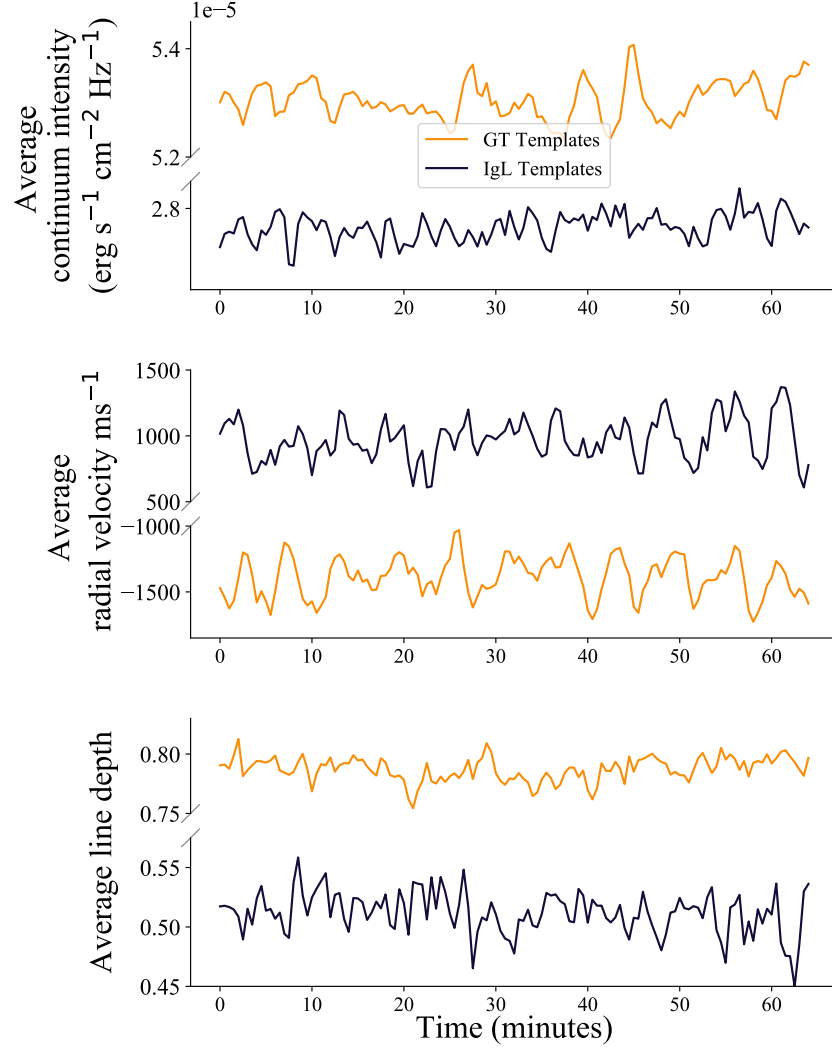


Figure 7.5: The evolution of averaged parameters for each initial template group with time. Template groups are defined as the brightest and darkest 2% of pixels in each snapshot. The bright templates represent Granular Tops (GTs) and the dark templates represent Intergranular Lanes (IgL). The periodic instances seen here are an artifact of p-modes. Radial velocity is calculated by cross correlating the line profile from each pixel with the total temporal and spatially averaged line profile.

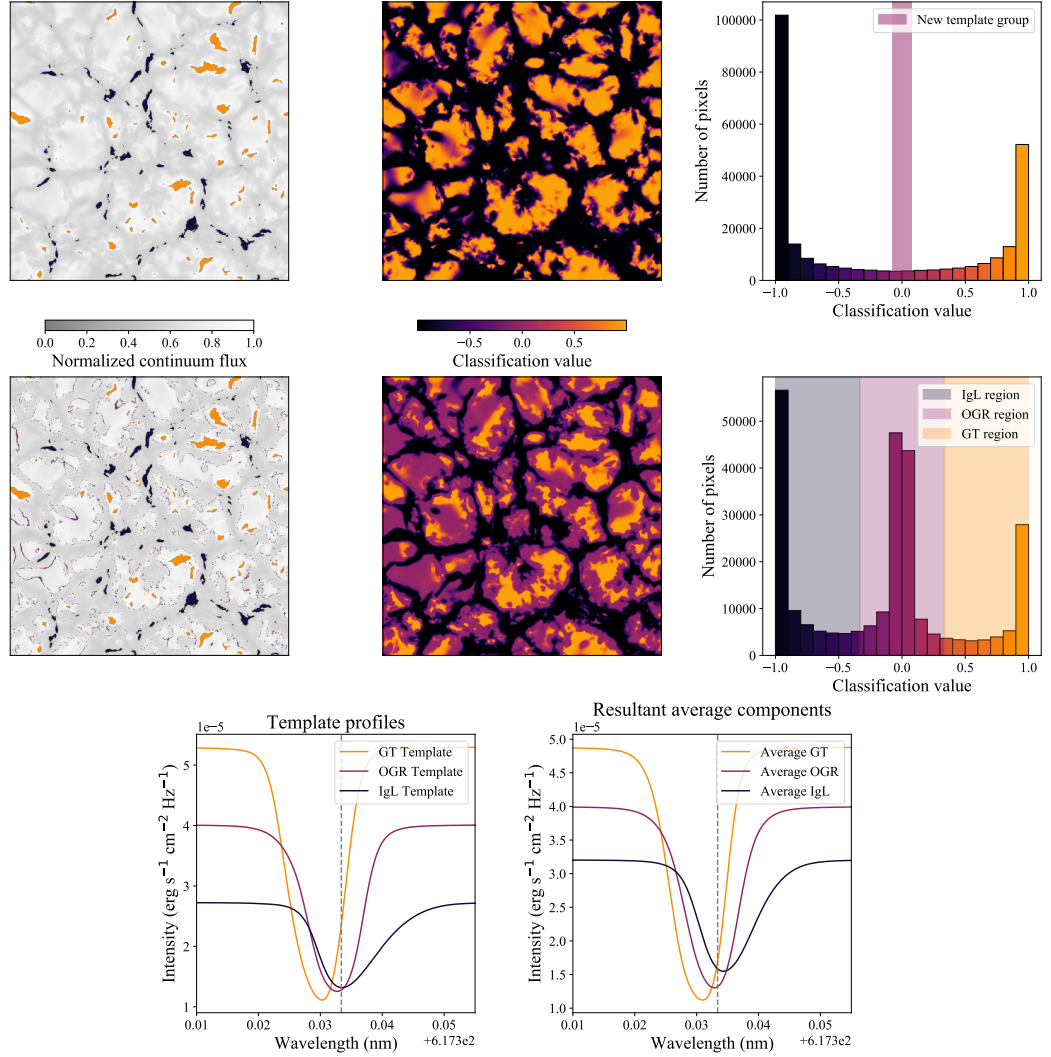


Figure 7.6: The parameterisation method demonstrated on a single snapshot, using the FeI 617nm line. *Top row:* The top left corner plot shows the locations of the Granular Top (GT) template pixels in orange and the Intergranular Lane (IgL) template pixels in black, overlaid on the normalised continuum flux. To the right of this are the resulting classification values for every pixel from the logistic regression model trained on the template pixels. Highlighted in purple in the top right plot is the region from which Outer Granular Region (OGR) template pixels are selected. *Middle row:* The leftmost plot again shows the locations of the templates, this time including the OGR template group in purple. To the right of this are the final classification values determined by the retrained logistic model including all three components. *Bottom row:* The bottom two plots show the spatially averaged template line profiles on the left and the resultant spatially averaged components on the right. The grey dotted lines indicate the rest wavelength of the line.



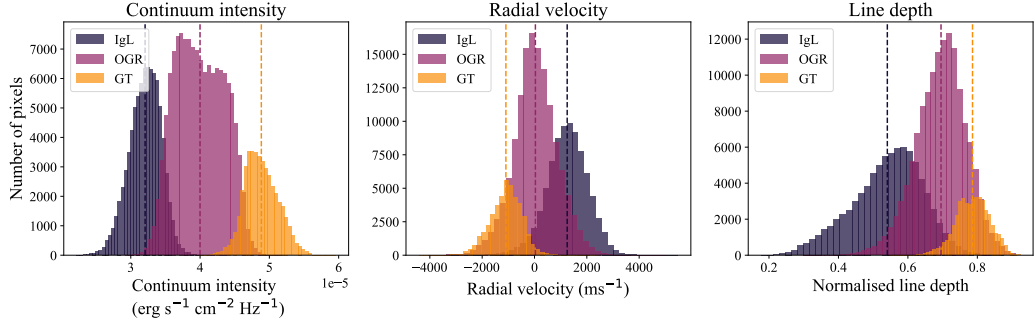


Figure 7.7: Distributions of selected parameters for each component for one snapshot at disc centre ( $\mu = 1.0$ ). The dotted lines indicate the mean value of each component. Note that radial velocity here is calculated relative to the time averaged profile across all snapshots (which itself exhibits a convective blueshift).

$$\text{Final classification} = P(\text{GT}) - P(\text{IgL})$$

This again results in a range from -1 (definitely an IgL) to 0 (definitely a OGR) to 1 (definitely a GT). Pixels are then assigned a group based on their classification value. GTs have values between  $1/3$  and 1, OGRs between  $-1/3$  and  $1/3$ , and IgLs between -1 and  $-1/3$ . The final classification results are shown in the second row of Figure 7.6. The bottom row of Figure 7.6 shows the average line profiles of the template pixels along with the resultant averaged group components. These spatially averaged group components are calculated for each snapshot individually and then are averaged again over time to remove the effects of p-modes.

The decision to populate each of our template groups with 2% of the available pixels is somewhat arbitrary. We tested the process also using 3% and 5%, and whilst there is a difference in initial classification result, as long as the percentage used is matched in the third template group, there is minimal difference in the determined final classification values.

Figure 7.7 shows the distributions of the chosen key line-shape parameters for each group in one snapshot. It is evident here that the classification method successfully separates all three parameters into groups that are as distinct as possible, prioritising continuum intensity since this parameter has the highest feature importance.

The entire classification process is run separately for each of the four lines, at each

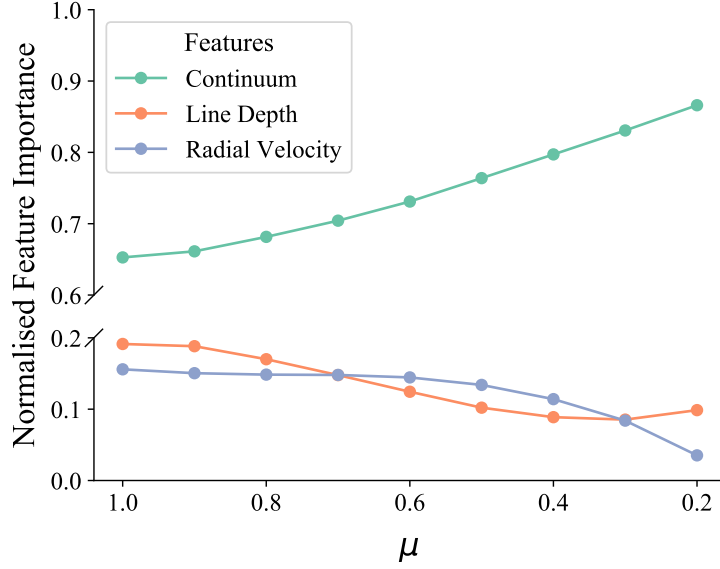


Figure 7.8: Average normalised absolute feature importance values at different limb angles. Each value has been divided by the sum of feature importance values to demonstrate the relative contributions of each feature and averaged over time. A high feature importance value indicates a strong weighting for the feature in the classification model.

$\mu$ . Note that a pixel assigned to one group for one line may not necessarily be of the same group for a different line due to changing formation heights and differing contrast levels between granules and lanes.

### 7.3.2 Pixel classification at different inclinations

The classification method remains robust across different inclinations, as the templates are data driven and inherently adapt to the specific characteristics of each cube. By defining GT and IgL templates directly from the data at each inclination, the method ensures that classifications are accurately aligned with the unique distribution of line shape parameters.

Figure 7.8 illustrates the variation in feature importance (FI) values assigned by the logistic regression model at different inclinations. The FI value determines the relative weight of each feature in the classification of individual pixels. A higher FI indicates a stronger correlation between the feature and the classification outcome. Each point in the plot represents the absolute value of the FI for a feature,

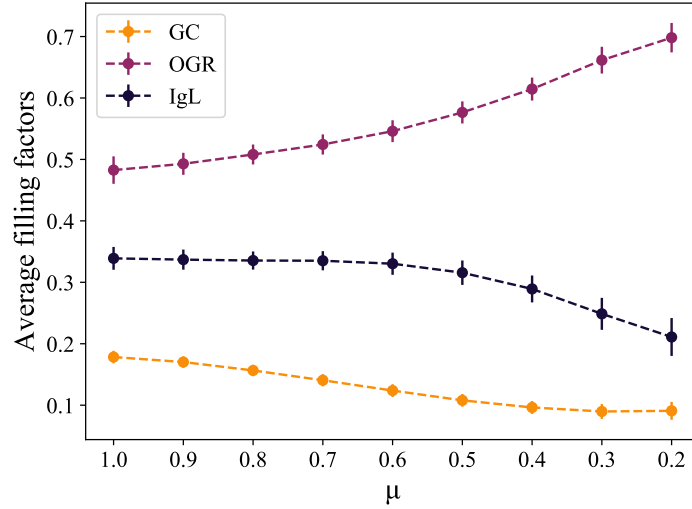


Figure 7.9: Time averaged filling factors of each component against limb angle for Fe I 617 nm. The error-bars represent the standard deviation of each result.

normalized by the sum of all FI values, and averaged over time. This reveals the relative contribution of each feature to the classification decisions. It is clear that continuum intensity consistently plays the dominant role in pixel classification, with this influence becoming more pronounced towards the limb. As higher atmospheric layers are probed, and horizontal velocity flows are incorporated, the distinction between the velocities and line depths of different components diminishes. Therefore the values become less important for classification purposes.

Another consequence of viewing the cube from an inclined angle is a change in component filling factors. Figure 7.9 shows the average filling factor for each component at each limb angle. Note that as expected, we see an increase in OGR filling factor as we get closer to the limb due to extremities (IgLS and GTs) being concealed by the edges and peaks of the corrugated optical surface.

The results for the spatially averaged GT, OGR and IgL components are plotted in Figure 7.10 at three limb angles, along with a time series of the filling factors. Scatter in velocity and intensity seen in the top two panels of this figure are a result of the p-modes. The reduction in contrast between component features can be clearly seen here in the profiles and bisectors at  $\mu = 0.3$ . More discussion on changes to granule/lane contrast towards the limb can be found in Section 7.5.

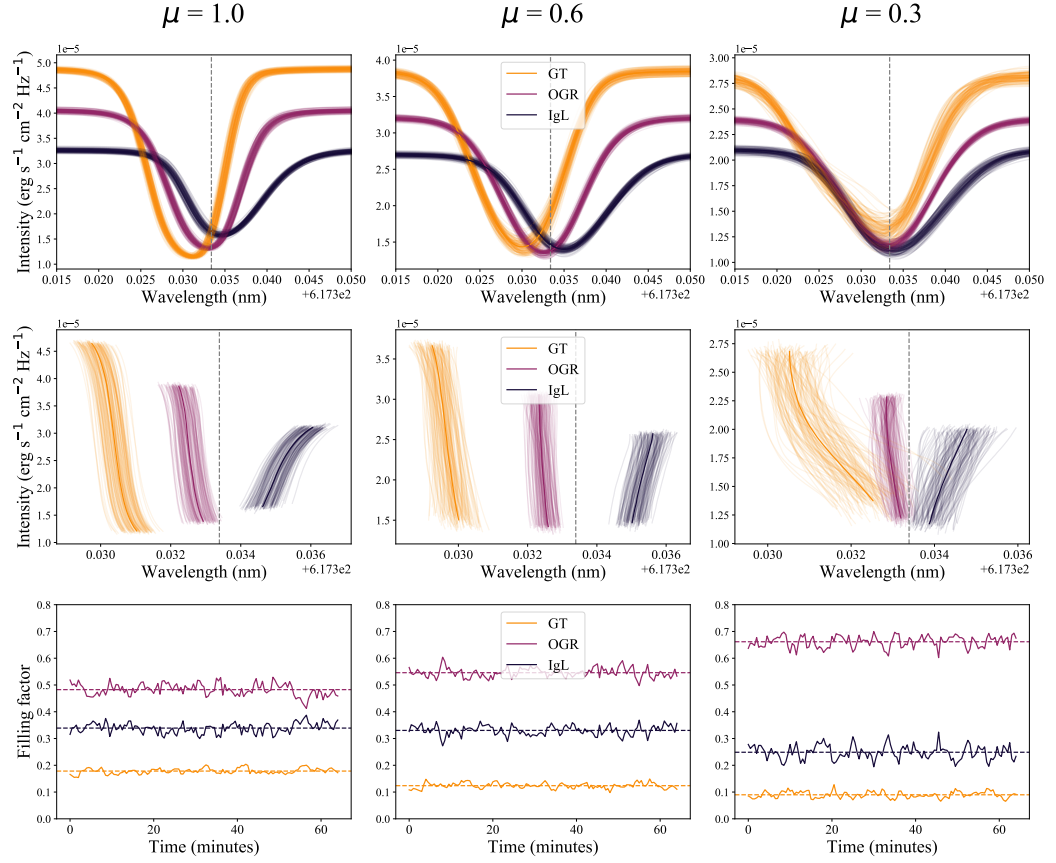


Figure 7.10: The parameterisation results for Fe I 617 nm. *Top row:* The spatially averaged components for every snapshot plotted on top of one another. *Middle row:* The bisectors of the profiles above, with the bold lines indicating the time averaged result. Vertical gray dotted lines indicate the rest wavelength of the line. *Bottom row:* The evolution of filling factors for each component over time. The horizontal dotted lines indicate mean values.

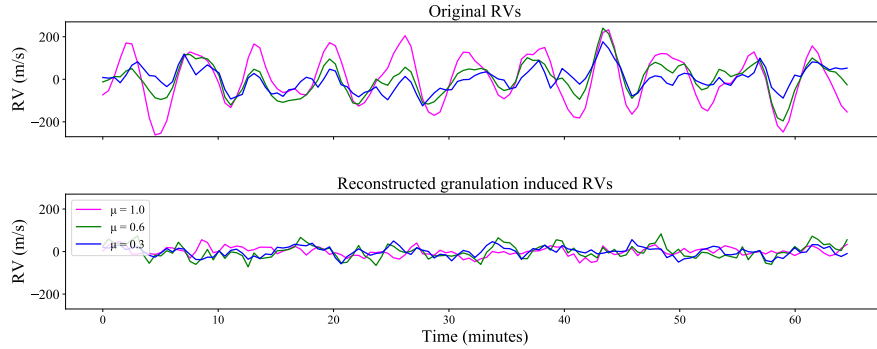


Figure 7.11: Line of sight radial velocities calculated by cross-correlating each profile with the time-averaged profile at the relevant limb angle. The top plot shows velocities from the original dataset that includes contributions from both granulation and p-modes. The bottom plot shows velocities from the reconstructed dataset, in which the p-modes have been removed.

## 7.4 Reconstructing the time series

We reconstruct our line profiles using the time averaged component line profiles coupled to the component filling factors obtained from each HD snapshot. As previously discussed in Section 7.3, the time averaging of components will eliminate the effects of p-modes, whilst the granulation signature is retained within the filling factors. Therefore by performing this reconstruction, we recreate the original time series but without p-mode effects, thus isolating the impact of granulation. Figure 7.11 shows the original RVs that include effects from both p-modes and granulation, and the RVs from the reconstructed time series, that include only granulation induced effects. As a reminder, RVs in this work are calculated using cross-correlation with a time averaged profile as the template. Figure 7.11 shows that the periodic oscillations caused by p-modes have been removed in the reconstructed time series.

### 7.4.1 Validation via power spectra comparisons with observations

Recent work by Al Moulla et al. [2023] separated stellar signal components by fitting analytical functions to radial velocity power spectral densities (VPSDs; Lefebvre et al. 2008). Other examples of this method can be found in Cegla et al. 2018, Kallinger et al. 2014 and Michel et al. 2009. Here, we use similar techniques to validate our reconstruction method.

Our HD simulations include p-mode oscillations and granulation. If the reconstruc-

tion using the parameterised line profiles is successful, the reconstructed time series should exclude p-mode contributions while preserving the granulation signature. We characterize the granulation contribution to the VPSD and validate our reconstruction method against observations of the solar VPSD, described below.

The observation and data-reduction procedures for the LARS data used in this section are described in greater detail in Löhner-Böttcher et al. [2017] and Löhner-Böttcher et al. [2019]. Here, we use eight time series observed at solar disc center that are centered on the FeI 617 nm line. In the analysis presented in Palumbo et al. 2024, these data were binned to a 15-second cadence; here we use the unbinned data that were observed at a 1.5-second cadence (0.5 seconds exposure + 1.0 second overhead). The baselines of the time series vary somewhat, but the longest covers  $\sim 29$  minutes and the shortest 17 minutes. We calculate separate VPSDs for each of the eight time series, from which we calculate a final VPSD by binning into 30 logarithmically equidistant frequency bins. As for the simulations, we calculate velocities by cross-correlating the time-averaged line profile with each epoch of the time series and derive the VPSD from this.

Following the methodology within Lefebvre et al. [2008], we model the granulation component of each of the VPSDs using a function of the form:

$$VPSD_g(\nu) = \frac{A_g}{1 + (\tau\nu)^\alpha}, \quad (7)$$

where  $A_g$  is the amplitude,  $\tau$  is the characteristic timescale, and  $\alpha$  is the power-law slope. Following Al Moulla et al. [2023], we fix the power-law slope  $\alpha = 2$ .

We describe the p-mode component of the VPSDs with a Lorentzian function:

$$VPSD_p(\nu) = \frac{A_p\Gamma^2}{(\nu - \nu_0)^2 + \Gamma^2}, \quad (6)$$

where  $A_p$  is the amplitude,  $\Gamma$  is the full-width at half-maximum (FWHM), and  $\nu_0$  is the central frequency.

For the simulated data, we perform a simultaneous joint fit to the original and reconstructed datasets using MCMC sampling. The original data is modeled with  $VPSD_g + VPSD_p$ , while the reconstructed data is fitted with  $VPSD_g$ , ensuring shared parameters for  $VPSD_g$  between the datasets. We model the observed VPSD from LARS separately with  $VPSD_g + VPSD_p + C$ , where  $C$  is a constant relating

to the photon noise.

The log-likelihood for each fit is defined as:

$$\ln \mathcal{L} = -\frac{1}{2} \sum_i \left[ \frac{(\log_{10}(y_i) - \text{model}_i)^2}{\sigma_i^2} + \ln(2\pi\sigma_i^2) \right], \quad (7.1)$$

where:

- $y_i$  is the observed data for dataset  $i$ ,
- $\text{model}_i$  is the corresponding model prediction,
- $\sigma_i$  represents the uncertainty in the data for dataset  $i$ .

The  $\sigma_1$  and  $\sigma_2$  parameters correspond to the uncertainties (standard deviations) of the two datasets and are treated as free parameters in the MCMC sampling. The python package `emcee` [Foreman-Mackey, 2014] was used for MCMC analysis, employing 32 walkers and 10,000 steps per walker, with a burn-in phase of 1500 steps. Table 7.2 outlines the priors for the parameters, while Table 7.3 presents the best-fit results for both the simulated and observed dataset. Note that the characteristic timescale of granulation ( $\tau$ ) will be affected by the spatial scale of observations. The values presented here for disc center calculations should not be compared to those from disc-integrated studies (e.g: Al Moulla et al. [2023]). The fact that our  $\tau$  result from our synthetic dataset shows a strong agreement with that derived from disc center solar observations indicates that our granulation extraction method accurately captures the temporal evolution.

The wavelengths of the dominant p-modes in our simulations are defined by the vertical extent of the HD box. In addition, there are artificial modes excited during the relaxation process. We therefore do not expect the p-mode component of our simulated dataset to match observations (see Zhou et al. 2021). However, if our reconstruction method has successfully eliminated the artificial p-mode contribution, we expect the granulation component of the two datasets to be consistent. Comparing absolute amplitudes is not meaningful here, instead we care about the contribution of granulation towards the total amplitude. We therefore normalise all data and fitted components by the relevant  $A_p + A_g + C$  (in the case of simulation,  $C = 0$ ). The results are shown in Figure 7.12, with the bottom plot showing the granulation component fitted to our reconstructed data along with the component

| Parameter                        | Description              | Prior (simulated)                 | Prior (observed)                  |
|----------------------------------|--------------------------|-----------------------------------|-----------------------------------|
| <b>P-mode Parameters</b>         |                          |                                   |                                   |
| $A_p [(ms^{-1})^2 Hz^{-1}]$      | Amplitude                | $U[5 \times 10^7, 2 \times 10^8]$ | $U[5 \times 10^7, 2 \times 10^8]$ |
| $\Gamma [mHz]$                   | FWHM                     | $U[0, 0.3]$                       | $U[0, 0.3]$                       |
| $\nu_0 [mHz]$                    | Central frequency        | $U[2.8, 3.5]$                     | $U[2.8, 3.5]$                     |
| <b>Granulation Parameters</b>    |                          |                                   |                                   |
| $A_g [(ms^{-1})^2 Hz^{-1}]$      | Amplitude                | $U[2 \times 10^4, 5 \times 10^5]$ | $U[2 \times 10^4, 5 \times 10^5]$ |
| $\tau [mHz^{-1}]$                | Characteristic timescale | $U[0.1, 1.0]$                     | $U[0.1, 1.0]$                     |
| <b>Constants</b>                 |                          |                                   |                                   |
| $C [(ms^{-1})^2 Hz^{-1}]$        | Photon noise             | N/A                               | $U[1 \times 10^2, 1 \times 10^5]$ |
| <b>Uncertainties</b>             |                          |                                   |                                   |
| $\sigma_1 [(ms^{-1})^2 Hz^{-1}]$ | Uncertainty in dataset 1 | $U[10^{-3}, 10]$                  | $U[10^{-3}, 10]$                  |
| $\sigma_2 [(ms^{-1})^2 Hz^{-1}]$ | Uncertainty in dataset 2 | $U[10^{-3}, 10]$                  | N/A                               |

Table 7.2: Priors for MCMC parameters.  $U[\text{min}, \text{max}]$  denotes a uniform prior.



| Parameter                        | Best Fit (simulated)  | Uncertainty (simulated)                     | Best Fit (observed)   | Uncertainty (observed)                      |
|----------------------------------|-----------------------|---------------------------------------------|-----------------------|---------------------------------------------|
| <b>P-mode Parameters</b>         |                       |                                             |                       |                                             |
| $A_p [(ms^{-1})^2 Hz^{-1}]$      | $1.10 \times 10^8$    | $6.51 \times 10^7 / 1.68 \times 10^8$       | $1.01 \times 10^8$    | $6.28 \times 10^7 / 1.63 \times 10^8$       |
| $\Gamma [mHz]$                   | $5.60 \times 10^{-2}$ | $4.17 \times 10^{-2} / 7.66 \times 10^{-2}$ | $7.58 \times 10^{-2}$ | $5.50 \times 10^{-2} / 1.05 \times 10^{-1}$ |
| $\nu_0 [mHz]$                    | 2.96                  | 2.88/3.05                                   | 3.25                  | 3.19/3.31                                   |
| <b>Granulation Parameters</b>    |                       |                                             |                       |                                             |
| $A_g [(ms^{-1})^2 Hz^{-1}]$      | $1.43 \times 10^5$    | $9.59 \times 10^4 / 2.13 \times 10^5$       | $3.28 \times 10^5$    | $2.12 \times 10^5 / 4.34 \times 10^5$       |
| $\tau [mHz^{-1}]$                | $3.25 \times 10^{-1}$ | $2.55 \times 10^{-1} / 4.18 \times 10^{-1}$ | $3.60 \times 10^{-1}$ | $2.12 \times 10^{-1} / 4.34 \times 10^{-1}$ |
| <b>Constants</b>                 |                       |                                             |                       |                                             |
| $C [(ms^{-1})^2 Hz^{-1}]$        | N/A                   | N/A                                         | $2.85 \times 10^3$    | $1.99 \times 10^3 / 3.96 \times 10^3$       |
| <b>Uncertainties</b>             |                       |                                             |                       |                                             |
| $\sigma_1 [(ms^{-1})^2 Hz^{-1}]$ | $5.55 \times 10^{-1}$ | $5.08 \times 10^{-1} / 6.08 \times 10^{-1}$ | $3.21 \times 10^{-1}$ | $2.82 \times 10^{-1} / 3.69 \times 10^{-1}$ |
| $\sigma_2 [(ms^{-1})^2 Hz^{-1}]$ | $6.79 \times 10^{-1}$ | $6.22 \times 10^{-1} / 7.46 \times 10^{-1}$ | N/A                   | N/A                                         |

Table 7.3: Best fit parameters and uncertainties from MCMC sampling. The uncertainties represent the 16th and 84th percentiles of the posterior distributions.

extracted from the observed data. We find a strong match to observations, confirming that our parameterisation and reconstruction method effectively isolates the granulation signature from our simulated data.

## 7.5 Center to limb effects of granulation

In this section, we use our reconstruction results to analyse granulation effects across the stellar limb for our four chosen lines. As briefly discussed in Section 7.3.2, the act of inclining our line of sight changes what areas are visible due to the corrugated nature of the stellar surface. It also changes the atmospheric layer visible to us; higher inclinations probe higher altitudes, which are on average cooler and contain different velocity fields. A key consequence of this is a change in contrast between granules and lanes, which affects the bisector asymmetry and RV root mean square (rms) as a function of limb angle.

Figure 7.13 illustrates the evolution of bisector shape and Doppler velocity for each component at different limb angles. The components displayed here are from the spatially and temporally averaged profiles solved for in Section 7.3. The rightmost plots in this figure show the total bisectors calculated from the combination of these components. The strong characteristic C-shape at limb angles close to disc center are a direct result of the contrast in brightness and velocity of the granular and lane components. The C-shape diminishes towards the limb as the contrast decreases. Note that the bisector shapes of Fe I 627 nm, the weakest line, resemble the upper portions of the stronger line bisectors, as is presented in Gray [2005]. A similar behavior can be seen in the “Fe I, G1V” plot in Figure 6 in Dravins et al. [2021]. However, it is shown in Palumbo et al. [2024] that this effect is not universal across all line profiles.

The top panel in Figure 7.14 shows the velocity contrast between Igls and GTs as a function of  $\mu$ . The velocities are derived by cross-correlating the component profiles with the time-averaged original profile at each  $\mu$ . Note that the contrast is larger for weaker lines. You can observe the reason for this in Figure 7.13, as it is the component cores that are most similar in velocity, and weaker lines only retain the upper portion of the stronger bisectors. This contrast is a strong indicator of granulation induced RV rms, as can be seen in the bottom plot of Figure 7.14. These rms values are calculated using the RVs from the reconstructed time series and indicate

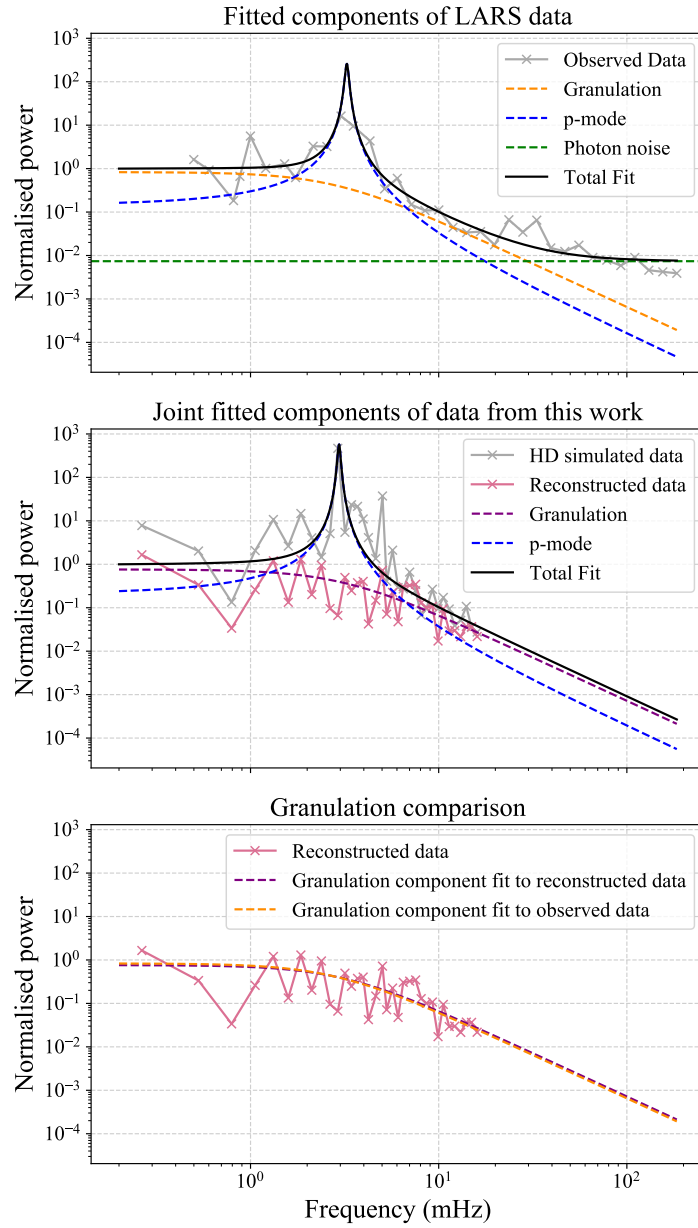


Figure 7.12: Velocity power spectral density and fits to simulated and observed datasets. The bold, black lines show the total fits to the data, while the dotted lines show the components within this fit. The top plot displays observational data from LARS. The middle plot shows both the original HD and reconstructed versions of our simulated dataset. In this case, a joint fit was performed, with the assumption that the reconstructed data represented the granulation component of the original data. The bottom plot shows the reconstructed data from our simulations with both granulation components from the plots above.

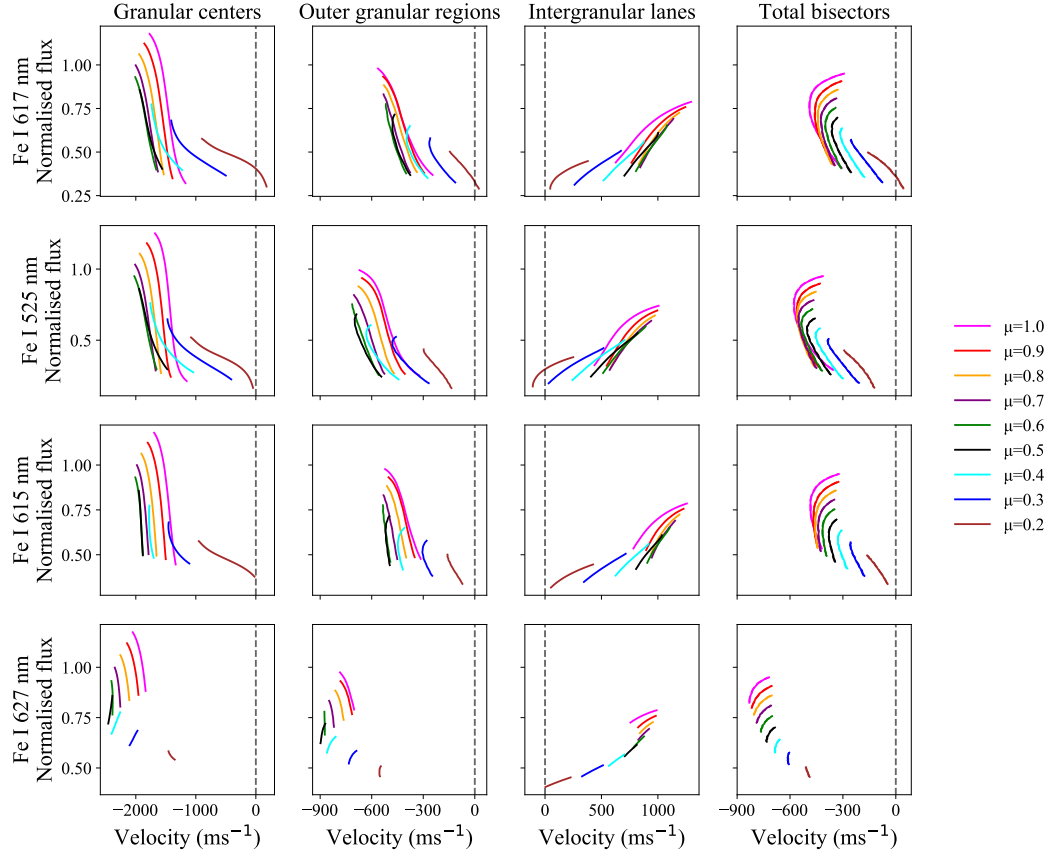


Figure 7.13: Bisectors of the average component profiles for each line and limb angle. Flux has been normalised relative to the continuum intensity of the total average profile at disc center (hence flux values greater than 1 can be seen in components brighter than the average). Velocity here is the Doppler velocity. The rightmost plots show the total bisectors found by combining the components multiplied by the relevant filling factors. The gray vertical dashed line indicates a velocity of 0 m/s.

the variability we see in the convective blueshift (CB) caused by granulation. This decrease in granular contrast for stronger lines is in agreement with Dravins et al. [2021], who points out that in solar-like G-type stars, the amplitudes of granule brightness and velocities are somewhat obscured beneath line-forming layers. The contrast therefore decreases with height, and so stronger lines, which form higher up in the photosphere, exhibit less granular contrast. It is for this same reason that the contrast in all lines decreases so rapidly towards the limb, where higher atmospheric layers are probed.

The actual values of CB at each  $\mu$  are shown in Figure 7.15. These velocities are calculated by taking the mean bisector Doppler velocity of the time-averaged profile, where Doppler velocity is calculated relative to the rest wavelength of the line. We perform the same calculations on time-averaged disc-resolved profiles from LARS and IAG. Instead of trying to match the absolute values between our models and the observations, we focus on comparing the center-to-limb variation in CB. We therefore shift the observational results for each line to match the mean CB across  $\mu$  values of simulations. The observational results are also plotted in Figure 7.15, with dashed lines being IAG and dotted LARS. Evidently, our results retain the observed relationship between  $\mu$  and CB, with velocity increasing at an accelerating rate when moving towards the limb.

Finally, in Figure 7.16, we plot the bisector wavelength span (BIS) and bisector curvature (BC) [Povich et al., 2001] against limb angle. These parameters are a way of quantifying the asymmetry of the line. They are defined as follows:

- **BIS:** The average bisector wavelength within the bottom portion of the bisector subtracted from the average wavelength in the top portion. The regions are defined as 10%-40% and 55%-90% of the line depth.
- **BC:** The bisector is split into three regions and the average wavelength is calculated for each (top, middle, bottom). BC is calculated with top + bottom -  $2 \times$  middle. Regions are defined as 80%-90%, 40%-60% and 10%-20%.

We calculate these measures for each profile in our reconstructed time series for each limb angle. The points plotted in Figure 7.16 are the mean values over time, and the errorbars are the standard deviations. The dashed lines show results calculated as defined above using profiles from IAG, and the dotted lines using profiles from LARS. In this plot, the observed values have not been shifted. Overall, our results

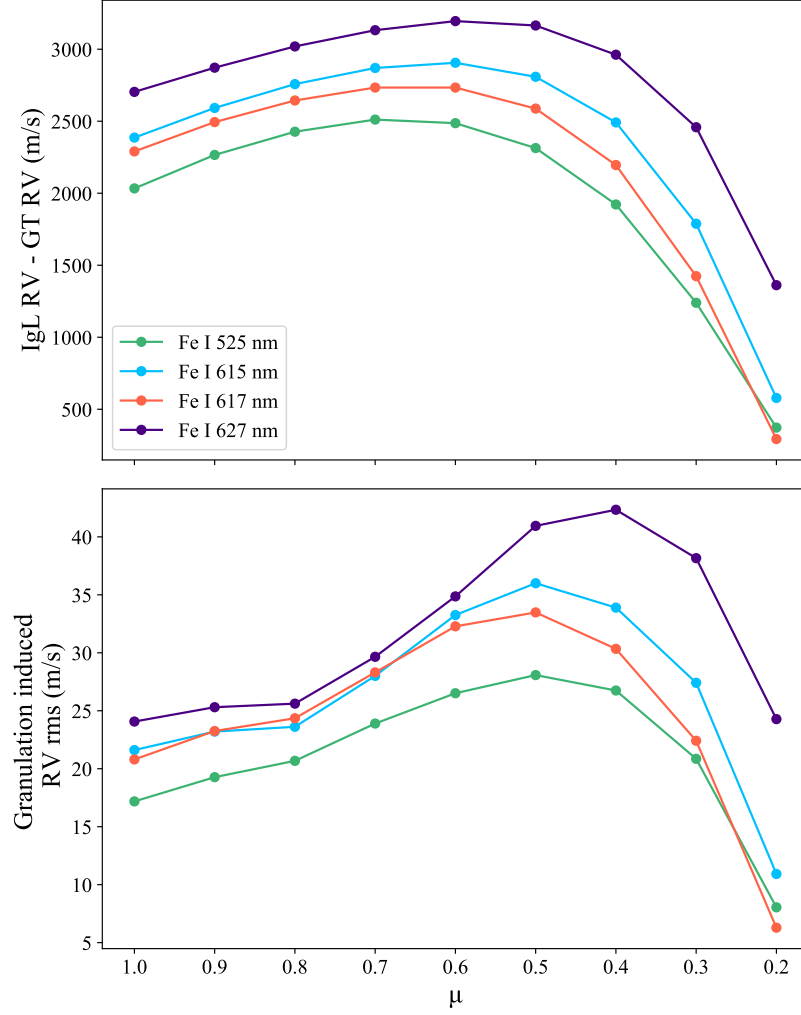


Figure 7.14: The top panel shows the difference in RV between intergranular lanes and granular tops for each line at different limb angles. The RVs are calculated by cross-correlating the relevant average component profile with the average total profile at each  $\mu$ . Note that Fe I 627 nm is the weakest line and Fe I 525 nm is the strongest. The bottom panel shows the changes in granulation induced RV rms. This is calculated using RVs from the reconstructed time series and indicates the level of variation between lines in granulation induced convective blueshift.

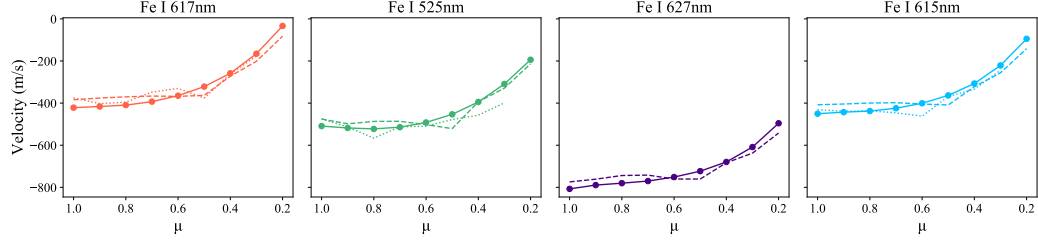


Figure 7.15: Variation of relative convective blueshift with limb angle, with comparisons to observations. Velocities here are the mean bisector Doppler shifts. Solid lines shows results from the reconstructed data from this work, dotted lines show results from LARS, dashed lines show results from IAG. Both observational results have been shifted to match the mean velocity across limb angles to our data. The focus of this comparison is center-to-limb variations rather than absolute velocity values.

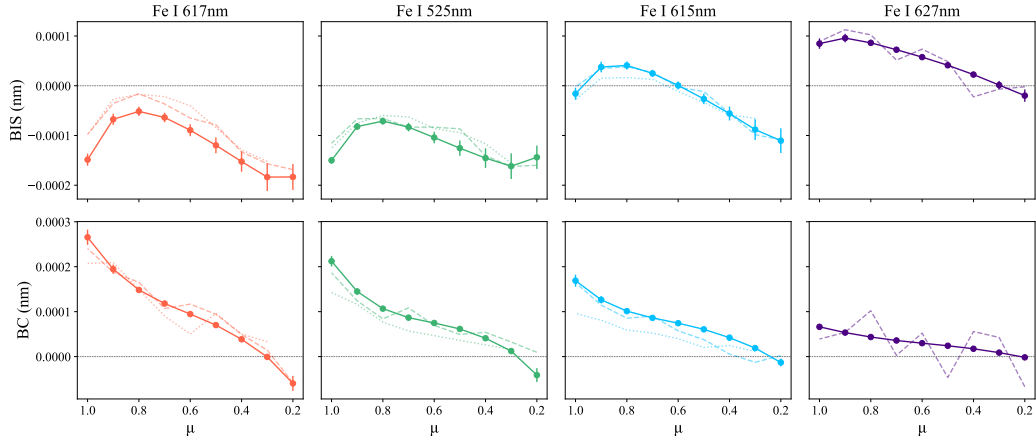


Figure 7.16: Bisector asymmetry measures plotted against limb angle for each line, with comparisons to observations. Bisector invserse slope (BIS) refers to the difference in average wavelength between the top (55-90%) and bottom (10-40%) of the bisector. Bisector curvature (BC) is the sum of the average wavelength in the top (80-90%) and bottom (10-20%) with the average wavelength in the middle (40-60%) subtracted. Errorbars indicate the standard deviation across snapshots. Solid lines show results from the reconstructed data from this work. Dashed lines show results from IAG observations. Dotted lines show results from LARS observations.

align well with observations.

## 7.6 Chapter summary and conclusions

In this chapter, we synthesised time series of four selected Fe I lines (Fe I 525 nm, Fe I 615 nm, Fe I 617 nm, and Fe I 627 nm) at nine limb angles across the surface of a solar-type star. The simulations are based on three-dimensional hydrodynamic cubes produced by MURaM, coupled with radiative transfer calculations performed using MPS-ATLAS. For each spectral line, the resulting dataset consists of 129 snapshots with a cadence of 30 seconds, spanning just over one hour of stellar surface evolution.

These synthetic time series inherently contain contributions from both p-mode oscillations and granulation. The primary objective of this chapter was to disentangle these two phenomena and isolate the signatures of granulation. To achieve this, we introduced a parameterisation framework based on spatial variations across the granulation pattern. The stellar surface was divided into three physically motivated components: granular tops, outer granular regions, and intergranular lanes. Classification into these components was performed using three spectral diagnostics: continuum intensity, radial velocity, and line depth. This allows for a classification scheme that is both line- and inclination-dependent, while remaining insensitive to the phase of pressure modes.

The mitigation of p-modes was achieved by averaging the spectral properties of each component over time, thereby removing oscillatory signals while preserving granulation signatures through time-varying filling factors. The reconstructed line profiles were then obtained by combining these averaged component profiles weighted by their corresponding filling factors at each snapshot. This process yielded a time series that isolates the effects of granulation alone.

We validated this approach by computing the velocity power spectral density (VPSD) of the reconstructed disc-centre Fe I 617 nm time series and fitting a Lorentzian profile. The resulting VPSD shows excellent agreement with the granulation component extracted from *LARS* observations of the same line at solar disc centre, providing strong evidence that the method successfully isolates granulation.

Using these isolated granulation time series, we investigated the center-to-limb vari-



ation of granulation-induced effects. We found that the velocity contrast between granules and intergranular lanes increases from disc centre to  $\mu \approx 0.7$ , after which it flattens and then decreases sharply towards  $\mu \approx 0.5$ . This behaviour is found to depend on line strength, with weaker lines exhibiting stronger contrast and consequently larger granulation-induced radial velocity scatter. The variation of convective blueshift with limb angle is also broadly consistent with observational results.

Finally, we quantified line bisector asymmetry using two complementary metrics, revealing both line-dependent behaviour and systematic centre-to-limb trends. These results show strong agreement with observations, further supporting the physical realism of the reconstructed granulation signals.

## Chapter 8

# The Isolation of Granulation in *Disc-Integrated* Spectral Lines

*“Geronimo!”*

---

*The doctor, Doctor Who*

### Note

This chapter is a reproduction of Frame et al. [2026], titled “Synthetic disc-integrated absorption lines isolating stellar granulation for high-precision RV studies”, originally published in March 2026 in Monthly Notices of the Royal Astronomical Society (MNRAS). All of the analysis and writing in this chapter was conducted by myself, with input and advice from co-authors.

### 8.1 Introduction

This chapter builds directly on the results of Chapter 7, in which disc-resolved spectral line profiles were used to isolate and characterise granulation across the stellar surface. While that analysis provided detailed insight into the centre-to-limb behaviour of granulation and its imprint on individual absorption lines, high-precision radial velocity (RV) observations are inherently disc-integrated. A key outstanding challenge is therefore to understand how these spatially resolved granulation signatures combine across the stellar disc, and how they manifest in integrated spectra relevant for exoplanet detection.

A limitation of empirically driven approaches is the difficulty in isolating pure granulation signals. Observational spectra are invariably contaminated by residual p-mode oscillations, telluric absorption, and overlap between granulation and supergranulation. They also contain instrumental uncertainties, caused by both instrument stability and observing conditions and are limited in resolution and precision. As a result of this, the intrinsic amplitude of granulation-induced velocity fluctuations remains poorly constrained. Current estimates of the solar RV rms caused by granulation range from  $\sim 0.3 \text{ m s}^{-1}$  [Elsworth et al., 1994; Dalal et al., 2023; Lakeland et al., 2024] to  $\sim 0.4 \text{ m s}^{-1}$  [Collier Cameron et al., 2019] to  $\sim 0.8 \text{ m s}^{-1}$  [Meunier et al., 2015] (as discussed in Chapter 4).

Cegla et al. [2013, 2018, 2019] developed a method of tiling a stellar grid with absorption lines synthesized from 3D magnetohydrodynamic (MHD) simulations produced with MURaM [Vögler et al., 2005] and 1D radiative transfer (RT) calculations from NICOLE [Socas-Navarro, 2015b; Socas-Navarro et al., 2015]. The goal of this approach was to construct disc-integrated line profiles containing only the effects of granulation. Their study focused on a single spectral feature, Fe I 630.2 nm, using MHD boxes representing the solar surface, with an initially imposed 200 G magnetic field.

Building on this, Frame et al. [2025] (hereafter F25, discussed in Chapter 7) used updated hydrodynamic (HD) MURaM simulations [Witzke et al., 2024] also for the solar case but with no magnetic field, together with MPS-ATLAS [Witzke et al., 2021] RT calculations to extend the analysis to four Fe I lines. Crucially, F25 introduced an updated parameterisation that explicitly removes the artificial p-mode oscillations present in HD simulations; this is an essential step given that the p-mode filtering in Cegla et al. [2013] was only adequate for the more strongly damped oscillations in MHD boxes. This refinement ensures a clean isolation of granulation signatures, overcoming a key limitation of observational data in which granulation is blended with p-modes, tellurics, and supergranulation.

F25 also investigated the center-to-limb dependence of granulation, showing that bisector shape, convective blueshift, and RV rms each exhibit non-trivial, line-dependent relationships with limb angle. Similar behavior was reported by Cegla et al. [2018], motivating the use of fine  $2^\circ$  sampling when tiling the stellar surface in subsequent simulations [Cegla et al., 2019]. Such sampling is fully adequate for capturing granulation signals, but is extremely computationally expensive, particu-

larity for multi-line analyses.

In this chapter, we adopt a continuous sampling approach using an interpolation scheme implemented in DISCO (disc Integrated Stellar CONvection)<sup>1</sup>, a Python framework developed in this work and made publicly available for generating and analysing disc-integrated stellar absorption line profiles. DISCO is capable of computing time-varying line profiles at arbitrary limb angles without the need for additional radiative transfer calculations. This approach reduces computational expense while maintaining the accuracy of the disc-integration process by enabling continuous and physically consistent coverage of the stellar disc.

It is worth briefly contrasting this framework with other tiled stellar surface models used in the literature. Statistical approaches such as that of Meunier et al. [2015] describe granulation through prescribed distributions of granule properties (e.g. size, velocity field, and lifetime), rather than through explicit synthesis of spectral line profiles at the tile level. Forward models such as SOAP are primarily designed to capture the effects of magnetic active regions and do not currently model time-resolved granulation-driven line profile variability, while empirical tools such as GRASS require observed time series as input and are therefore not predictive in the absence of suitable data. The approach adopted here is closely related to that of Cegla et al. [2019], but differs in our use of a line-profile-based parameterisation of unresolved granulation combined with continuous limb-angle interpolation, as discussed earlier.

In this chapter, we use this new interpolation-based tiling scheme to construct time-varying, disc-integrated stellar absorption line profiles that contain only the effects of granulation. This allows us to isolate the intrinsic velocity variability caused by granulation and to assess, under idealised conditions, the extent to which it can be mitigated using common spectral diagnostics. We test both bisector asymmetry and full-line shape metrics across four Fe I lines to determine their ability to trace and correct convective variability. By subsequently introducing realistic instrumental resolution and injecting various levels of photon noise, we evaluate the practical limits of these diagnostics and quantify the residual RV scatter that would remain in high-precision observations. Through this approach, we aim to establish both the theoretical lower bound on granulation-induced velocity noise and the observational requirements needed to overcome it.

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<sup>1</sup><https://github.com/ginger-frame/DISCO>

Table 8.1: Summary of simulation and line synthesis setup.

| Property              | Value / Description                              |
|-----------------------|--------------------------------------------------|
| Simulation code       | MURaM [Vögler et al., 2005; Witzke et al., 2024] |
| Simulation duration   | $\sim 1$ hour                                    |
| Cadence               | 30 seconds                                       |
| Horizontal extent     | $9 \times 9 \text{ Mm}^2$                        |
| Horizontal resolution | $512 \times 512$ pixels                          |
| Vertical extent       | 5 Mm*                                            |
| Vertical resolution   | 500 pixels                                       |
| Line synthesis code   | MPS-ATLAS [Witzke et al., 2021]                  |
| Spectral resolution   | $R = 2,000,000$                                  |

\* 1 Mm of atmosphere above the photosphere and 4 Mm of sub-photosphere and convection zone of a solar type star.

A summary of the data used in this chapter is provided in Section 8.2. For a more in-depth description, as well as a full explanation of the parameterisation process, we refer the reader to F25 (Chapter 7). Section 8.3 outlines our interpolation scheme for generating profiles at arbitrary limb angles. Section 8.4 describes our stellar grid set up. Section 8.5 explains the calculation of our disc-integrated profiles using DISCO. Section 8.6 explores techniques for the mitigation of granulation induced RVs under idealised circumstances. Section 8.7 investigates the impact of signal-to-noise ratio (SNR) on our ability to trace granulation signatures in stellar spectra.

## 8.2 Data

All absorption line profiles in this work were synthesised from a time series of 3D hydrodynamic simulation boxes. To produce line profiles at different positions on the stellar disc and account for changes in limb darkening and convective blueshift, the hydrodynamic quantities of the 3D cubes were tilted and interpolated onto rays parallel to the desired limb angle, prior to line synthesis (see Smitha et al. 2025 for a description of this process). For details on our data and line synthesis method, see Section 7.2. A summary of the simulation properties is provided in Table 8.1.

Line synthesis for the full time series was performed for the following lines: Fe I 525.0 nm, Fe I 615.2 nm, Fe I 617.3 nm, Fe I 627.1 nm. For the atomic properties of these lines, see Table 7.1.

### 8.3 Producing profiles at arbitrary limb angles

In F25, we demonstrated that absorption line profiles at different limb angles can be parameterized into three components: granular tops (GTs), outer granular regions (OGRs), and intergranular lanes (IgLS). By averaging these component profiles over time and space, we effectively remove p-mode oscillations while preserving the granulation signal in the component filling factors. This yields a valuable dataset consisting of time-averaged component profiles and their corresponding filling factor distributions. By sampling new filling factors from these distributions and combining them with the component profiles, we can synthesize additional accurate line profiles. In this work, we show that we are able to construct highly accurate line profiles at any given limb angle for unlimited instances in time.

We analysed the filling factor distributions from F25 and found a strong linear correlation between OGR and IgL filling factors, but no significant correlation involving GT filling factors. Based on this, we produce new synthetic profiles by independently sampling GT filling factors from their distribution, and separately sampling from the distribution of the OGR-to-IgL filling factor ratio.

A random instance of a line profile at a given limb angle  $\theta$  (see Section 8.4.3 for  $\theta$  definition) is then given by:

$$I(\theta) = I_{\text{GT}}(\theta)\epsilon_1 + I_{\text{OGR}}(\theta)\frac{\epsilon_2(1 - \epsilon_1)}{1 + \epsilon_2} + I_{\text{IgL}}(\theta)\frac{(1 - \epsilon_1)}{1 + \epsilon_2} \quad (8.1)$$

$$\epsilon_1 \sim \mathcal{D}_{\text{GT}}(\theta)$$

$$\epsilon_2 \sim \mathcal{D}_{\text{OGR/IgL}}(\theta)$$

where each  $I_C(\theta)$  ( $C \in \{\text{GT}, \text{OGR}, \text{IgL}\}$ ) is the average component profile and each  $\mathcal{D}(\theta)$  is the probability distribution from which the relevant filling factor  $\epsilon$  is pulled.

To be able to generate  $I(\theta)$  at any given  $\theta$ , we must be able to interpolate on  $\theta$  each  $I_C(\theta)$  and  $\mathcal{D}(\theta)$ . To do this we first define the optimum set of training limb angles, based upon the trade-off between computation time and minimisation of root mean square error (rmse) in the disc-integrated profile. We find the optimal training set consists of 16 angles (in degrees): 0, 2, 6, 9, 13, 17, 20, 23, 27, 35, 50, 60, 68, 81, 82, and 83. For a description of the method used to determine these angles, see

Section 8.9.1.

In F25, calculations were performed from  $\mu = 1.0$  to  $\mu = 0.2$  in steps of 0.1, where  $\mu = \cos(\theta)$ . Other than  $\mu = 1.0$  ( $\theta = 0^\circ$ ) and  $\mu = 0.5$  ( $\theta = 60^\circ$ ), the results in F25 are not included in the training set for this work. We therefore use these results as our validation set to check the interpolation is working as expected.

### 8.3.1 Interpolating average component profiles

To interpolate the component line profiles across different stellar limb angles, we employ Principal Component Analysis (PCA). This allows us to reduce the dimensionality of the line profiles and interpolate their variation smoothly with angle.

PCA identifies a set of orthogonal basis functions called principal components (PCs), or eigenprofiles, that capture the main variations in the profiles across different limb angles. Each original profile can then be approximated as a weighted sum of these components, plus a mean profile that represents the average shape across all angles. The weights (also called PCA coefficients or scores) vary with limb angle and describe how much each principal component contributes to a given profile. Each coefficient  $a_k(\theta)$  is interpolated as a smooth function of  $\theta$  using cubic splines.

Figure 8.1 shows the first three PCs for the three average components in the Fe I 617 nm line, along with the variation of the coefficients with  $\theta$ . In practice, we retain seven PCs for each component, which we find provides a good balance between capturing the relevant variability in the data and avoiding overfitting. See Appendix 8.9.1 for more details.

At an arbitrary  $\theta$ , each component profile is constructed as:

$$I_C(\theta) \approx \bar{I}_C + \sum_{k=1}^7 \tilde{a}_k(\theta) \phi_k. \quad (8.2)$$

where  $\bar{I}_C$  is representative of the mean profile over all  $\theta$ ,  $\tilde{a}_k(\theta)$  is the spline-interpolated coefficient for component  $k$ , and  $\phi_k$  is the PC.

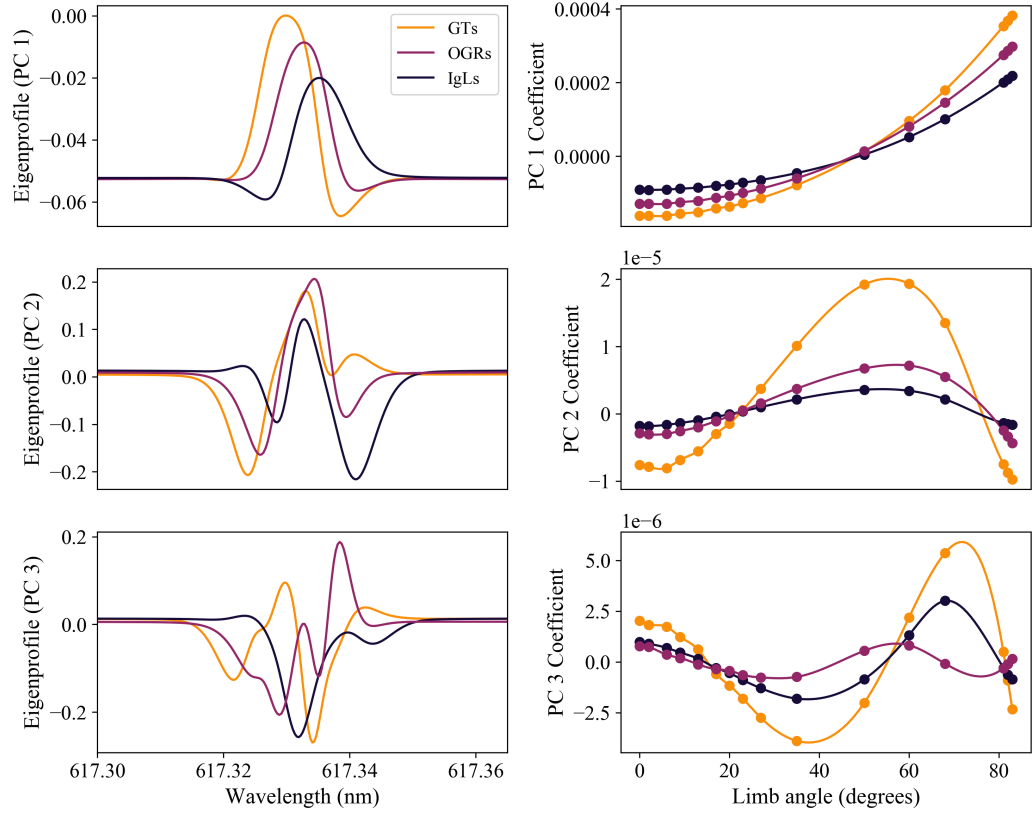


Figure 8.1: First three eigenprofiles (principal components) of each component profile (left column) and the associated coefficients and their variation with limb angle (right column) for Fe I 617.3nm. The circular points show results for the training set of limb angles from which the interpolation is based on.



### 8.3.2 Characterising and interpolating filling factor distributions

In F25, we established that granulation-induced velocity and line-shape variations are preserved in our time series of filling factors. It is therefore crucial to accurately maintain the underlying statistical distributions when drawing new samples.

Following the approach of Cegla et al. [2019], one option of characterising the filling factor distributions is to fit generalised logistic functions to the cumulative distribution functions (CDFs). While this method performs well when fitting each training angle independently, we find that the resulting fit parameters do not vary smoothly with limb angle, making interpolation problematic.

To address this, we instead model the distribution of filling factors at each training angle using a skewed Gaussian distribution, characterised by three parameters: shape  $\alpha$  (controlling skewness), location  $\zeta$  (analogous to the mean), and scale  $\omega$  (analogous to the standard deviation). Although this model is simpler than the generalised logistic function, it proves sufficiently flexible for our application. Specifically, a Kolmogorov–Smirnov (KS) test between samples drawn from the fitted skewed Gaussian and the original training data consistently passes at all limb angles, confirming the model’s adequacy.

All choices regarding the interpolation of the skewed Gaussian parameters are guided by the success of the KS test applied to the validation set of limb angles. It is important to note that this validation set is entirely excluded from the fitting procedure and serves solely to assess generalization. Specifically, for each validation angle, we draw 129 random samples from the interpolated distribution, matching the size of the validation set, and repeat this sampling process 1000 times. The KS test is performed on each sample set, guiding interpolation choices to ensure statistical consistency at unseen angles. The KS test returns two key metrics: the D statistic, which quantifies the maximum difference between the cumulative distributions (with 0 indicating a perfect match and values closer to 1 indicating large discrepancies), and the p-value, which estimates the likelihood of observing such a difference under the assumption that both samples are drawn from the same distribution. A p-value greater than 0.05 typically indicates that the null hypothesis (that the distributions match) cannot be rejected. When we refer to the KS test ‘passing’, we mean that the p-value is over 0.05 and the difference between the distributions are not statistically significant.

For both  $\mathcal{D}_{\text{GT}}$  and  $\mathcal{D}_{\text{OGR/IgL}}$ , we find that the shape parameter  $\alpha$  must be interpolated over  $\theta$  using a second-order polynomial. Although this provides only a modest fit to the training data, increasing the polynomial order leads to overfitting. While the training RMSE continues to decrease, the RMSE evaluated on the validation set increases. Omitting the skewness term altogether significantly degrades the results. To mitigate the impact of this suboptimal fit to the shape parameter, we fix  $\alpha$  to its interpolated value and then refit the location and scale parameters accordingly.

The location parameter  $\zeta$  is well captured by a 10th-order polynomial in both distributions. For the scale parameter  $\omega$ , the optimal interpolation method differs between the two cases. In  $\mathcal{D}_{\text{GT}}$ , we achieve the best results by normalizing  $\omega$  by the corresponding  $\zeta$ , and fitting the normalized scale using a sum of two exponential functions. In contrast, for  $\mathcal{D}_{\text{OGR/IgL}}$ , the best fit is obtained by applying the sum of exponentials directly to the unnormalized scale parameter.

Figure 8.2 shows the fitted parameters and their interpolation curves for both distributions. The colored points correspond to fits from the validation sample and are not used in constructing the interpolation, serving as an independent check of the model’s performance.

For  $\mathcal{D}_{\text{OGR/IgL}}$ , the interpolated distributions pass the KS test in more than 97% of trials at all validation angles. The results for  $\mathcal{D}_{\text{GT}}$  are similarly robust, with success rates exceeding 97% except at  $\mu = 0.3$  ( $\theta = 72.54^\circ$ ) and  $\mu = 0.2$  ( $\theta = 78.46^\circ$ ), where the pass rate decreases to approximately 70%. However, at such extreme limb angles, the GT component contributes minimally to the overall disc-integrated signal with filling factors  $< 0.1$ , therefore this decline in fit quality is not expected to significantly impact the final disc integrated results. Note also that tiles towards the limb are heavily limb-darkened and fore-shortened, and so their accuracy holds less weight than those nearer disc center when it comes to preserving disc-integrated accuracy.

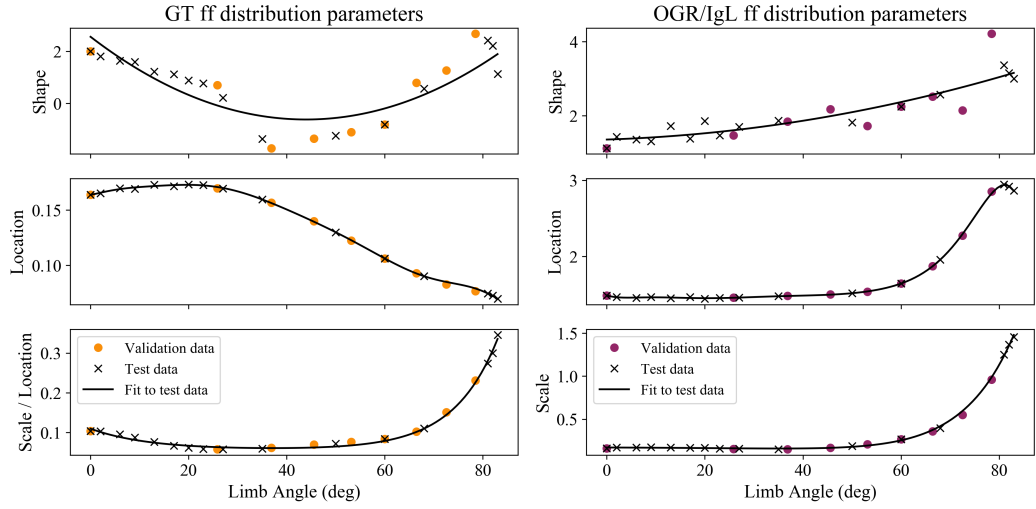


Figure 8.2: Model fits to the parameters required to build skewed Gaussian distributions for both the GT filling factors (left column) and the ratio OGR/IgL filling factors (right column) for Fe I 617.3nm. The black crosses show the best fit parameters to the test-set distributions, and the black line is the model fit to these data. The colored circles show best fit parameters to the validation-set distributions, these values are not included in the fitting. Note that for the GT filling factor distribution the scale parameter is normalised by the location parameter. This is not the case for the OGR/IgL filling factor distribution.

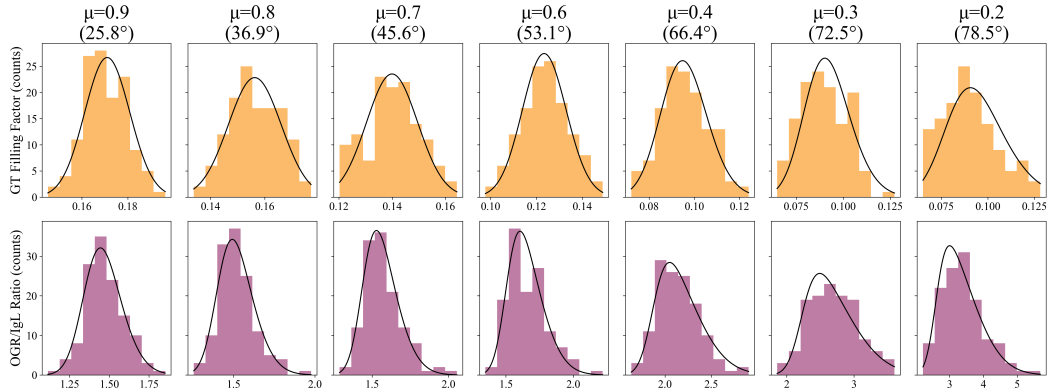


Figure 8.3: Histograms of GT filling factors and OGR/IgL ratio filling factors for the validation set of angles for Fe I 617.3nm. Overplotted in black are the predicted skewed Gaussian distributions using parameters derived through the interpolation procedure using a separate set of training angles. These Gaussians are not fit to the data shown and serve as a test of whether distributions at the validation angles are being correctly captured.

Figure 8.3 shows the predicted skewed Gaussian distributions for the validation set of angles based on the interpolation procedure. The distributions are overplotted on histograms of the actual distributions within the validation set. The predicted distributions appear to effectively contain the real distributions, suggesting the interpolation of parameters has been successful. Some degradation of effectiveness is evident towards the limb, as discussed above. For an alternative test of our ability to correctly capture the filling factor distributions, see Section 8.9.2 for Quantile-Quantile (Q-Q) plots.

### 8.3.3 Validation of interpolation

Using our interpolated components from Section 8.3.1 and our interpolated distributions from Section 8.3.2 we construct a sample of profiles for each validation angle using equation 8.1, matching the size of the validation time series (129 instances). Figure 8.4 shows the bisectors from these samples, alongside the bisectors from the validation data for Fe I 617 nm. This plot serves as a visual demonstration that general bisector shapes and velocities are being preserved in the interpolated samples.

To assess how accurately the velocity distributions are preserved, we use the peak of a cross-correlation function (CCF) as a measure of radial velocity. We calculate the CCF using the relevant time-averaged validation profile as a template, and measure the peak with a second order polynomial fit to 3 data points. For each validation angle, we perform KS tests comparing the validation velocities to 1000 independently generated sample velocity distributions of matching size. The results are summarized in Table 8.2. Note that for a two-sample KS test where each sample has a size 129, the critical D value lies at  $\sim 0.169$ , and so any D value falling under this provides evidence for matching distributions. Across all validation angles, the majority of tests return  $p > 0.05$ , with pass rates in the range 82-96%. The pass rates are not expected to be 100%: even two draws from the same underlying distribution will fail a KS test a non-negligible fraction of the time when the sample size is modest. The observed pass rates include expected statistical fluctuations associated with repeated finite sampling, and do not indicate systematic discrepancies in the interpolated distributions. Overall, we find that the interpolation preserves the underlying velocity statistics to within the limits imposed by finite-sample effects.

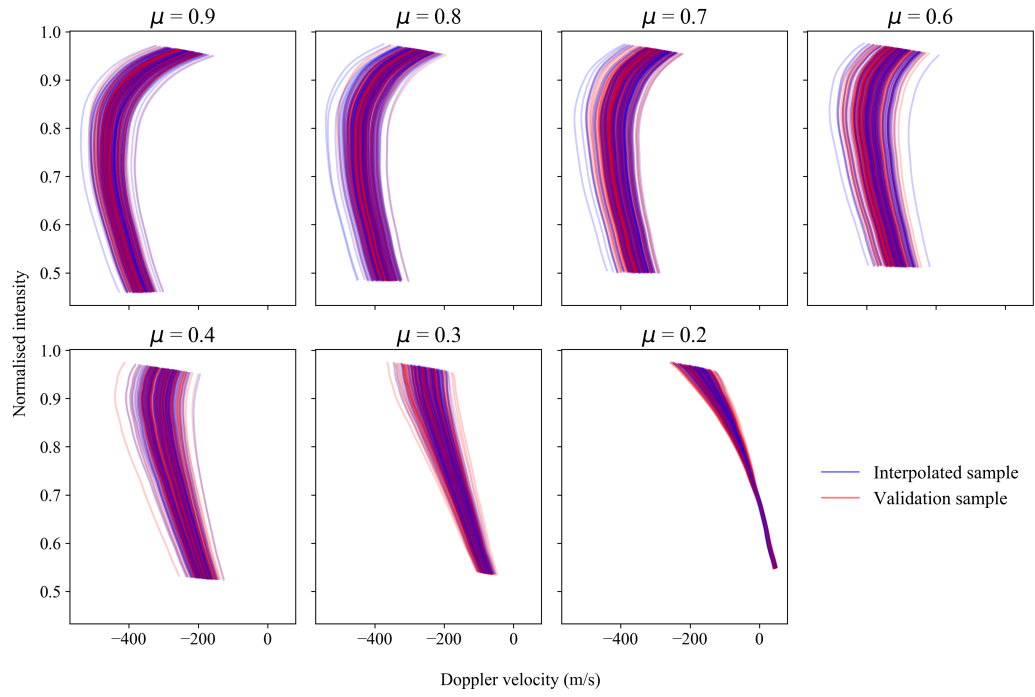


Figure 8.4: Fe 617.3 nm bisectors from an example sample pulled from the interpolation method at each validation limb angle. Bisectors from the validation time series are overplotted. The interpolation and validation sample at each angle are of equal size. In an attempt to mitigate overlap, we alternate plotting interpolated and validation bisectors. The intensity values have been normalised in each case by the maximum intensity value in the validation sample at the relevant angle.

Table 8.2: Results of a 2-sample KS test performed on velocity values calculated using the validation set and a randomly generated sample using the interpolation procedure. For each limb angle ( $\theta$ , also displayed as  $\mu = \cos(\theta)$ ), the test is run 1000 times using unique occurrences of the generated samples (see Section 8.3.3).

| $\mu$ | $\theta$ (deg) | Passed (%) | Avg. D | Avg. p-value |
|-------|----------------|------------|--------|--------------|
| 0.9   | 25.8           | 92.1       | 0.1222 | 0.3593       |
| 0.8   | 36.9           | 90.5       | 0.1191 | 0.4057       |
| 0.7   | 45.6           | 82.2       | 0.1313 | 0.3175       |
| 0.6   | 53.1           | 87.8       | 0.1268 | 0.3386       |
| 0.4   | 66.4           | 96.0       | 0.1161 | 0.4042       |
| 0.3   | 72.5           | 82.7       | 0.1390 | 0.2308       |
| 0.2   | 78.5           | 90.6       | 0.1349 | 0.2385       |

## 8.4 Producing the stellar grid

We follow the methodology in Cegla et al. [2019] for the production of our stellar grid. See also Vogt et al. [1987] and Piskunov & Kochukhov [2002] for similar procedures. The python scripts used to create the grid are available for use, stored in the DISCO repository.

We construct a sphere of radius  $R_{\odot}$  with tiles of size  $9 \times 9 \text{ Mm}^2$  to match the surface area of our MURaM simulation boxes. We then project the visible half of the sphere onto 2D space. For each visible tile we calculate and store the line of sight velocity, projected area and limb angle. The calculations and uses for each of these parameters are described in the subsections below. Figure 8.5 depicts an example grid color-coded by each parameter. The tiles in this figure have been made larger for demonstrative purposes, and the star has been inclined by  $70^\circ$ . The true setup used in this study contains  $\sim 37,000$  visible tiles and has an inclination of  $90^\circ$  (face on).

### 8.4.1 Line of sight velocity

We use the solar differential rotation model from Snodgrass & Ulrich [1990] to calculate the angular rotational velocity  $\omega$  as a function of latitude  $\phi$ :

$$\begin{aligned}
\omega(\phi) &= A + B \sin^2(\phi) + C \sin^4(\phi) \\
A &= 2.773 \times 10^{-6} \text{ rad s}^{-1} \\
B &= -4.84 \times 10^{-7} \text{ rad s}^{-1} \\
C &= -3.61 \times 10^{-7} \text{ rad s}^{-1}
\end{aligned} \tag{8.3}$$

where we have subtracted Earth's orbital angular velocity from the constant coefficient  $A$  to convert from sidereal to synodic velocity.

The tangential velocity  $v_t(\phi)$  at each latitude is given by  $R_\odot \omega(\phi) \cos(\phi)$ . The velocity value that we want to store is the tangential velocity projected along the line of sight to the observer. This is calculated as follows:

$$v_{los}(\phi, \lambda) = v_t(\phi) \cdot \sin(\lambda) \sin(i) \tag{8.4}$$

where  $\lambda$  is the longitude and  $i$  is the stellar inclination.

#### 8.4.2 Projected area

To cover the stellar surface with approximately square tiles, we sample the surface at a discrete set of latitudes  $\{\phi_j\}$  uniformly spaced between  $-90^\circ$  and  $+90^\circ$ , with the spacing chosen such that the arc length of each latitudinal slice is approximately equal to the simulation box size (9 Mm). At each discrete latitude  $\phi_j$ , the number of tiles along the corresponding parallel is given by:

$$N_{\phi_j} = \frac{2\pi R_\odot \cos \phi_j}{9\text{Mm}}. \tag{8.5}$$

where  $N_{\phi_j}$  is rounded to the nearest integer. Longitude is sampled at discrete points  $\{\lambda_k\}$  along each parallel such that the horizontal extent of each tile is also approximately 9 Mm. The surface area of an individual tile is then obtained by dividing the area of the latitudinal slice at  $\phi_j$  by  $N_{\phi_j}$  along that parallel.

The projected area refers to the portion of the tile visible to an observer when the 3D sphere is projected onto the 2D sky plane. Cartesian coordinates for each grid point are computed as:

$$\begin{aligned}
x &= R_{\odot} \cos(\phi) \sin(\lambda) \\
y &= R_{\odot} [\sin(\phi) \sin(i) - \cos(\phi) \cos(\lambda) \cos(i)] \\
z &= R_{\odot} [\cos(\phi) \cos(\lambda) \sin(i) + \sin(\phi) \cos(i)]
\end{aligned} \tag{8.6}$$

where the  $xy$ -plane is the plane of the sky, and the  $z$ -axis points towards the observer. The coordinate system is defined such that when  $i = 90^\circ$ , the point at  $(\phi, \lambda) = (0, 0)$  maps to  $(x, y, z) = (0, 0, R_{\odot})$ .

The projected area  $A_p$  of a tile is then calculated as:

$$A_p = V A_t \sqrt{1 - \left(\frac{x_c}{R_{\odot}}\right)^2 - \left(\frac{y_c}{R_{\odot}}\right)^2} \tag{8.7}$$

where  $A_t$  is the surface area of the tile, and  $(x_c, y_c)$  are the coordinates of its center. The factor  $V$  is the visibility factor, representing the fraction of the tile that lies on the visible hemisphere. Points with  $z > 0$  are considered visible. To determine  $V$ , we compute  $z$  for all four corners of the tile:

- If all corners are visible,  $V = 1$
- If none are visible,  $V = 0$
- If partially visible, we subdivide the tile into 100 smaller sub-tiles and compute the fraction with visible centers. This fraction becomes  $V$ .

Enforcing approximately square tiles on a spherical surface introduces small geometric discontinuities near the rotational poles, where the number of tiles per latitudinal slice decreases. These discontinuities are visible upon inspection in Figure 8.5, they are however visually exaggerated due to the tiles having been significantly enlarged. Because tile areas are defined analytically from each latitudinal slice, the total surface area per slice is conserved by construction, even if gaps or overlaps between tiles occur. For viewing geometries close to edge-on ( $i \simeq 90^\circ$ ), the impact of the discontinuities are further suppressed by geometric foreshortening and limb darkening. While their contribution may increase for non-face-on configurations, the large number of tiles and the conservation of total surface area should ensure that their effect on disc-integrated quantities remains negligible.



### 8.4.3 Limb angle

The limb angle  $\theta$  refers to the angle between the surface normal and the line of sight:

$$\theta = \cos^{-1} \left( \frac{z}{\sqrt{x^2 + y^2 + z^2}} \right) \quad (8.8)$$

where  $x, y, z$  are as defined in Equation 8.6.

## 8.5 Disc integrated profiles with DISCO

DISCO generates a profile  $I(\theta)$  using Equation 8.1 for each tile on the stellar grid. Note that  $\epsilon_1$  and  $\epsilon_2$  are random variables sampled from the generated distributions, and it is this that drives the granular variability. Our method does not impose filling factor correlations between neighbouring tiles. This reflects the fact that solar granules are small and short-lived features, with typical horizontal scales of order 1 Mm and lifetimes of only a few minutes. Granular evolution is dominated by local conditions, and there is no widely accepted mechanism that would maintain coherent behaviour between granules separated by several megametres. The tiles in our model span horizontal scales of 9 Mm, corresponding to approximately 5–10 granule diameters in the solar case. Observational studies of time-averaged solar velocity fields have identified persistent up- and down-flow structures on scales of only 2–4 Mm (e.g. Baudin et al. 1997; Hirzberger et al. 1997), which are significantly smaller than our tiles. Any such correlations are therefore expected to be contained within individual tiles rather than extending between neighbouring tiles. In addition, there is no clear observational evidence for a distinct mesogranular flow pattern [Rincon & Rieutord, 2018], supporting the assumption that tile-to-tile correlations can be neglected.

In each tile, the generated profile  $I(\theta)$  is shifted in velocity space by the line of sight stellar rotational velocity calculated as in Section 8.4.1 and multiplied by  $A_p/\pi R_\odot^2$ , where  $A_p$  is the projected area from Section 8.4.2. The final disc integrated profile is then generated by summing over all of the visible tiles.

Figure 8.6 shows our disc-integrated results (the mean of 1000 instances) compared to observations from the Institut für Astrophysik, Göttingen (IAG) solar atlas [Reiners et al., 2016], as well as simulated results from Palumbo et al. [2024]. In this plot, all profiles have been shifted so that the mean Doppler velocity of the bisector is 0 m/s. In the profiles themselves, we find a strong match to observations other than

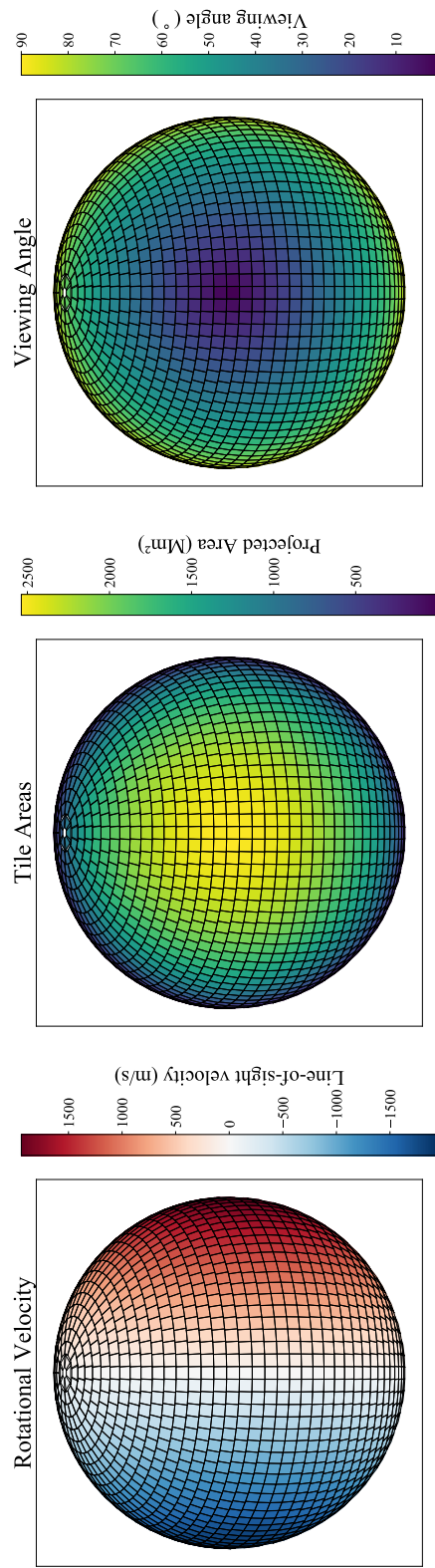


Figure 8.5: An example stellar grid with enlarged tiles and slight inclination for demonstrative purposes. The left hand plot shows the line of sight stellar rotational velocity at each tile, including differential rotation. The middle plot shows the projected area of each tile. Note that these are enlarged tiles, hence the inflated area values. The rightmost plot shows the limb angle at each tile.

our depth appears slightly shallower in all but Fe I 627 nm. The depth mismatch is not introduced by the disc-integration procedure, as a similar, though much smaller, difference is already present when comparing disc-resolved profiles to observations. This suggests that the discrepancy originates in the local line synthesis, potentially due to uncertainties in the atomic data or missing physical effects such as magnetic fields, and is subsequently amplified through disc integration.

In the bisectors, we find strong matches to the telluric-corrected IAG solar atlas from Baker et al. [2020]. Note that the ‘wiggles’ in the observational bisectors are due to the wavelength grid being saved in single precision and are not physical. As is evident from this plot, despite this wavelength region containing no strong telluric absorption lines, even tiny contaminants can cause velocity shifts of up to  $10 \text{ m s}^{-1}$  at specific intensity levels. Our results are inherently telluric free as they are not influenced in any way by observational data. This agreement with the telluric-corrected dataset is an excellent indication that our interpolation across the stellar disc works as expected.

By repeating calculations of disc integrated profiles over a number of iterations, we are able to ascertain the RV variability caused by the pure surface convection on a sun-like star. Our approach ensures that we have no contamination from p-modes, spots, faculae, super-granulation, meridional flows and tellurics, all of which will be present to some extent in observationally driven strategies. We also are free from concerns regarding instrumental precision and observing conditions.

Figure 8.7 shows histograms of disc-integrated RVs for 1000 iterations of each line. The RVs here are calculated by cross-correlating each profile with the mean profile over all iterations. To extract the RV we fit a second order polynomial to the peak of the cross-correlation function. We find, as expected due to results reported in F25, that RV rms increases as lines get weaker. Our weakest line (Fe I 627 nm) has an RV rms of  $0.21 \text{ m s}^{-1}$  whereas our strongest line (Fe I 525 nm) has only  $0.16 \text{ m s}^{-1}$ . All results are however lower than are reported in many empirically driven studies such as Palumbo et al. [2024]. We believe this is largely due to the true isolation of granulation impact. However, it is worth pointing out that our study ignores magnetic effects and the impact of this will require further investigation.

Finally, we emphasize that the filling factors used in DISCO are drawn independently for each iteration, with no memory of previous realizations. As a result, the

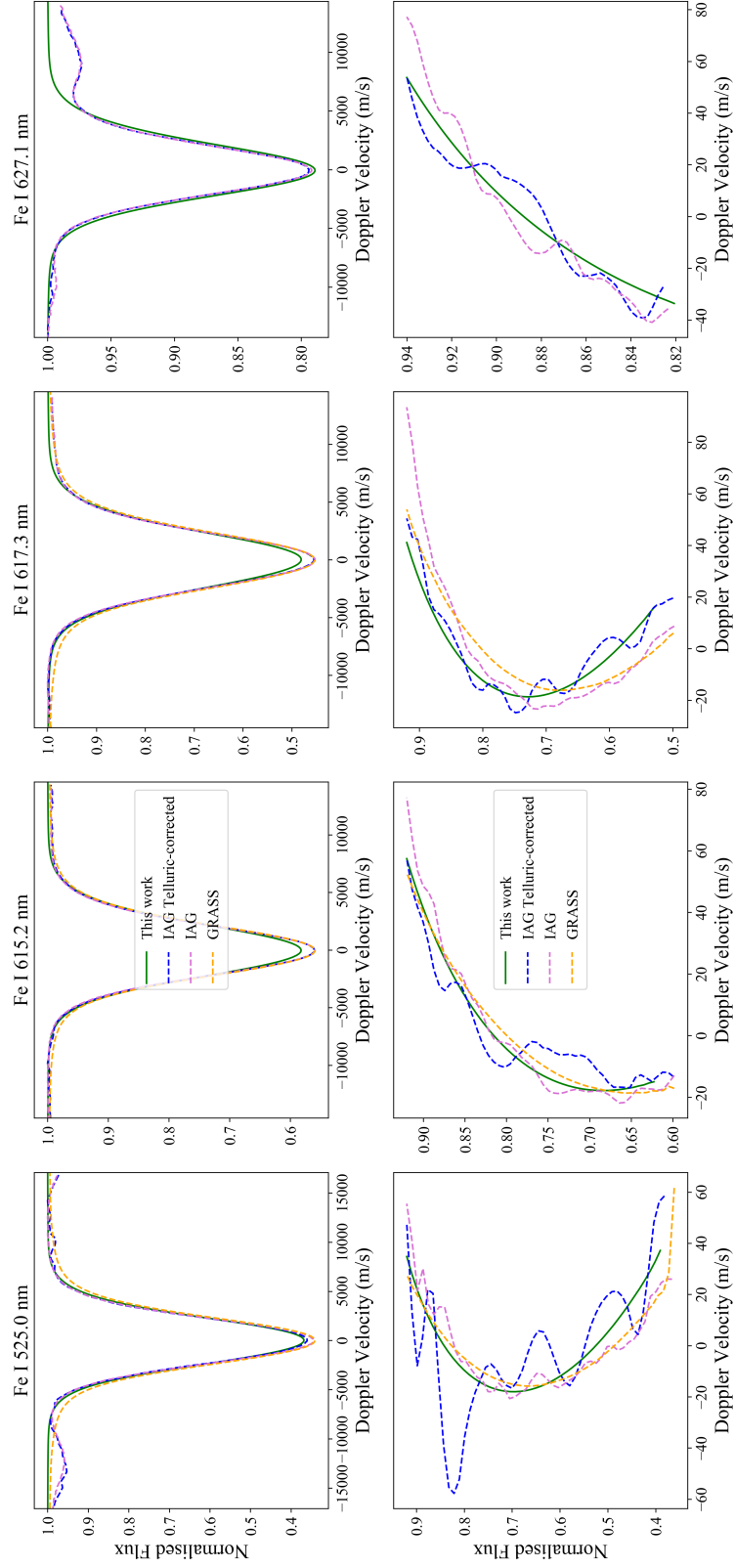


Figure 8.6: Comparisons of disc integrated results from this work with data from the IAG solar atlas [Reiners et al., 2016], the telluric-corrected version of the IAG solar atlas [Baker et al., 2020] and results from GRASS [Palumbo et al., 2024]. Note there is no GRASS result available for Fe I 627.1nm, hence the omission. All data has been shifted so that the mean Doppler velocity of the bisector is 0 m/s. Wiggles in the bisectors of the telluric-corrected data are due to the wavelength grid being stored in single precision. Note that the flux axis for each line has a different scale.

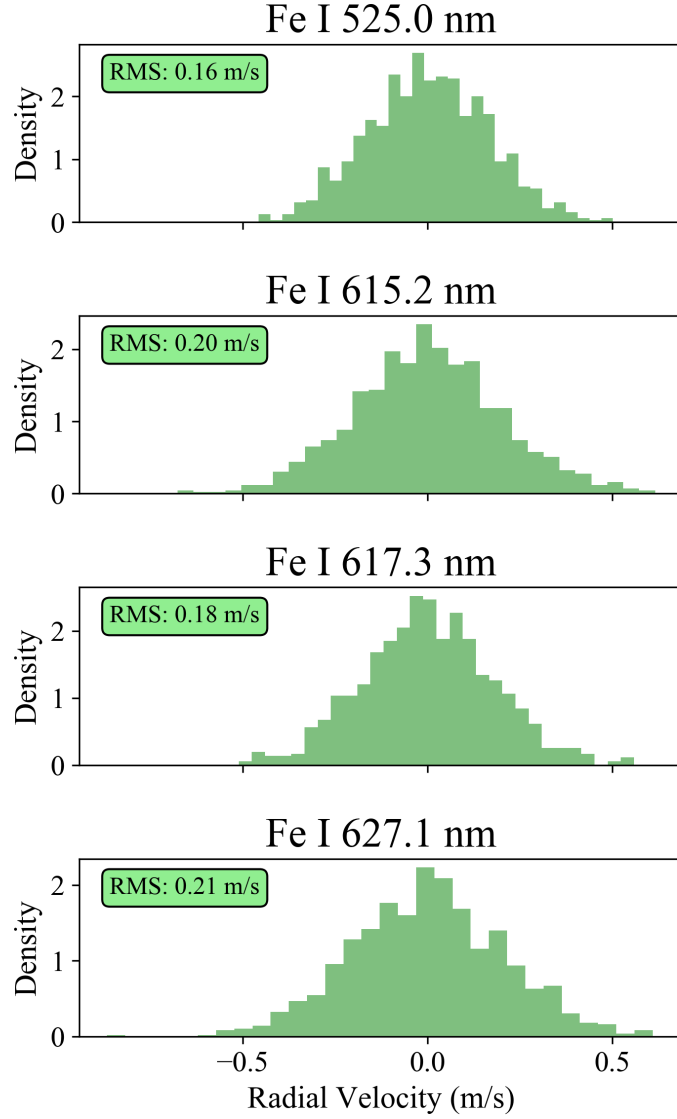


Figure 8.7: Granulation-induced velocity distributions across 1000 disc-integrated line profiles for each spectral line. The velocity values are calculated using a CCF with the mean profile. The RMS value of each distribution is printed in the green boxes.

framework does not generate temporally connected time series, but instead produces statistically independent disc-integrated spectra. While this is sufficient for quantifying the intrinsic RV variability induced by granulation, it precludes the study of characteristic timescales or temporal correlations in the velocity signal. Extending this approach to produce physically motivated time series, for example by introducing random-walk or correlated stochastic evolution of the filling factors, represents a promising avenue for future work.

## 8.6 Correcting for granulation-induced RV

Whilst we have shown that granulation-induced RV rms may be lower than expected, it is still a contributing factor towards obscuring the  $0.09 \text{ m s}^{-1}$  RV signal imposed by an Earth twin. In this section we explore how effectively we can remove granulation-induced RV signals from a profile based only on the shape of the line.

### 8.6.1 Bisector asymmetry correlations

In previous works such as Cegla et al. [2019] and Palumbo et al. [2024], correlations between bisector shape and granulation-induced RV have been used to mitigate velocity scatter. A key diagnostic of bisector asymmetry is the bisector inverse span (BIS), defined as the difference in the mean wavelength (or velocity) between an “upper” and “lower” region of the bisector. The conventional choice is 10–40% and 55–90% of the line depth. Both cited studies, however, report that the BIS–RV correlation for granulation can be significantly improved by fine-tuning these regions for each line profile.

Following the optimisation strategy outlined in Cegla et al. [2019], we iteratively explore the parameter space from 5% to 95% of the line depth, subject to the constraints that each region spans at least 5 percentage points and that the two regions are separated by at least 5 percentage points. We choose our optimal regions based on maximising the absolute pearsons R value for the correlation between BIS and RV. Surprisingly, our optimal regions differ substantially from those reported by Palumbo et al. [2024] for the same lines. For bisectors with a pronounced “C-shape,” we find that both optimal regions lie below the C-bend, while for shallower lines without a C-shape both regions lie above 70% of the line depth.

In terms of scatter reduction, our BIS–RV correlations are broadly consistent with

Palumbo et al. [2024], yielding a  $\sim 30\%$  reduction in RV rms for strong lines with C-shaped bisectors and  $\sim 13\%$  for weaker lines. These improvements remain below those reported by Cegla et al. [2019] for the Fe I 630.2 nm line. A summary of our results is illustrated in Figure 8.8. We note that all of our optimised regions have a width of 10% and are separated by 5%. This pattern arises naturally from the optimisation and was not imposed as a constraint in the procedure.

We find that this method of reducing RV rms is highly sensitive to the precise definition of the bisector regions. Moreover, the signal-to-noise ratio of typical observational data is insufficient to determine BIS values accurately on a line-by-line basis. As noted by Palumbo et al. [2024], the only viable observational application would involve grouping lines with similar sensitivity to bisector asymmetry and combining their signals. Although we achieve similar scatter reduction in our noise-free high resolution profiles to Palumbo et al. [2024], the optimal regions we uncover cover much less of the bisectors shape than is traditional and therefore is much more impacted by noise and resolution.

We therefore view the BIS metric as a challenging diagnostic of granulation-induced variability. Its effectiveness is heavily dependent on the precise choice of regions and on the intrinsic shape of the spectral line, and it becomes increasingly unreliable at lower spectral resolution or in the presence of noise, since the interpolation required to construct the bisector amplifies measurement uncertainties.

The BIS is, however, only one possible measure of line asymmetry. Other asymmetry diagnostics, such as those explored in Cegla et al. [2019] have been shown to offer complementary and in some cases more robust sensitivity to granulation driven line distortions. A full exploration of the broader space of asymmetry based indicators is beyond the scope of this work, but represents an important direction for future studies. For the remainder of this paper, we restrict our analysis to simpler, widely used line-shape metrics.

### 8.6.2 Fundamental line shape diagnostics

Ground-based spectroscopy does not retain information on the absolute continuum intensity. This limits the available line shape diagnostics to relative measures, such as equivalent width (EW), normalised line depth, and full width at half maximum (FWHM). We test the correlation of each of these diagnostics with the net convec-

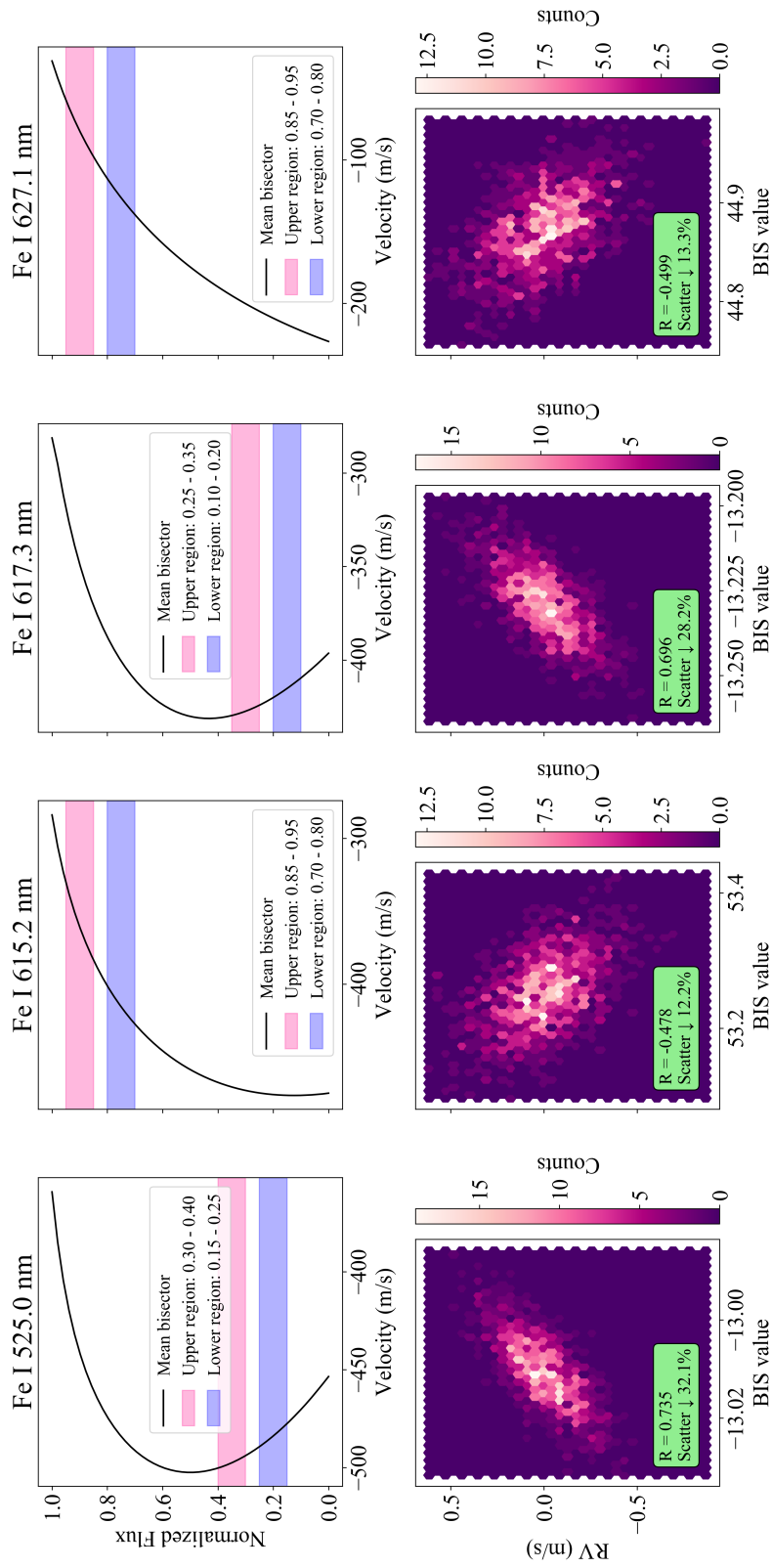


Figure 8.8: **Top panel:** Mean bisectors of each line. Shaded regions show the upper and lower regions that maximise the correlation between BIS values and granulation-induced velocity shifts. Normalised flux has been normalised according to the line depth. **Bottom panel:** Hexbin plots showing the relationship between BIS and RV for 1000 profiles for each spectral line. The Pearson's R value of the correlation, along with the resulting decrease in RV scatter after correction is displayed in the textboxes.



tive blueshift across our line sample.

We find that the strongest correlation is obtained with the equivalent width. The granulation induced RV scales tightly with EW, consistent with previous results [Alende Prieto & Garcia Lopez, 1998; Ramírez et al., 2008; Reiners et al., 2016; Cegla et al., 2019]. This relation is physically motivated: granules contribute line profiles that are both deeper and broader than those formed in intergranular lanes, mostly due to their strong temperature gradient, which leads to the line core forming at much cooler temperatures than the continuum. A larger filling factor of granules therefore yields both an increased EW and a stronger blueshift. In our dataset we find a Pearson correlation coefficient of  $\sim -0.9$ , corresponding to a scatter reduction of  $\sim 50\text{--}60\%$  depending on the line. This highlights EW as the most effective full line shape diagnostic for mitigating convective blueshift variability.

For the normalised line depth we find only a weak correlation with granulation induced RV, with Pearson coefficients of  $\sim -0.4$ , corresponding to a scatter reduction of around 10%. The FWHM shows an even weaker correlation, with no significant improvement in scatter. See Figure 8.9 for the relationships and linear fits for each line and diagnostic. We find the un-normalised line depth has a much stronger correlation, suggesting the EW variation is largely driven by continuum changes. High-precision photometry may therefore offer a promising complementary avenue for tracing granulation in future work.

We are able to further improve the scatter reduction by combining the information from all three diagnostics in a linear regression model. To simulate realistic observational conditions, we degrade our high-resolution, noise-free profiles to match the spectral resolution and sampling of the ESPRESSO spectrograph. Each simulated line profile is convolved with a Gaussian line-spread function (LSF) corresponding to the resolving power of the selected ESPRESSO mode ( $R = 70,000$ ,  $140,000$ , or  $190,000$  for moderate, high and ultra-high resolution, respectively). Following convolution, the spectra are flux-conservingly rebinned onto a logarithmic wavelength grid, sampled at approximately four pixels per LSF FWHM. The rebinning procedure integrates overlapping wavelength intervals between the input and output grids, ensuring that total flux is conserved across bins. The resulting profiles thus reproduce the resolution and sampling characteristics expected from ESPRESSO observations under ideal, noise-free conditions. The linear regression model is trained on 1000 instances and tested on a separate set of 1000 instances, with the resulting

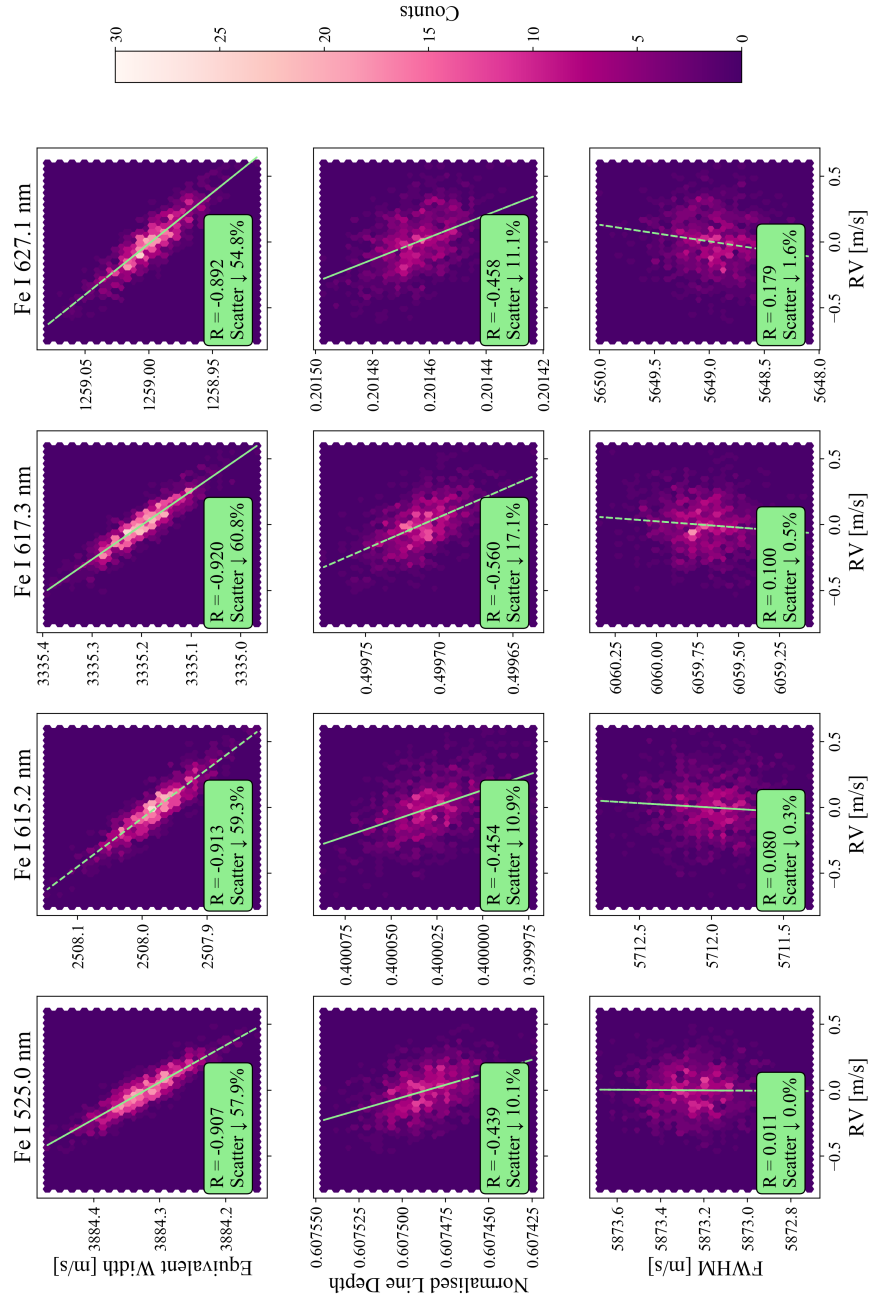


Figure 8.9: Relationships between granulation induced RV and some line shape diagnostics available through ground-based spectroscopy. The green line is a linear fit to the data and printed in the green box is the pearson R coefficient along with the RV rms reduction achievable using this result.

Table 8.3: Scatter reduction (%) for each spectral line across ESPRESSO modes, after applying a linear regression model based on combined line shape diagnostics.

| Line             | RV rms reduction (%) |      |      |
|------------------|----------------------|------|------|
|                  | MR                   | HR   | UHR  |
| Fe I 525.0 nm    | 61.9                 | 62.5 | 62.2 |
| Fe I 615.2 nm    | 71.5                 | 72.0 | 71.9 |
| Fe I 617.3 nm    | 70.5                 | 72.2 | 72.3 |
| Fe I 627.1 nm    | 63.2                 | 68.0 | 68.1 |
| MR: R = 70,000   |                      |      |      |
| HR: R = 140,000  |                      |      |      |
| UHR: R = 190,000 |                      |      |      |

scatter reduction for each mode summarised in Table 8.3. We find that spectral resolution has a negligible impact on these diagnostics, likely because the equivalent width is conserved through resolution changes.

However, the results presented in this section correspond to ideal, noise-free conditions and serve only to demonstrate that the correlations exist in principle. In practice, observational noise will significantly hinder their recovery, and substantial work remains to assess their observability. The following section investigates how the model performs under realistic signal-to-noise ratios (SNR) and how the inclusion of additional spectral lines influences this behaviour.

## 8.7 Effect of Photon Noise and Synthetic Spectra Generation

The addition of photon noise to the line profiles reduces our ability to detect subtle correlations between line-shape diagnostics and granulation-induced radial velocities. In this study, we assume that the noise is dominated by photon noise, which scales with the signal intensity. To assess its impact, we inject Gaussian noise into the synthetic line profiles by perturbing each intensity value with  $\mathcal{N}(0, \sigma^2)$ , where  $\sigma = I/\text{SNR}$ . Here,  $I$  denotes the continuum-normalised intensity at each pixel, and SNR is the per-pixel signal-to-noise ratio. This represents a simplified treatment of realistic observational noise, as we assume a constant SNR across all wavelengths in our synthetic spectra.

We find that the correlations identified in Section 8.6.2 rapidly diminish as noise

increases, requiring an SNR greater than 100,000 for the relationships to remain discernible. It is important to note, however, that our analysis considers single-line diagnostics, whereas real observations typically encompass wide band spectra. The inclusion of multiple lines would introduce additional information and thus reduce the required per-pixel SNR.

To approximate a more realistic multi-line observation, we follow the procedure outlined in Palumbo et al. [2024] and construct synthetic spectra by replicating each single-line profile multiple times with wavelength offsets that include small random perturbations. Each replicated profile preserves the same granulation-induced Doppler shift and line-shape variations; only the photon-noise realisation differs between repetitions. This process extends each time-step spectrum into a broader wavelength range containing several copies of the same line, separated by a fixed amount but slightly perturbed to avoid aliasing. Alongside these extended spectra, we generate a corresponding template mask by placing Gaussian features at the rest wavelength of the line and then repeating them using the wavelength shifts applied in the synthetic spectra. This ensures the template is aligned with the artificial line pattern and provides a suitable reference for cross-correlation. The resulting synthetic spectra and template are then used to compute CCFs, allowing us to analyse how line-shape variations and noise influence the measured CCF and inferred velocity shifts. The more lines we include in our extended synthetic spectra, the more information is retained in our CCF, as noise contributions begin to average out.

Varying both the SNR and the number of lines, we retrain and re-test the linear regression model introduced in Section 8.6.2, this time on the CCF rather than individual profiles. For consistency, we use the granulation-induced RVs derived from the noise-free spectra as the true targets, rather than recalculating RVs from the noisy spectra. Figure 8.10 presents the resulting granulation induced RV scatter reduction achieved under different conditions. The outcomes are discouraging: even when combining 1000 strong lines at an SNR of 1000, the model achieves only a modest 8-11% reduction in granulation induced RV scatter, with weaker lines yielding even poorer performance. These findings indicate that with these simple line shape diagnostics, granulation signatures are effectively obscured within the CCF shapes at realistic noise levels, rendering them undetectable with current instrumentation. This is in-keeping with results in Sulis et al. [2023], who had difficulty isolating RV and CCF shape correlations in ESPRESSO spectroscopy for solar-like stars. Advances in either photon noise mitigation strategies, higher SNR observations, or the

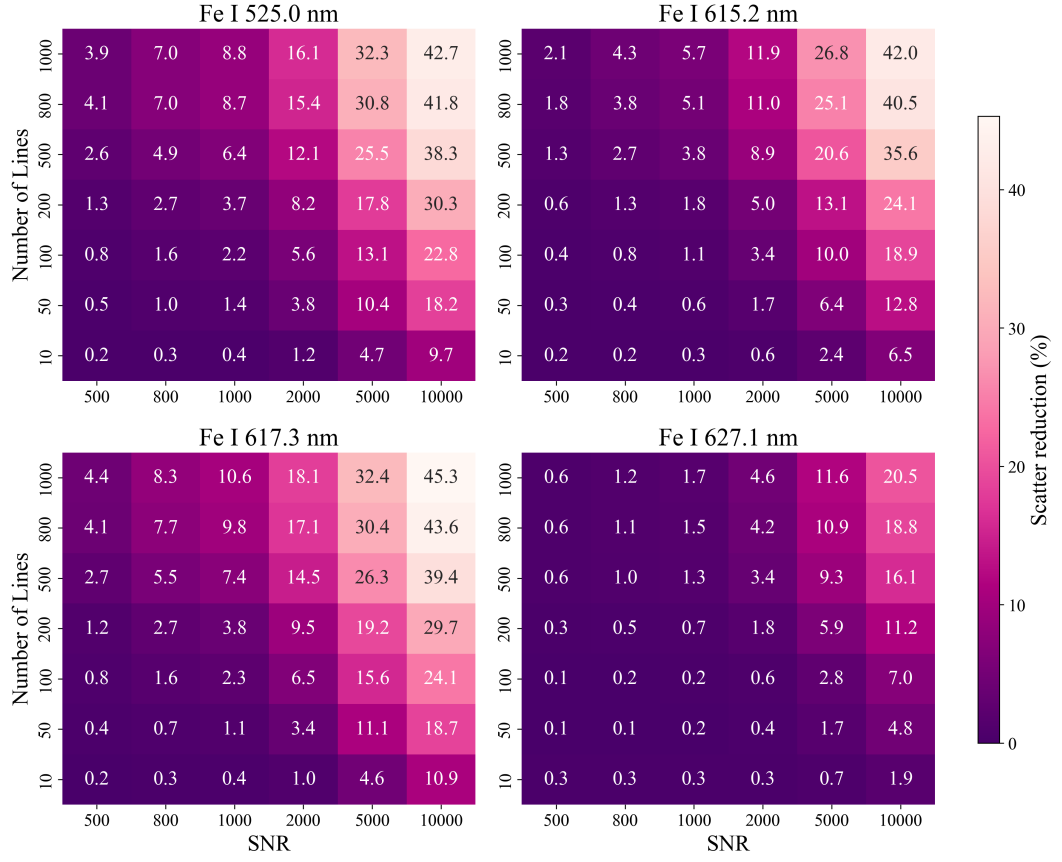


Figure 8.10: Heatmaps of RV rms scatter reduction for each line after a linear regression model trained on CCF shape diagnostics is applied. Results here have been averaged over 100 iterations. Varied parameters are the SNR per pixel and the number of lines included in the synthetic spectra.

development of more sensitive diagnostics will be necessary to recover these subtle signals.

The data presented in this chapter is stored in the public DISCO repository. All python scripts used to generate and analyse the profiles are also included. We welcome community suggestions or attempts to more effectively trace granulation signatures in the presence of photon noise.

## 8.8 Chapter summary and conclusions

This chapter builds on Frame et al. [2025] (F25, discussed in Chapter 7), which demonstrated that parameterisation can be used to construct disc-resolved spectral absorption lines containing only the effects of granulation. In this chapter, we have introduced an interpolation method that enables these profiles to be mapped onto a stellar grid with high accuracy.

We parameterised line profiles into three components representing the intensity outputs of granular tops, outer granular regions and intergranular lanes. We interpolated the time-averaged component profiles and sets of parameters from which we constructed the filling-factor distributions for each component. The interpolation was trained on 16 limb angles, with 7 additional angles withheld for validation. As shown in Figure 8.4, combining the interpolated profiles with the independently interpolated filling-factor distributions reproduces realistic profile samples at arbitrary limb angles, preserving the center-to-limb variations. This allowed us to generate unlimited high-accuracy, time-varying profiles at minimal computational expense.

We tiled a stellar grid with profiles generated in this manner and produced 1000 random instances of disc-integrated profiles for each of the four spectral absorption lines: Fe I 525.0 nm, Fe I 615.2 nm, Fe I 617.3 nm, Fe I 627.1 nm. The scripts to generate these profiles are available within the `DISCO` repository. These profiles are, by design, free from any contamination via p-modes, tellurics, meridional flows, instrumental noise and supergranulation; they contain only the effects of granulation. As a consequence of this, we were able to probe the velocity variations imposed by granulation, unencumbered by other effects. We found granulation induced RV rms values to be lower than is reported elsewhere, with values ranging from  $0.16 \text{ m s}^{-1}$  for our strongest line (Fe I 525.0 nm) to  $0.21 \text{ m s}^{-1}$  for our weakest (Fe I 627.1 nm).

We found that at individual disc positions, the optimal regions for BIS–RV correlations correspond to the traditional upper and lower parts of the bisector, yielding strong and consistent correlations. However, when integrating over the stellar disc, these clear relationships vanish. The optimal BIS regions in the disc-integrated profiles occupy only narrow portions of the bisector, making them highly sensitive to spectral resolution and noise. Although our results reproduce the magnitude of scatter reduction reported by previous studies for noise-free profiles, the correlations we obtain are less robust to noise. A more in-depth investigation of the effectiveness

of alternative asymmetry measures is left for future work. We chose to focus on simpler metrics such as equivalent width, normalised line depth and full width at half maximum.

Across our line sample, the equivalent width emerged as the most reliable diagnostic of granulation-induced velocity shifts, showing strong correlations with convective blueshift and reducing granulation induced RV scatter by up to 60%. In contrast, normalised line depth and FWHM exhibited only weak or negligible correlations. Combining all three diagnostics in a linear regression model further improved performance, achieving up to 70% scatter reduction in ideal, noise-free conditions, with negligible dependence on instrumental resolution. However, when realistic noise was introduced, these relationships rapidly degraded, remaining detectable only at unrealistically high signal-to-noise ratios ( $\text{SNR} \sim 100,000$ ) for single line analysis. Even when averaging over thousands of lines in synthetic multi-line spectra, scatter reductions remained below 10% at SNRs typical of current high-resolution spectrographs. These results demonstrate that while these simple line-shape diagnostics contain valuable information on convective variability in principle, their practical utility is severely limited by observational noise and instrumental precision.

To conclude, more powerful and noise-robust diagnostics will be essential for mitigating granulation signatures in observational data. The framework presented here enables the generation of an effectively unlimited training set of high-accuracy, disintegrated line profiles that contain only granulation signals and come with known convective velocities. Such uncontaminated synthetic data provide a valuable resource for developing and benchmarking future mitigation strategies.

## 8.9 Additional Content

### 8.9.1 Determination of Training Angles

#### Constructing a Ground Truth

To establish a reference for evaluating our dimensionality-reduction approach, we selected four random snapshots from the time series and synthesised Fe I 617 nm line profiles in  $1^\circ$  increments from disc centre to a limb angle of  $84^\circ$ . The mean of the four snapshots at each angle was adopted as a proxy for the time-averaged profile.

To determine the optimal number of principal components to retain when applying PCA to reconstruct time-averaged profiles at arbitrary angles, we employed  $k$ -fold cross-validation with  $k = 7$  [Stone, 1974]. In this procedure, the set of limb angles was partitioned into seven folds, and the PCA model was trained iteratively, each time withholding one fold as a validation set. For each iteration, reconstruction accuracy was quantified by computing the root mean squared error (RMSE) between the predicted validation profiles and their synthesised counterparts. This process was repeated for component numbers ranging from 3 to 20. The cross-validation results indicated that retaining 14 components yielded the lowest average RMSE, corresponding to an average reconstruction error of only 0.02% in normalised flux. This choice thus provides a good balance between reducing dimensionality and avoiding overfitting.

Using this optimal PCA representation, we tiled the stellar grid and computed the disc-integrated profile following the procedure outlined in Section 8.5, training the PCA model on all 84 angular positions with 14 retained components. For the full time series, however, it is computationally infeasible to synthesise profiles at every angular step. It is therefore necessary to identify a reduced set of training angles that can still capture the essential variability in the line profiles. The ground truth constructed above serves as a benchmark for this purpose, enabling a systematic comparison of different candidate training sets and the identification of an optimal subset of angles.

### **Selection of Optimal Training Angles**

To identify the optimum reduced set of training angles, we adopted an iterative elimination strategy. Starting from the full set of 84 limb angles, we performed the disc integration repeatedly, each time withholding a single angle. In each case, the disc-integrated profile was reconstructed using PCA with seven retained components, and the reconstruction error was quantified via the RMSE relative to the ground truth profile defined in the previous section.

The reduction from fourteen to seven retained components was motivated by the smaller training sets encountered during this optimisation. Retaining too many components in this context increases the risk of overfitting, whereas seven components provided a robust representation of the profiles while still capturing the majority of the variance.



At each iteration, the angle whose removal caused the smallest increase in RMSE was permanently excluded from the training set. This process was repeated iteratively until only 15 angles remained. The resulting subset therefore represents the angular positions that contribute most significantly to preserving reconstruction accuracy while substantially reducing the computational expense of synthesising the full time series. Figure 8.11 illustrates the selected training angles and compares the resulting disc-integrated profiles against the ground truth. The relative RMSE between the ground truth profile and the reconstruction using only the 15 selected angles is approximately 0.0006%, indicating an excellent reconstruction.

Rather than repeating this computationally intensive procedure for each spectral line, we verified that the angle set derived for Fe I 617 nm performs equally well for other lines. Computing the ground truth and reconstructing profiles using the 15 angles for additional lines yielded excellent agreement in all cases, with relative RMSE values remaining below  $\sim 0.001\%$ .

In practice, interpolation must be performed on component profiles and granule filling factor parameters rather than a single time-averaged profile. To avoid any extrapolation issues at the disc centre, we therefore added  $0^\circ$  to the training set, extending it to 16 angles. The final set of training angles is: 0, 2, 6, 9, 13, 17, 20, 23, 27, 35, 50, 60, 68, 81, 82,  $83^\circ$ . For angles beyond  $83^\circ$  (up to  $90^\circ$ ), we treat them as  $83^\circ$  to avoid extrapolation. This is acceptable because the contribution from this extreme limb region is minimal due to its small projected area and strong limb darkening, and therefore has a negligible impact on the disc-integrated profile.

### 8.9.2 Testing the recreation of filling factor distributions at arbitrary limb angles

Figure 8.12 shows Q–Q plots comparing our interpolated skew-normal model to the empirical data at each validation angle. The black dashed line indicates the ideal  $y = x$  reference; a perfect model fit would result in points closely following this line. Overall, the model shows good agreement, with a slight deviation toward the limb, as discussed in Section 8.3.2. Deviations at the distribution tails are likely due to under-sampling in the empirical dataset; 129 data points are likely insufficient to fully capture tail behavior.

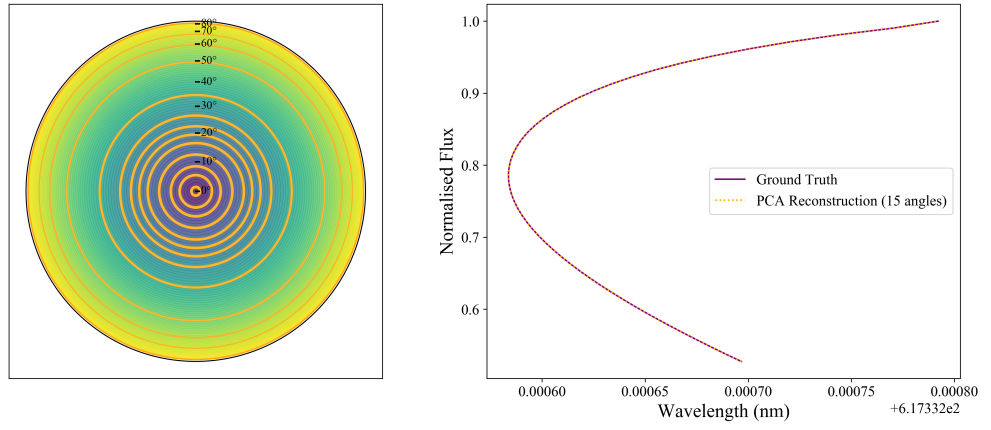


Figure 8.11: **Left plot:** Depiction of limb angle rings on the stellar grid. Colors represent the changing limb angle. Highlighted in orange are the 15 selected optimal training degrees for construction of the disc-integrated profile through PCA. **Right plot:** Bisector of disc integrated profiles using PCA trained on all angles with 14 components (Ground truth) versus the selected 15 angles with 7 components. The difference is indiscernible.

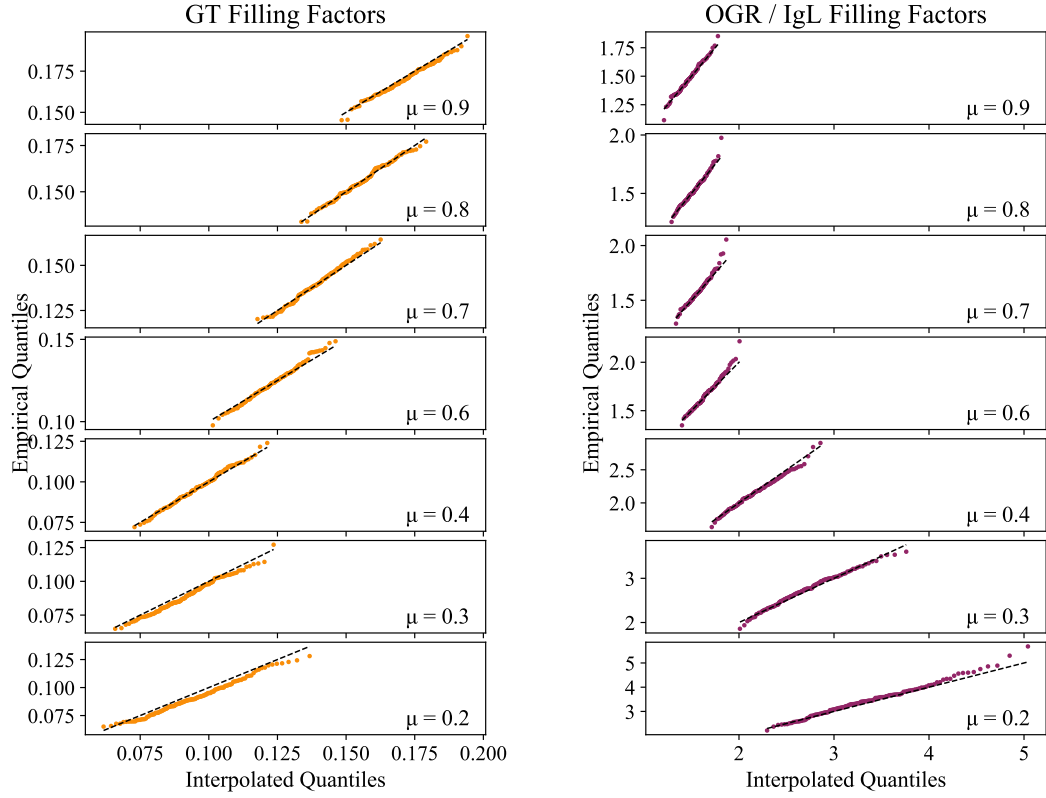


Figure 8.12: QQ plots showing the difference between interpolated and empirical quantiles for the GT and OGR/IgL filling factor distributions at different limb angles. The black dotted line indicates  $y=x$ , which is where the datapoints should lie if the interpolated and empirical distributions were exactly the same. The data shown here is from the validation set of limb angles and so has not been included in any training.

## Chapter 9

# Ongoing and future applications of work from this thesis

*“The most important step a man can take. It’s  
not the first one, is it? It’s the next one.  
Always the next step, Dalinar”*

---

*Brandon Sanderson, Oathbringer*

### 9.1 Granulation-induced variability across the optical spectrum

**Note:** This section summarises work from Lagae [2026], titled “Towards understanding stellar variability at the sub m/s level: granulation-induced variability across the optical spectrum”, submitted to MNRAS. I am the second author of this publication. The analysis presented here was performed by Cis Lagae, building directly on the modelling framework developed in Chapter 7. My contribution to this work lies in the development of the methodology and computational tools enabling this analysis, together with close collaboration and scientific input during the course of the project.

In Chapter 7, I presented a parameterisation method that enabled the isolation of granulation signatures in four Fe I lines. That work demonstrated that granulation-induced variability, including the RV rms, is line dependent. However, a sample of only four lines is insufficient to draw statistically robust conclusions about the physical drivers of this variability or to assess whether different spectral lines behave coherently.

Lagae [2026] extends this framework to a much larger and more diverse sample of 72 unblended spectral lines across two optical wavelength regions (550-560nm and 610-620nm). Synthetic spectra from these regions is generated using the same solar MURaM simulations as outlined in Table 8.1. The parameterisation method from Chapter 7 is adapted and applied to the spectra, isolating granulation-driven variability from p-mode oscillations at a much larger scale. This enables a systematic investigation of how RV, equivalent width, and line depth vary as a function of line properties such as strength, excitation potential, and atomic species.

This expanded analysis reveals clear trends that were not accessible in the smaller sample. In particular, weaker lines are found to exhibit significantly larger RV variability than stronger lines, while strong lines show enhanced variability in equivalent width (EW). Moreover, both equivalent width and line depth are often strongly correlated with granulation-induced RV shifts, reinforcing their potential as diagnostics for mitigating stellar noise. Figure 9.1 shows the relationship between  $RV_{\text{Bouchy}}$  (a measure of RV; see Bouchy et al. [2001]) and EW for different lines.

A particularly important result of this work is the high degree of temporal coherence observed across spectral lines. As shown in Figure 9.2, granulation-induced RV variations evolve in a highly correlated manner across lines with differing depths, excitation potentials, and atomic species. This indicates that granulation imprints a shared temporal signal, with differences between lines arising primarily in amplitude rather than in the underlying variability. This implies that line blending will not fundamentally distort the granulation signal, but instead preserves its coherent structure while modifying only absolute measured quantities. This is particularly important for real observations, where spectral lines are rarely isolated.

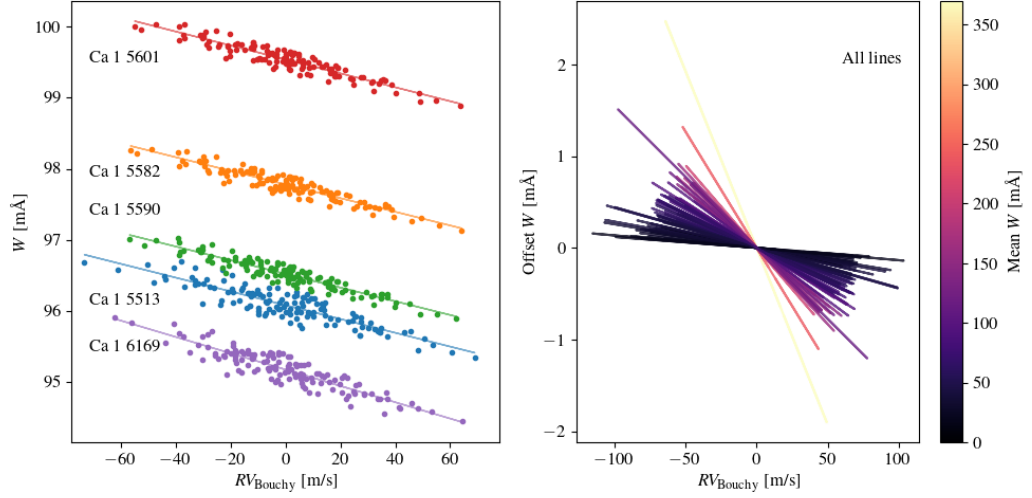


Figure 9.1: **Figure and caption from Lagae [2026]** Equivalent width as a function of  $RV_{\text{Bouchy}}$  for each point in the reconstructed timeseries. A subset of five lines are shown in the left panel, with their best fitting linear regression model shown as a solid line. In the right panel, the best fitting linear regression model for all lines are shown, offset by the intercept for ease of comparison. All linear regressions in the right panel are colour coded by their mean equivalent width.

Most importantly, the shared temporal behaviour across lines provides a strong motivation for multi-line approaches to modelling and mitigating stellar variability. By combining information from many spectral features, it becomes possible to enhance signal-to-noise and more robustly isolate the granulation signal.

Future extensions of this work will explore the granulation signal across different stellar types and in the presence of magnetic fields, where additional physical processes such as faculae and magnetic suppression of convection may alter both the amplitude and structure of the variability (discussed in the following section).

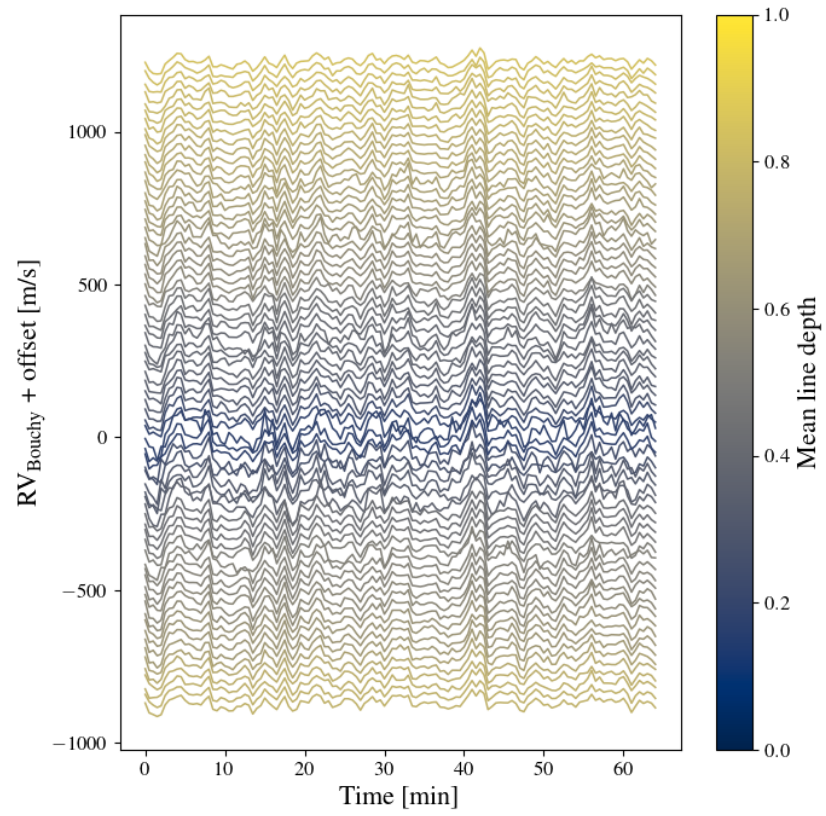


Figure 9.2: **Figure and caption from Lagae [2026].** Temporal evolution of the RV computed for each spectral line plus an arbitrary offset of  $\pm 30 \text{ m s}^{-1}$  to visualise the coherency between lines. The lines are sorted and colour coded by mean line depth.

## 9.2 Magnetic Effects

An important extension of this work is the inclusion of magnetic fields and their impact on spectral line formation. While the present study focuses on purely HD simulations, real stellar photospheres exhibit magnetoconvective behaviour, where magnetic fields interact with convective flows to modify both the thermodynamic structure and velocity field of the atmosphere. In particular, magnetic regions inhibit convective motions, leading to a reduction in the net convective blueshift, which is a dominant source of RV variability in solar-type stars [Meunier et al., 2010, 2017; Miklos et al., 2020]. In addition to this, magnetic fields directly influence spectral line formation through Zeeman splitting, which broadens and distorts absorption line profiles depending on the field strength and the magnetic sensitivity of the absorption line [Reiners, 2012; Stenflo, 2013].

MURaM MHD simulations are available for a range of average magnetic field strengths (both small-scale dynamo simulations and uniform field strengths), providing a realistic framework for studying these effects. In parallel, the new **MPS-STOKES-ATLAS** code [Holzreuter et al., 2026, in preparation], allows for the synthesis of spectral lines including the full treatment of Zeeman splitting and polarisation. This enables modelling of magnetically sensitive line profiles across the stellar disc.

The parametrisation framework developed in this thesis is, in principle, directly applicable to such MHD simulations. The classification of surface components, statistical modelling of their filling factors, and interpolation of line profiles across limb angle do not fundamentally depend on the absence of magnetic fields. Instead, these methods operate on the emergent spectra and underlying surface structures, both of which are naturally extended in MHD contexts to include magnetic features such as magnetic bright points and magnetised intergranular lanes.

Applying this framework to MHD simulations would enable the isolation and quantification of magnetic contributions to RV variability in a manner analogous to the granulation-only case presented here. This would provide a powerful tool for disentangling convective and magnetic signals, and for assessing the extent to which line-shape diagnostics remain effective in the presence of magnetic broadening and asymmetries.



### 9.3 Supergranular flows with DISCO

As discussed in Chapter 8, DISCO provides a flexible framework for generating arbitrarily large samples of disc-integrated spectral line profiles that isolate the effects of stellar granulation. These synthetic datasets offer a controlled environment in which mitigation strategies can be developed and tested. Results from Chapter 8 indicate that the radial velocity variability induced by granulation alone is relatively modest ( $\sim 20 \text{ cm s}^{-1}$ ), and that, under realistic observing conditions, photon noise imposes significant limitations on our ability to detect and characterise these signals in individual spectral diagnostics.

These findings suggest that, in the hydrodynamic regime considered here, granulation is unlikely to represent a dominant barrier to the detection of Earth-analogue planets when considered in isolation. Rather than diminishing its importance, this result helps to place granulation within a broader hierarchy of stellar variability sources, highlighting that its impact may be sub-dominant compared to other processes under realistic conditions. In this context, the role of larger-scale convective patterns, in particular supergranulation, becomes especially important.

Unlike granulation, supergranulation operates on larger spatial and temporal scales and is associated with horizontal velocity flows that may imprint more significant signatures on disc-integrated spectra. These effects remain comparatively under-explored. A natural extension of the DISCO framework is the inclusion of supergranular velocity fields, for example by incorporating solar Dopplergram measurements. This would enable the generation of synthetic datasets that simultaneously capture both granular and supergranular variability, providing a more complete representation of convective noise. Such developments will form the basis of future work, including a planned PhD project by Brandon Rajkumar.

## Chapter 10

# Thesis conclusions

*“Amaze amaze amaze!”*

---

*Rocky, Project Hail Mary*

The discovery and characterisation of a short-period planet within the Neptune desert presented in this thesis contributes to the ongoing effort to map the architecture of exoplanet populations and understand the physical processes that shape them. By occupying a relatively underpopulated region of parameter space, this system provides an additional benchmark for models of planetary formation and evolution, particularly those concerned with atmospheric loss and migration pathways. Owing to its comparatively large mass and short orbital period, I was able to detect this planet readily with current observational techniques, producing a clear and robust radial velocity signal.

In contrast, detecting Earth-like planets remains significantly more challenging. Such planets induce radial velocity amplitudes of tens of centimetres per second or below, placing them well beneath the level of intrinsic stellar variability. Stellar surface phenomena, including oscillations, magnetic activity, and convective processes, introduce complex, time-varying distortions to spectral line profiles that can mimic or obscure planetary signatures. As instrumental precision continues to improve, stellar variability has emerged as the fundamental limiting factor in the detection of low-mass exoplanets. In this thesis, I have focused on one such source of variability: stellar granulation. Granulation arises from convective motions in the stellar photosphere and imprints characteristic asymmetries and velocity shifts on spectral absorption lines.

To address this challenge, I developed a novel parameterisation framework to isolate and model granulation-driven variability using three-dimensional hydrodynamic simulations of the solar surface. By decomposing the stellar photosphere into physically distinct components and describing their statistical behaviour, this approach enables the generation of realistic, time-varying spectral line profiles without requiring full simulation outputs. I further incorporated dimensionality reduction techniques to efficiently interpolate these profiles across the stellar disc, facilitating the construction of disc-integrated spectra.

Using this framework, I generated an effectively unlimited set of synthetic observations, enabling a controlled investigation of granulation-induced radial velocity variability. Across four Fe I lines, I found that the intrinsic granulation signal introduces velocity scatter at the level of  $\sim 0.16\text{--}0.21 \text{ m s}^{-1}$  under idealised conditions. Importantly, I showed that both the magnitude and characteristics of this variability depend on the strength of individual spectral lines, highlighting the limitations of treating stellar variability as a wavelength-independent noise source.

These synthetic datasets also allowed me to systematically explore line-shape diagnostics as potential tracers of granulation. I identified strong correlations between certain diagnostics (such as equivalent width) and the underlying granulation-induced velocity in the absence of observational noise. However, these relationships degrade significantly when realistic noise levels are introduced, underscoring the practical challenges associated with granulation mitigation in real observations. These results emphasise the need for both high signal-to-noise data and carefully selected spectral diagnostics when attempting to correct for stellar variability.

Overall, this work quantifies the impact of granulation on spectral absorption lines while providing a framework to isolate, understand, and ultimately mitigate this source of noise. The methods developed here offer a pathway towards more physically grounded corrections for stellar variability, complementing existing empirical approaches.

Looking forward, several avenues for future work present themselves. Extending this framework to a broader range of stellar types will be essential for generalising these results beyond the solar case. Incorporating additional sources of variability, such as magnetic activity and supergranulation, will allow for a more complete representation of stellar signals. Furthermore, integrating these physically motivated

models into radial velocity pipelines and machine learning frameworks may provide new opportunities to disentangle planetary signals from stellar noise.

As the field moves towards the detection of true Earth analogues, the ability to model and correct for stellar variability at the centimetre-per-second level will become increasingly critical. This thesis represents a step towards that goal, demonstrating both the scale of the challenge and the potential for physically motivated solutions.



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