

Supplementary wavelength calibration methods for SALT/RSS spectropolarimetric observations

Justin Cooper

B.Sc. (Hons)

Submitted in fulfillment of the requirements for the degree

Magister Scientiæ

in the Faculty of Natural and Agricultural Sciences

Department of Physics

University of the Free State

South Africa

Date of submission: June 5, 2024

Supervised by: Prof. B. van Soelen, Department of Physics

Abstract

TODO:

- Done last
- Flow from use of SALT and pipeline and basics of its science implementations into why a more streamlined wavelength calibration is an improvement.
- Give summary of results.
- Aim for a paragraph (~ 600) without going too in-depth into anything specific.
- Brian's comment: Abstract should summarize paper. Include results, conclusions, etc.

Keywords:

TODO:

- Add Keywords → look up the astronomy journal keywords
- Look up keywords for pipeline development and data reduction.
- I.E. Polarization: optical, Calibration: wavelength, galaxies: AGN, Blazars, Pipeline, SALT, etc.

Acknowledgements

I hereby acknowledge and express my sincere gratitude to the following parties for their valuable contributions:

- **TODO: Add acknowledgements!**

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Chapter 1

Introduction

TODO: Very short intro to Spectroscopy, Polarization, and Spectropolarimetry and their importance in astronomy

TODO: Problem Statement, VERY IMPORTANT, roughly a sentence but problem thoroughly fleshed out.

TODO: Focus on AGN implications and implementations such as the types of objects and a short history for each type of object, Blazar focus with specification on BL Lacs and FSRQs, the Unified Model, ~~The Blazar sequence~~

TODO: Brian's comment: Highlight importance of polarimetry for understanding emission and how that plays a role in AGN.

TODO: Basics of modelling (Different energy/wavelength ranges used and what the models tell us about emission processes/structure) so that Hester's results can be noted for applications of the pipeline.

TODO: General layout of Dissertation

Chapter 2

Spectropolarimetry and the SALT RSS

This chapter gives an overview of the basics of spectropolarimetry (§ 2.3), and how it functions, following from the principles of both spectroscopy (§ 2.1) and polarimetry (§ 2.2). Further, it is discussed how these techniques are practically implemented for Southern African Large Telescope (SALT) (§ 2.4), using the Robert Stobie Spectrograph (RSS) (§ 2.4.3), and how the spectropolarimetric reduction process is completed (§ 2.4.3).

2.1 Spectroscopy

Spectroscopy originated in its most basic form with Newton's examinations of sunlight through a prism (Newton and Innys, 1730) but came to prominence as a field of scientific study with Wollaston's improvements to the optics elements (Wollaston, 1802), Fraunhofer's use of a diffraction grating instead of a prism (der Wissenschaften, 1824), and Bunsen and Kirchoff's classifications of spectral features to their respective chemical elements (Kirchhoff and Bunsen, 1861).

The simplest spectrometer schematic, as shown in Figure 2.1, consists of incident light collected from the telescope's optics, labelled A, being focused onto a slit, B, and passed through a collimator, C. The collimator collimates the light allowing a dispersion element, D, to disperse the light into its constituent wavelengths. The resultant spectrum is focused by camera optics, E, onto a focal plane, F. Viewing optics are situated at the focal plane in the case of a spectroscope and a detector is situated at the focal plane in the case of a spectrograph.

2.1.1 Telescope Optics

The telescope optics refers simply to all the components of a telescope necessary to acquire a focal point at the spectrometer entrance, labelled B. The focal point in most traditional telescope designs is fixed relative to the telescope and so the spectrometer may be mounted at that point. In cases where the telescope is designed to have a moving focal point relative to the telescope (see Buckley et al., 2006; Cohen, 2009; Ramsey et al., 1998), the spectrometer, or a signal transfer method such as a fibre feed to the spectrometer, must also move along the telescope's focal path.

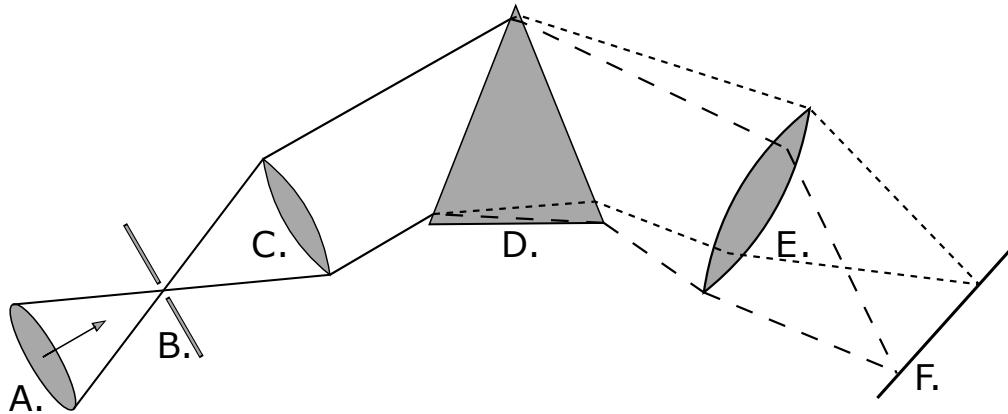


Figure 2.1: Layout depicting the light path through a spectrometer. Diagram adapted from Birney et al. (2006).

2.1.2 Slit

The slit's function is to control the amount of incident light entering a spectrometer and, along with the exposure time of the detector, prevents over-exposures of bright sources on highly sensitive detectors (Tonkin, 2013). If a source is spatially resolvable, or larger than the seeing conditions, the slit additionally acts to spatially limit the source to increase the spectral resolution, resulting in sharper features in the resultant spectrum. Without the slit the spectral resolution would be determined by the projected width of the source on the detector, or the seeing if the source was a star-like point source. Increasing the spectral resolution comes with the trade-off of decreasing the light collected from the source and thus acquiring a less intense resultant spectrum. Multiple spectra may be acquired simultaneously when the slit is positioned such that collinear sources lie along the slit.

The spectrometer is usually situated at the focal point. In cases where this is not feasible due to restrictions, for example restrictions of weight or size, a fibre feed may be situated behind the slit on the telescope. This allows the signal to be routed away from the telescope to a controlled environment with only minuscule losses.

2.1.3 Collimator

The collimators function is to collimate the focused light from the telescope, ensuring that all light rays run parallel before reaching the dispersion element. The focal ratio of the collimator (f_c/D_c , where f refers to the focal length and D refers to the diameter) should ideally match the focal ratio of the telescope (f_T/D_T).

2.1.4 Dispersion Element

Including a dispersion element in the optical path is what defines a spectrometer. As the name suggests, a dispersion element disperses the light incident on it into its constituent wavelengths and produces a spectrum. There are two types of dispersion elements, namely the prism and the diffraction grating, which operate on different principles, as discussed in § 2.1.7.

2.1.5 Camera Optics

The lens functions similarly to that of the telescope's optics but in this case focuses the dispersed light onto a receiver situated at the focal plane. As mentioned previously, an eye piece is fixed to the focal point for a spectroscope while a spectrograph employs a detector.

2.1.6 Detector

The two most prevalent detector types in spectroscopy are the Charged-Coupled Device (CCD) and Complementary Metal-Oxide-Semiconductor (CMOS) detectors. In astronomical spectroscopy however, sources are fainter and exposure times are much longer and so the CCD detectors are by far the preferred detector as their output has a higher-quality and lower-noise when compared to CMOS cameras under the same conditions (Janesick et al., 2006).

The CCD is a detector composed of many thousands of pixels which can store a charge so long as a voltage is maintained across the pixels. Each pixel detects incoming photons using photo-sensitive capacitors through the photoelectric effect and converts the photons to a charge (Buil, 1991). There are also thermal agitation effects which introduce noise to the charge accumulated by a pixel, further discussed in § 2.1.8. Once the exposure is finished the accumulated charge is read column by column, row by row, through an Analog-to-Digital Converter (ADC) which produces a two-dimensional array of ‘counts’.

2.1.7 Dispersion of Light

Light can be broken up into its constituent wavelengths through two different physical phenomena, namely dispersion and diffraction, which dispersive elements use to create spectra. Dispersive prisms and diffractive gratings each have their strengths and weaknesses and a wide spectrum of instruments exist which implement either, or both, concepts. Regardless of the specific element, dispersive elements all have a resolving power, R , and an angular dispersion. Generally, while the angular dispersion is a more involved process to determine, the resolving power of a spectrograph can be measured as:

$$R = \frac{\lambda}{FWHM}, \quad (2.1)$$

where λ is the wavelength of an incident monochromatic beam and Full Width at Half Maximum (FWHM) refers to the width of the feature on the detector at half of its maximum intensity.

Prism

The prism operates on the principle that the refractive index of light, n , varies as a function of its wavelength, λ . Prisms were the only dispersive elements available for early spectroscopic studies, but they were not without flaw. The angular dispersion of a prism is given by:

$$\frac{\partial\theta}{\partial\lambda} = \frac{B}{a} \frac{dn}{d\lambda}, \quad (2.2)$$

where θ is the angle at which the refracted light differs from the incident light, λ is the wavelength of the incident light, B is the longest distance the beam would travel through

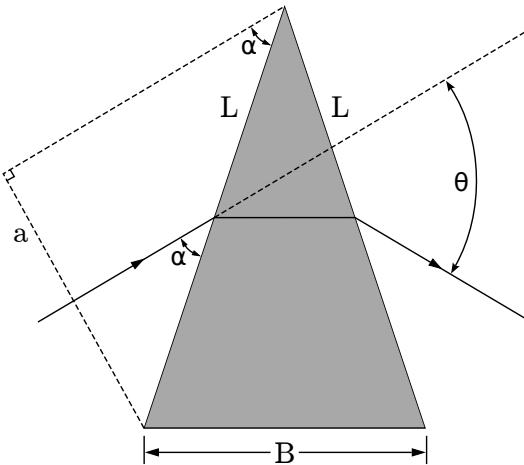


Figure 2.2: Geometry of a prism refracting an incident monochromatic beam at a minimum deviation angle. Diagram adapted from Birney et al. (2006).

the prism. $a = L \sin(\alpha)$ is the maximal beam width that would fit onto a prism with a transmissive surface of length L for a given angle, α , at which a beam would strike the transmissive surface, as shown in Figure 2.2.

The refractive index of a material as a function of its wavelength, $n(\lambda)$, can be approximated by Cauchy's equation:

$$n(\lambda) = A_C + \frac{B_C}{\lambda^2} + \frac{C_C}{\lambda^4} + \dots, \quad (2.3)$$

where A_C, B_C, C_C are the Cauchy coefficients and have known values for certain materials. Cauchy's equation is a much simpler approximation of the refractive index that remains very accurate at visible wavelengths (Jenkins and White, 1976). Taking only the first term of the derivative of the Cauchy equation allows us to approximate the angular dispersion of a prism,

$$\frac{\partial \theta}{\partial \lambda} = -\frac{B}{a} \frac{2B_C}{\lambda^3} \propto -\lambda^{-3}, \quad (2.4)$$

which shows that the angular dispersion of a prism is wavelength dependent and furthermore that longer wavelengths are dispersed less than shorter wavelengths (Birney et al., 2006; Hecht, 2017). The dependence of the angular dispersion, $d\theta/d\lambda$, on the wavelength, λ , is crucial for the formation of a spectrum but this cubic, non-linear, relation results in a non-linear spectrum. Since prisms rely on the refractive index of the material they are made of, they have low angular dispersions.

Multiple prisms can be used to increase the angular dispersion but as the dispersion is non-linear it becomes increasingly more difficult to calibrate. The more material and material boundaries the light must pass through, the more its intensity decreases due to attenuation effects and Fresnel losses. Even so, the transmittance of modern prisms for their selected wavelength range is generally very high due to improved manufacturing methods as well as improved transmitting materials.¹

¹See manufacturers technical specifications, THORLABS, or Edmund Optics for example.

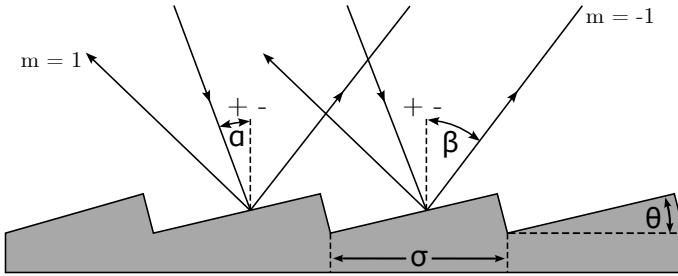


Figure 2.3: Geometry of a reflective blazed grating refracting an incident monochromatic beam. Diagram adapted from Birney et al. (2006).

Diffraction Grating

The alternative dispersing element is a diffraction grating, which operates on the principle that as light interacts with a grating where the groove size is comparable to the light's wavelength, the light is dispersed through constructive and destructive interference. This interference results in multiple diffracted beams m , called orders, either side of a central reflected, or transmitted, beam such that $m \in \mathbb{Z}$, where $m = 0$ is the non-dispersed, or reflected, beam.

An example of a reflective blazed grating is illustrated in Figure 2.3. Here a monochromatic beam is incident on the grating at an angle of α from the grating normal. Due to the interference, a diffracted beam of wavelength λ is found at an angle of β from the grating normal. The relation between the incident and diffracted beams is given by the grating equation:

$$m\lambda = \sigma(\sin(\alpha) \pm \sin(\beta)), \quad (2.5)$$

where σ is the groove spacing of the grating and m is the order of the diffracted beam being considered. The grating equation also applies to transmission gratings, though care should be taken for the signs of α and β .

Equation 2.5 also shows that different diffracted beams may share an angle of dispersion for beams not in the same order. The regions of an order that do not overlap with another order are called free spectral ranges. An order-blocking filter may be used to account for the overlaps and increase the free spectral range. A diffraction grating can also be blazed by an angle θ , as illustrated in Figure 2.3. Blazing refers to the fact that the grooves on the surface of the grating are not symmetrical. The asymmetry of the grooves diffracts the incident beam such that most of the beam's intensity is found in a reflected, zeroth order, beam. The wavelength at which a blazed spectrograph is most effective is called the blaze wavelength, λ_b , which is determined by:

$$\begin{aligned} m\lambda_b &= 2\sigma \sin(\theta) \cos(\alpha - \theta), \text{ where} \\ 2\theta &= \alpha + \beta. \end{aligned} \quad (2.6)$$

Taking the derivative of Equation 2.5 with respect to λ while keeping α constant, allows us to determine the angular dispersion of a diffraction grating,

$$\frac{\partial \beta}{\partial \lambda} = \frac{m}{\sigma \cos(\beta)}. \quad (2.7)$$

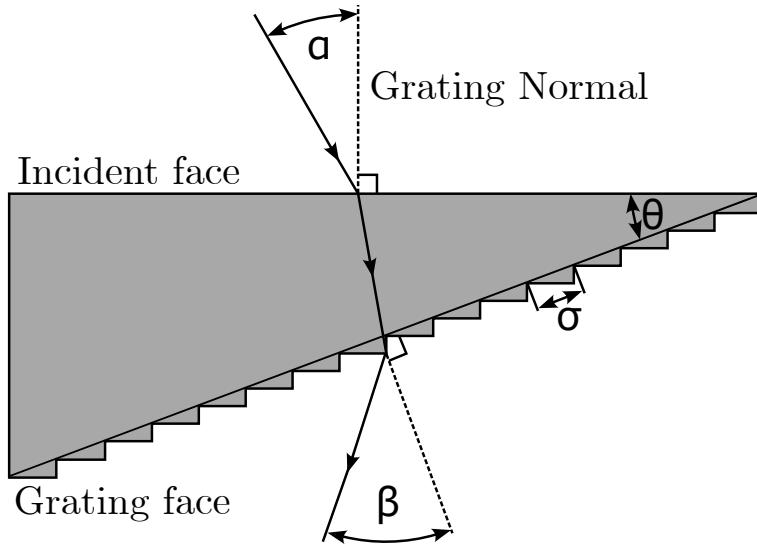


Figure 2.4: Diagram of a grism for an incident monochromatic beam of light and a diffracted beam of order $m = 1$. Diagram adapted from Birney et al. (2006).

Substituting m/σ with the grating equation results in

$$\frac{\partial \beta}{\partial \lambda} = \frac{\sin(\alpha) + \sin(\beta)}{\lambda \cos(\beta)} \propto \lambda^{-1}. \quad (2.8)$$

Similar to the dispersion of a prism, Equation 2.8 shows that the dispersion of a grating is wavelength dependent, but this dependence is only inversely proportional and thus more uniform across a wavelength range than that of a prism. Furthermore, shorter wavelengths are refracted less than longer wavelengths since there is no negative relation between the angular dispersion and the wavelength (Birney et al., 2006; Hecht, 2017).

Alternate Diffraction Elements

As mentioned before, multiple subgroups exist for both dispersive prisms and diffractive gratings. For prisms, along with the single and multiple prism setups mentioned, there also exists grisms and immersed gratings. A grism (Grating Prism), as shown in Figure 2.4, refers to a transmissive grating etched onto one of the transmissive faces of a prism and allows a single camera to capture both spectroscopic and photometric images without needing to be moved, with and without the grism in the path of the beam of light, respectively. An immersed grating refers to a grism modified such that the transmissive grating is coated with reflective material. The primary source of dispersion for both grisms and immersive gratings is the grating and any aberration effects from the prism are negligible in comparison.

Other types of gratings include the Volume Phase Holographic (VPH) grating as well as the echelle grating. The VPH grating consists of a photoresist, which is a light-sensitive material, sandwiched between two glass substrates. Diffraction is possible since the photoresist's refractive index varies near-sinusoidally perpendicularly to the gratings lines, as seen in Figure 2.5. This allows for sharper diffraction orders and low stray light scattering as compared to more traditional gratings but since blazing is not possible the

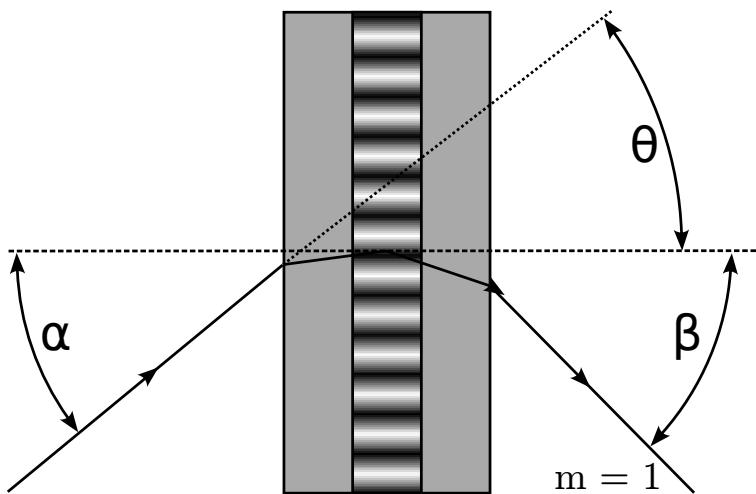


Figure 2.5: Diagram of a VPH grating for an incident monochromatic beam of light. Diagram adapted from Birney et al. (2006).

efficiency is decreased. An echelle grating refers to a diffraction grating with higher groove spacing which is optimized for use at high orders. The high order of the diffracted beam allows for greater angular dispersion which is most useful when combined with another dispersion element to cross-disperse a spectrum, resulting in a high resolution spectrum.

2.1.8 Detector and Spectroscopic Calibrations

Acquiring a spectrum from observations is more involved than simply reading out the data recorded on the CCD. A raw science image, which is the raw counts of the observed source read from the CCD with no calibrations applied, has on it a combination of useful science data as well as noise. The noise is a combination of random noise introduced through statistical processes and systematic noise introduced through the instrumentation and the observation conditions the source was observed under. This noise causes an uncertainty in the useful data and can be minimized, predominantly by calibrating for the systematic noise, but never fully removed (Howell, 2006).

The dominant source of noise in a raw image is detector noise. CCDs are manufactured to have a small base charge in each pixel, called the ‘bias’ current which allows the readout noise, a type of random noise, to better be sampled. There is also an unintentional additional charge which is linearly proportional to the exposure time and originates from thermal agitation of the CCD material, called the ‘dark’ current. The dark current can be minimized and possibly ignored if the CCD is adequately cooled. These types of noise add to the charge held by a pixel and are thus considered additive.

The CCD is not a perfect detector and the efficiency of it and the optics of the telescope also contribute noise to the image. The efficiency of a CCD is referred to as the Quantum Efficiency, and it is a measure of what percentage of light striking the detector is actually recorded and converted to a charge. The efficiency of the CCD and telescope optics is also wavelength dependent and so the noise that results from them is more complex than that of additive noise. This type of noise is referred to as multiplicative noise.

Additive noise, such as bias and dark currents, is inherent to CCD images, and as such

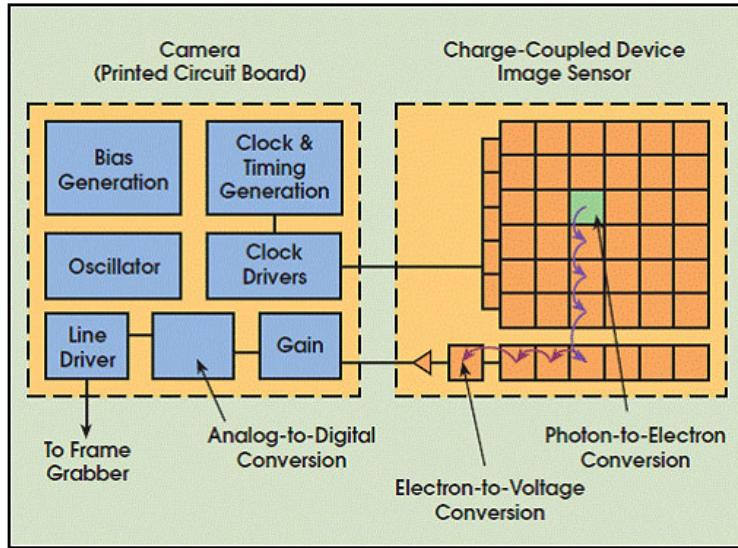


Figure 2.6: Diagram of the inner logic of a CCD. Figure adapted from Litwiller (2001).

needs to be subtracted out first when performing calibrations. Bias currents can be found by taking a bias image or by adding an overscan region to each image. A bias image is an image where the charges on the CCD are reset and then immediately read off without exposing anything on the detector, effectively taking an image with zero exposure time. Alternatively, to save time during an observational run, overscan regions may be added to the images. An overscan region refers to adding a few cycles to the readout of each column of the CCD such that the base current is read out and appended to each image.

Dark currents can be found by taking an image with nothing exposed onto the detector for a certain exposure time. This resultant dark image can then be scaled to the science images exposure time since the dark current should be linearly proportional to exposure time. When the detector is capable of being held at precise temperatures, dark images may be taken over multiple hours during the day to produce a high quality master dark image that may then be scaled and subtracted from all subsequent images.

Next, multiplicative noise, such as a CCD's pixel-to-pixel response, should be accounted for. This pixel-to-pixel response should be uniform across the image and to achieve this an average response may be divided out. The average response is referred to as a ‘flat’ image or flat-field and may be acquired by observing a uniformly illuminated surface to determine the pixel-to-pixel response.

Dome flats are images taken of a relatively flat surface, usually the inside a telescopes dome, and are used in both photometry and spectroscopy. The surface is uniformly and indirectly illuminated by a projector lamp, ideal for flat-field images. Alternate flat-fielding methods, such as night sky and twilight flats, are available but are suited solely for photometry. Night sky flats are produced from science images containing mostly sky. The science images are combined using the ‘mode’ statistic which removes any celestial objects at the cost of a low Signal-to-Noise Ratio (S/N) flat-field. Twilight flats are produced from images of the twilight (or dawn) sky. They are taken when the Sun has just set, in the opposite direction, at $\sim 20^\circ$ from zenith and provide a better S/Ns at the cost of careful timing of the images.

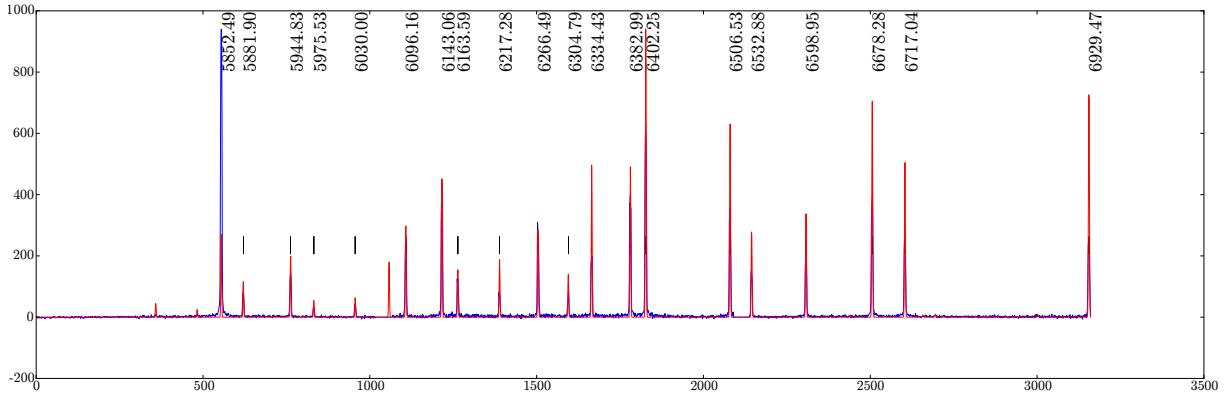


Figure 2.7: Example of an arc spectrum for NeAr taken with SALT’s RSS using the PG1800 grating at a grating angle of 34.625° , an articulation angle of 69.258° , and covering a wavelength range of $\sim 5600 - 6900 \text{ \AA}$. Plot adapted from SALT’s published Longslit Line Atlases, (2023).²

A flat-field must be normalized before being used to correct any science images since it only acts to account for the pixel-to-pixel response and not for the additive errors. A normalized spectroscopic flat image, $F_\lambda^n(x, y)$, can be calculated as:

$$F_\lambda^n(x, y) = \frac{F_\lambda(x, y) - B(x, y) - (\frac{t_S}{t_D})D(x, y)}{\text{med}_{lp}(F_\lambda(x, y) - B(x, y) - (\frac{t_S}{t_D})D(x, y))}, \quad (2.9)$$

where $F_\lambda(x, y)$ is the non-corrected flat image, $B(x, y)$ is the bias image, $D(x, y)$ is the dark image which is scaled by the exposure time of the science image, t_S , and the dark image, t_D . med_{lp} is a low-pass median filter which smoothes out any rapid changes in the pixel-to-pixel response, removing the illumination contribution.

The calibrated science image, $S_\lambda^*(x, y)$, which accounts for the bias and dark currents as well as the flat fielding can then be calculated as:

$$S_\lambda^*(x, y) = \frac{S_\lambda(x, y) - B(x, y) - (\frac{t_S}{t_D})D(x, y)}{F_\lambda^n(x, y)}. \quad (2.10)$$

When multichannel CCDs are used, which consist of multiple CCDs or a CCD with multiple output amplifiers, additional calibrations, specifically cross-talk corrections and mosaicking, are required. Cross-talk noise refers to contamination that occurs during readout in one channel from another channel with a high signal and occurs because the signals can not be completely isolated from one another. Cross-talk corrections therefore account for this signal contamination between channels being read out at the same time (Freyhammer et al., 2001). Mosaicking is necessary for multichannel CCDs since the digitized signal read out from the detector has no reference of the physical location of the pixel it was detected at. Mosaicking, therefore, correctly orients the data acquired from a multichannel detector so that a single correctly oriented image is produced.

Wavelength Calibration

Finally, since the dispersion element breaks the incident light into its constituent wavelengths non-linearly (§ 2.1.7), the relation between the pixel on a detector and the wavelength of the light incident on it is unknown. Ideally, the spectrometer’s optics would be

²NeAr plot sourced from <https://astronomers.salt.ac.za/data/salt-longslit-line-atlas/>

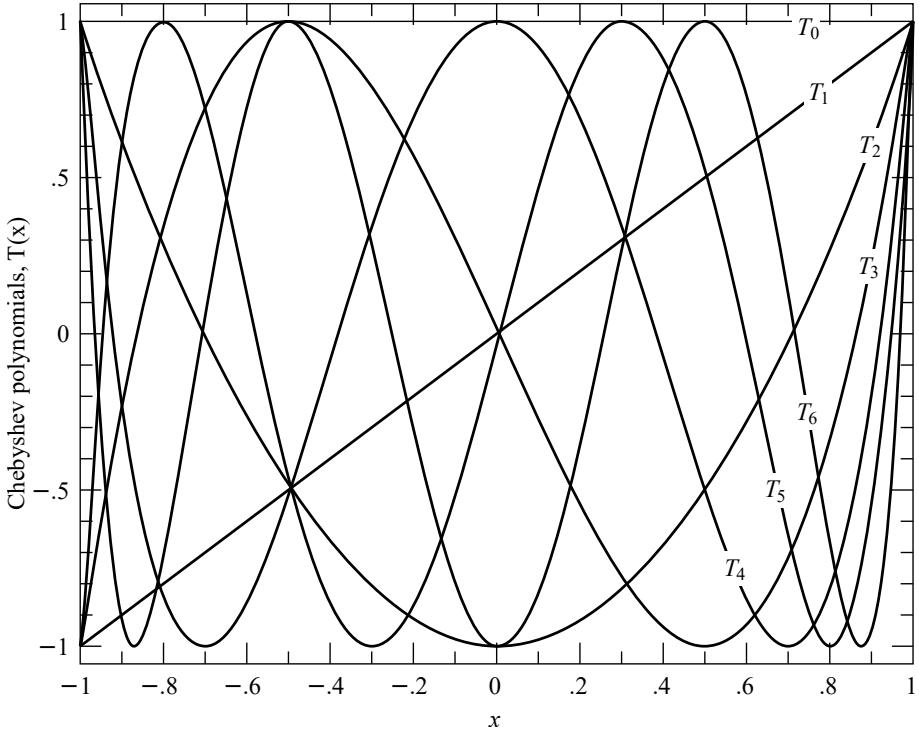


Figure 2.8: The first seven Chebyshev polynomials (T_0 through T_6) as defined by Equation 2.12 over the region $[-1, 1]$ for which they are orthogonal. Plot adapted from (Press et al., 2007) (2023)³

modelled to produce a reliable pixel to wavelength calibration (see E.g. Liu and Hennelly, 2022), but this becomes increasingly more difficult for spectrometers with complex, non-sedentary, optical paths. Alternatively, a source with well-defined spectral features, with said features evenly populating the wavelength region of interest, such as in Figure 2.7 may be observed. The observed frame is commonly referred to as an ‘arc’ frame, after the arc-lamps used to acquire the spectra, and should be observed alongside the science frames over the course of an observation run. It is important that the arc frame is observed at the same observing conditions and parameters as the science frames since the optical path will vary over the course of an observing run and for different observing parameters, invalidating previously acquired arc frames.

The wavelength calibrations then consist of defining a two-dimensional pixel-to-wavelength conversion function from the arc frame which may later be applied to calibrate the science frames. The two most common approximations for wavelength calibrations are the Chebyshev and Legendre polynomial approximations.

Chebyshev Polynomials The Chebyshev polynomials are defined explicitly as:

$$T_n(x) = \cos(n \cos^{-1}(x)) , \text{ or recursively as} \quad (2.11)$$

$$\begin{aligned} T_0(x) &= 1 , \\ T_1(x) &= x , \text{ and} \end{aligned} \quad (2.12)$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) , \text{ for } n \geq 1 ,$$

³Excellent resources on Chebyshev and Legendre polynomials are available digitally at www.numerical.recipes/book.

where T is a Chebyshev polynomial of order n .⁴ An important property of Chebyshev polynomials is that they are orthogonal polynomials. This means that the inner product of any two differing Chebyshev polynomials, $T_i(x)$ and $T_j(x)$, over the range $[-1, 1]$ is zero, as shown by:

$$\int_{-1}^1 T_i(x)T_j(x) \frac{1}{\sqrt{1-x^2}} dx = \begin{cases} 0, & i \neq j \\ \pi/2, & i = j \neq 0 \\ \pi, & i = j = 0 \end{cases}, \quad (2.13)$$

where $1/\sqrt{1-x^2}$ is the weighting factor for Chebyshev polynomials. This property is important because it means that the coefficients in the Chebyshev polynomial expansion are independent of one another, allowing for a unique solution when approximating an unknown function (Arfken and Weber, 1999; Press et al., 2007).

An approximation, using Chebyshev polynomials, of an unknown wavelength calibration function is given by:

$$f(x) \approx \sum_{i=0}^N c_i T_i(u), \text{ or} \quad (2.14)$$

$$F(x, y) \approx \sum_{i=0}^N \sum_{j=0}^M c_{ij} T_i(u) T_j(v), \quad (2.15)$$

for a one- or a two-dimensional wavelength surface function, respectively. Here N and M are the desired x and y orders, and c_i and c_{ij} are the Chebyshev polynomial coefficients (Florinsky and Pankratov, 2015; Leng, 1997). Since the orthogonality property of the Chebyshev polynomials only holds true over the range $[-1, 1]$, the $(x, y) \in ([0, a], [0, b])$ pixel coordinates must be remapped to $u, v \in [-1, 1]$ following the relation:

$$(u, v) = \frac{2(x, y) - a - b}{b - a}. \quad (2.16)$$

The Chebyshev polynomials are more suited for wavelength calibrations than standard polynomials since they are orthogonal and have minima and maxima located at $[-1, 1]$, as seen in Figure 2.8. This means that the Chebyshev approximation is exact when $x = x_n$, where x_n are the positions of the $n - 1$ x -intercepts of $T_N(x)$. These properties greatly minimize the error in the Chebyshev approximation, even at lower order approximations (Arfken and Weber, 1999).

Legendre Polynomials Similar to the Chebyshev polynomials, the Legendre polynomials may be defined explicitly as:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n, \text{ or recursively as} \quad (2.17)$$

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \text{ and} \end{aligned} \quad (2.18)$$

$$(n + 1)P_{n+1}(x) = (2n + 1)xP_n(x) - nP_{n-1}(x), \text{ for } n \geq 1,$$

⁴Chebyshev polynomials are denoted T as a hold-over from the alternate spelling of ‘Tchebycheff’.

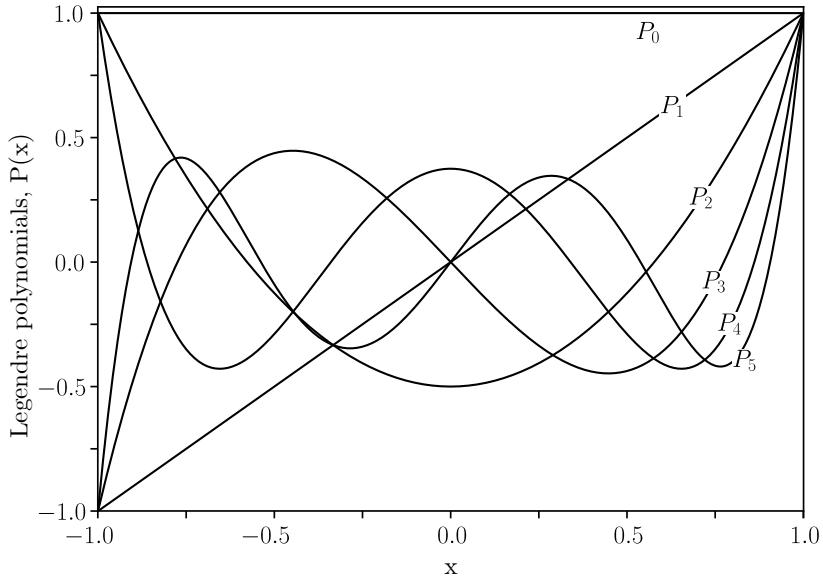


Figure 2.9: The first six Legendre polynomials (P_0 through P_5) as defined by Equation 2.20 over the region $[-1, 1]$ for which they are orthogonal. Plot adapted from Geek3, CC BY-SA 3.0, via Wikimedia Commons (2023).

where P is a Legendre polynomial of order n . Legendre polynomials also hold the property of orthogonality. This means that the inner product of any two differing Legendre polynomials, $P_i(x)$ and $P_j(x)$, over the range $[-1, 1]$ is zero, as shown by:

$$\int_{-1}^1 P_i(x) P_j(x) dx = \begin{cases} 0, & i \neq j \\ \frac{2}{2n+1}, & i = j \end{cases}, \quad (2.19)$$

where a weight of 1 is the weighting factor for Legendre polynomials (Dahlquist and Björck, 2003; Press et al., 2007).

An approximation, using Legendre polynomials, of an unknown wavelength calibration function is given by:

$$f(x) \approx \sum_{n=0}^N a_n P_n(u), \text{ or} \quad (2.20)$$

$$F(x, y) \approx \sum_{i=0}^N \sum_{j=0}^M a_{ij} P_i(u) P_j(v), \quad (2.21)$$

for a one-dimensional wavelength function or a two-dimensional surface function, respectively. Here N and M are the desired x and y orders, u and v are the same mapping variable as in Equation 2.16, and a_{ij} are the Legendre polynomial coefficients.

Legendre polynomials benefit from having the orthogonality condition with no weight necessary ($w = 1$) which makes their coefficients computationally easier to compute but increases the error in a Legendre approximation when compared to that of the error in a Chebyshev approximation for functions of the same order, N (Ismail, 2005).

Regardless of which method of polynomial approximation is chosen, the polynomials are fit by varying the relevant coefficients using the least squares method. The resultant

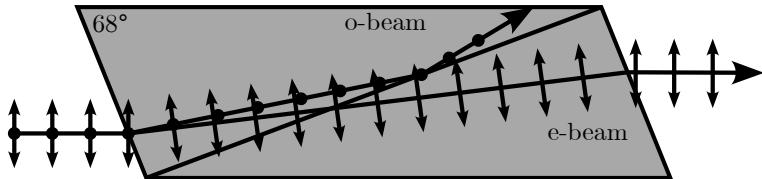


Figure 2.10: Diagram of a Nicol prism for incident non-polarized light. Diagram adapted from Fred the Oyster, CC BY-SA 4.0, via Wikimedia Commons (2023).

minimized function may then be used to convert the science frames from an (x -pixel, y -pixel) coordinate system to a (λ , y -pixel) coordinate system.

2.2 Polarimetry

Both Huygens and Newton came to the conclusion that light demonstrates transversal properties (Huygens, 1690; Newton and Innys, 1730), which was later further investigated and coined as ‘polarization’ by Malus (Malus, 1809). Malus also investigated the polarization effects of multiple materials including some of which were birefringent, such as optical calcite, which he referred to as Iceland spar after Bartholinus’ investigations of the material (Bartholinus, 1670).

Fresnel built on Malus’ work showing that two beams of light, polarized at a right angle to one another, do not interfere, conclusively proving that light is transversal in nature, opposing the widely accepted longitudinal nature of light due to the prevalent belief in the ether. He later went on to correctly describe how polarized light is reflected and refracted at the surface of optical dielectric interfaces, without knowledge of the electromagnetic nature of light. Fresnel’s equations for the reflectance and transmittance, R and T , are defined as:

$$\begin{aligned} R_s &= \left| \frac{Z_2 \cos \theta_i - Z_1 \cos \theta_t}{Z_2 \cos \theta_i + Z_1 \cos \theta_t} \right|^2, \\ R_p &= \left| \frac{Z_2 \cos \theta_t - Z_1 \cos \theta_i}{Z_2 \cos \theta_t + Z_1 \cos \theta_i} \right|^2, \\ T_s &= 1 - R_s, \text{ and} \\ T_p &= 1 - R_p, \end{aligned} \quad (2.22)$$

where s and p are the two polarized components of light perpendicular to one another, Z_1 and Z_2 are the impedance of the two media, and θ_i , θ_t , and θ_r are the angles of incidence, transmission, and reflection, respectively (Fresnel, 1870).

Nicol was the first to create a polarizer, aptly named the Nicol prism, where the incident light is split into its two perpendicular polarization components, namely the ordinary and extraordinary beams. Faraday discovered the phenomenon where the polarization plane of light is rotated when under the influence of a magnetic field, known as the Faraday effect. Brewster calculated the angle of incidence, $\theta_B = \arctan n_2/n_1$, at which incident polarized light is perfectly transmitted through a transparent surface, with refractive indexes of n_1 and n_2 , while non-polarized incident light is perfectly polarized when reflected and partially polarized when refracted.

Stokes’ work created the first consistent description of polarization and gave us the

Stokes parameters which describe an operational approach to measuring polarization (discussed further in § 2.2.1) (Stokes, 1852). Hale was the first to apply polarization to astronomical observations, using a Fresnel rhomb and Nicol prism as a quarter-wave plate and polarizer, respectively (Hale, 1908, 1979). Wollaston also created a prism, similarly named the Wollaston prism, which allowed simultaneous observation of the ordinary and extraordinary beams due to the smaller deviation angle (Wollaston, 1802). Finally, Chandrasekhar's work furthered our understanding of astrophysical polarimetry by explaining the origin of polarization observed in starlight as well as mathematically modeling the polarization of rotating stars, which came to be named Chandrasekhar polarization (Chandrasekhar, 1950).

2.2.1 Polarization

Maxwell's equations for an electromagnetic field propagating through a vacuum are given as:

$$\begin{aligned}\nabla \cdot \mathbf{E} &= 0, \\ \nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, \text{ and} \\ \nabla \times \mathbf{B} &= \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t},\end{aligned}\tag{2.23}$$

where \mathbf{E} and \mathbf{B} are the electric and magnetic field vectors, and c is the speed of light. In a right-handed (x, y, z) coordinate system, a non-trivial solution of an electromagnetic wave following Maxwell's Equations propagating along the z -axis, towards a hypothetical observer, is described by:

$$\begin{aligned}\mathbf{E} &= E_x \cos(kz - \omega t + \Phi_x) \hat{x} + E_y \cos(kz - \omega t + \Phi_y) \hat{y}, \text{ and} \\ \mathbf{B} &= \frac{1}{c} E_y \cos(kz - \omega t + \Phi_y) \hat{x} + \frac{1}{c} E_x \cos(kz - \omega t + \Phi_x) \hat{y},\end{aligned}\tag{2.24}$$

where E_x , E_y , Φ_x , and Φ_y are all parameters describing the amplitude and phase of the electric field vector in the (x, y) plane, and with the magnetic field vector proportional and perpendicular to the electric field vector (Griffiths, 2005).

Considering only the electric field component and rewriting Equation 2.24 using complex values allows us to simplify the form of the solution to:

$$\mathbf{E} = \Re(\mathbf{E}_0 e^{-i\omega t}),\tag{2.25}$$

where we only consider the real part of the equation, and where \mathbf{E}_0 is defined as:

$$\mathbf{E}_0 = E_x e^{i\Phi_x} \hat{x} + E_y e^{i\Phi_y} \hat{y},\tag{2.26}$$

and is referred to as the polarization vector since it neatly contains the parameters responsible for the polarization properties (Degl'Innocenti, 2014).

For an electric field vector with oscillations in some combination of the x and y axes, the tip of the vector sweeps out an ellipse, as depicted in Figure 2.11. This ellipse is referred to as the polarization ellipse and has the form:

$$\left(\frac{\mathbf{E}_x}{\mathbf{E}_{0,x}} \right)^2 + \left(\frac{\mathbf{E}_y}{\mathbf{E}_{0,y}} \right)^2 - \frac{2\mathbf{E}_x \mathbf{E}_y}{\mathbf{E}_{0,x} \mathbf{E}_{0,y}} \cos \Phi = \sin^2 \Phi,\tag{2.27}$$

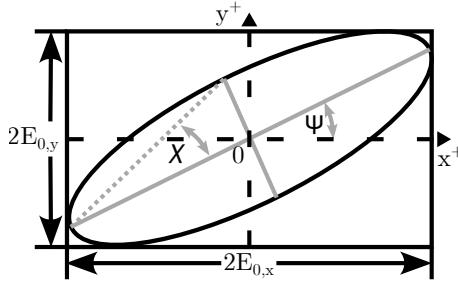


Figure 2.11: The polarization ellipse for an electric field vector propagating through free space. Diagram adapted from Inductiveload, PDM 1.0, via Wikimedia Commons (2023).

where $\Phi = \Phi_x - \Phi_y$ is the phase difference between the x and y phase parameters. The degree of polarization for the polarization ellipse is related to the eccentricity of the ellipse and the angle at which it is rotated relates to the polarization angle. Since $\mathbf{E}_{0,x}$, $\mathbf{E}_{0,y}$, Φ_x , and Φ_y describe the wave, the polarization ellipse that results from these parameters is fixed as the wave continues to propagate.

Since observations consist of images taken over a desired exposure time, time averaging of Equation 2.27 over the exposure time is necessary. Given the periodical nature and high frequencies of the fields, the time averaging may be found over a single oscillation using:

$$\langle \mathbf{E}_i \mathbf{E}_j \rangle = \lim_{dt \rightarrow \infty} \frac{1}{T} \int_0^T \mathbf{E}_i \mathbf{E}_j dt, \quad \text{for } i, j \in (x, y), \quad (2.28)$$

where T is the total averaging time over the electric field vectors \mathbf{E}_i and \mathbf{E}_j (Collett, 2005). Applying the time averaging to Equation 2.27 and simplifying results in:

$$(E_{0x}^2 + E_{0y}^2)^2 - (E_{0x}^2 - E_{0y}^2)^2 - (2E_x E_y \cos \Phi)^2 = (2E_x E_y \sin \Phi)^2. \quad (2.29)$$

The expressions inside the parentheses can be found through observation and may also be represented as:

$$\mathbf{S} = \begin{pmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{pmatrix} = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} = \begin{pmatrix} E_{0x}^2 + E_{0y}^2 \\ E_{0x}^2 - E_{0y}^2 \\ 2E_{0x} E_{0y} \cos \Phi \\ 2E_{0x} E_{0y} \sin \Phi \end{pmatrix}, \quad (2.30)$$

where S_0 to S_3 are referred to as the Stokes (polarization) parameters. The parameters describe the: S_0 , total intensity (often normalized to 1); S_1 , ratio of the Linear Horizontally Polarized (LHP) to Linear Vertically Polarized (LVP) light; S_2 , ratio of the Linear $+45^\circ$ Polarized ($L+45^\circ$) to Linear -45° Polarized ($L-45^\circ$) light; and S_3 , ratio of the Right Circularly Polarized (RCP) (clockwise) to Left Circularly Polarized (LCP) (counter-clockwise) light. When the intensity is normalized, the Stokes parameters range from 1 to -1 , based on the dominating component of the parameter (Chandrasekhar, 1950; Stokes, 1852).

From Equation 2.29 and 2.30, the polarization parameters are related by:

$$I^2 = Q^2 + U^2 + V^2, \quad (2.31)$$

for entirely polarized light. Only beams of completely polarized light could be accounted for before Stokes' work on polarization. Using the Stokes parameters, we can now account

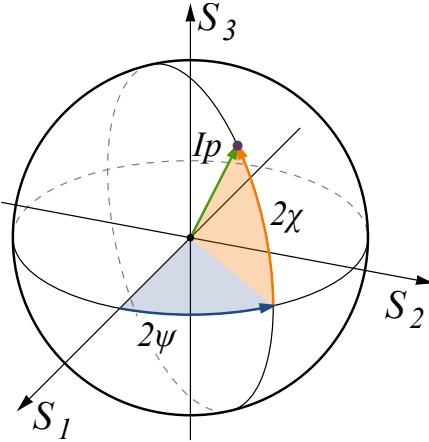


Figure 2.12: The Poincaré sphere describing the polarization properties of a wave-packet propagating through free space. Diagram adapted from Inductiveload, PDM 1.0, via Wikimedia Commons (2023).

for partially polarized light such that:

$$I^2 \geq Q^2 + U^2 + V^2, \quad (2.32)$$

where I , Q , U , and V are the normalized polarization parameters, often symbolized as

$$\bar{Q} = \frac{Q}{I}, \quad \bar{U} = \frac{U}{I}, \quad \text{and} \quad \bar{V} = \frac{V}{I}. \quad (2.33)$$

Similar to the polarization ellipse, the Stokes parameters may be depicted using the Poincaré sphere in spherical coordinates $(IP, 2\Psi, 2\chi)$, such that:

$$\begin{aligned} I &= S_0, \\ P &= \frac{\sqrt{S_1^2 + S_2^2 + S_3^2}}{S_0}, \text{ for } 0 \leq P \leq 1, \\ 2\Psi &= \arctan \frac{S_3}{\sqrt{S_1^2 + S_2^2}}, \text{ and} \\ 2\chi &= \arctan \frac{S_2}{S_1}, \end{aligned} \quad (2.34)$$

where I denotes the total intensity, P denotes the degree of polarization, or the ratio of polarized to non-polarized light in the wave-packet, χ denotes the polarization angle, and Ψ denotes the ellipticity angle of the polarization ellipse.

2.2.2 Polarization Measurement

Except for polarimetry in the radio-wavelength regime, the polarization of a beam can not be directly measured. The polarization properties may, however, be recovered from the beam through the manipulation of the four parameters given in Equation 2.24. This so-called manipulation is achieved by passing the beam through optical elements which vary the beam for differing amplitudes and phases. These matrix operations may be represented by their corresponding Mueller matrices.

For ideal components, the resultant beam \mathbf{S}' after passing through an optical element is given by $\mathbf{S}' = \mathbf{MS}$, where \mathbf{S} is the beam incident on the optical element and \mathbf{M}

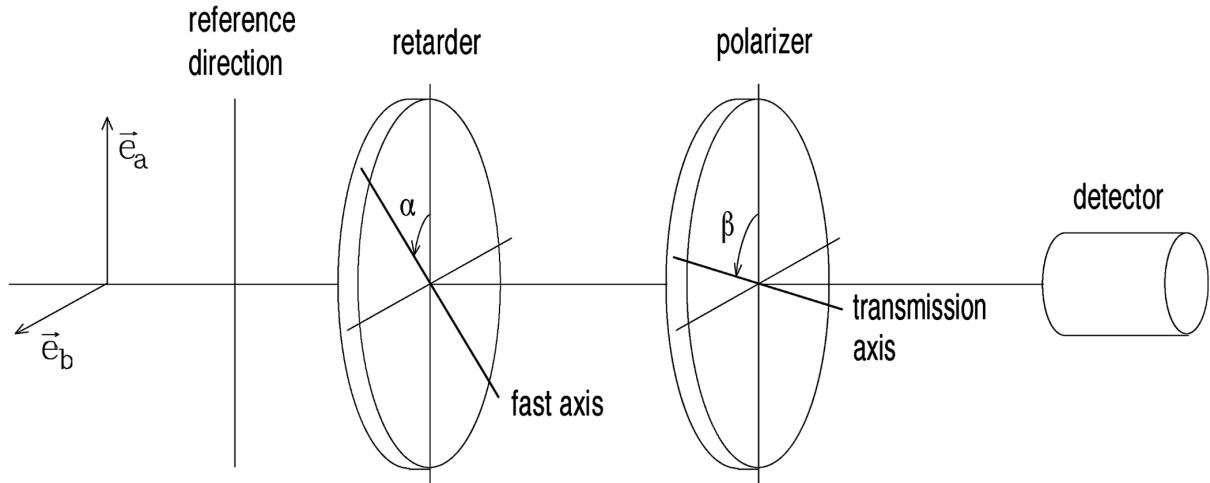


Figure 2.13: A diagram of an ideal polarimeter. Diagram adapted from Degl'Innocenti and Landolfi (2004).

represents the 4×4 Mueller matrix representing the optical element. Mueller matrices are especially useful when dealing with paths through optical elements as they observe the ‘train’ property (Priebe, 1969). This means that an incoming beam \mathbf{S} passing, in order, through elements with known Mueller matrices ($\mathbf{M}_0, \dots, \mathbf{M}_N$) results in an outgoing beam \mathbf{S}' such that:

$$\mathbf{S}' = \mathbf{M}_N \dots \mathbf{M}_0 \mathbf{S}. \quad (2.35)$$

Some Mueller Matrices are given below with angles related to those in Figure 2.13, measured counter-clockwise in a right-handed coordinate system.

General Rotation The Mueller matrix for coordinate space rotations about the origin by an angle θ ,

$$\mathbf{R}(\theta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\theta & \sin 2\theta & 0 \\ 0 & -\sin 2\theta & \cos 2\theta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad (2.36)$$

General Linear Retardance The Mueller matrix for retardance where α is the angle between the incoming vector and fast axis, and δ is the retardance introduced by the retarder,

$$\mathbf{W}(\alpha, \delta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos^2 2\alpha + \sin^2 2\alpha \cos \delta & \cos 2\alpha \sin 2\alpha(1 - \cos \delta) & \sin 2\alpha \sin \delta \\ 0 & \cos 2\alpha \sin 2\alpha(1 - \cos \delta) & \cos^2 2\alpha \cos \delta + \sin^2 2\alpha & -\cos 2\alpha \sin \delta \\ 0 & -\sin 2\alpha \sin \delta & \cos 2\alpha \sin \delta & \cos \delta \end{bmatrix}. \quad (2.37)$$

The retarder is often referred to by this retardance, e.g. if the retardance is $\delta = \pi$ or $\pi/2$, the retarder is referred to as a half- or quarter-wave plate, respectively.

General Linear Polarization The Mueller matrix for linear polarization where β is the angle between the incoming vector and transmission axis,

$$\mathbf{P}(\beta) = \frac{1}{2} \begin{bmatrix} 1 & \cos 2\beta & \sin 2\beta & 0 \\ \cos 2\beta & \cos^2 2\beta & \cos 2\beta \sin 2\beta & 0 \\ \sin 2\beta & \sin 2\beta \cos 2\beta & \sin^2 2\beta & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (2.38)$$

These matrices in combination with Equation 2.35 allow us to describe how the incoming Stokes parameters would change when passing through the various optical elements. For a setup similar to Figure 2.13, the detected Stokes parameters can be described by:

$$\begin{aligned} S'(\alpha, \beta, \gamma) \propto \frac{1}{2} \{ & I + [Q \cos 2\alpha + U \sin 2\alpha] \cos(2\beta - 2\alpha) \\ & - [Q \sin 2\alpha + U \cos 2\alpha] \sin(2\beta - 2\alpha) \cos \gamma \\ & + V \sin(2\beta - 2\alpha) \sin \gamma \}, \end{aligned} \quad (2.39)$$

where the retardance angle, α , polarization angle, β , for a wave plate with a relative phase difference, γ , may be varied to acquire a system of equations that can be solved to retrieve the Stokes polarization parameters (Bagnulo et al., 2009).

Several or more frames taken under differing configurations may be used to reduce a system of equations to extract all four Stokes polarization parameters, but it is possible to extract the I , Q and U polarization parameters using only four frames, or two dual-beam frames, for well-chosen configurations and assuming ideal components. This ideal configuration varies the retarder angle such that $\Delta\alpha = \pi/8$ while keeping the polarizer stationary. More frames for additional retarder angles are advisable and often necessary, however, as they correct for any differences in sensitivity, such as may arise in a polarized flat field and which is further discussed in § 2.2.3 (Patat and Romaniello, 2006).

From Equation 2.39 we see that the linear retarder element is the driving element of a polarizer as the first three Stokes parameters (S_{0-2} , or I , Q , and U) may be found by changing only the angle of retardance, α .

Wave Plates Wave plates, also commonly referred to as retarders, are generally made from optically transparent birefringent crystals. A wave plate has a fast and slow axis, which are perpendicular to one another and both perpendicular to an incident beam. Due to the birefringence of the wave plate medium, the phase velocity of the beam polarized parallel to the fast axis, namely the extraordinary beam, slightly increases while that of the beam polarized parallel to the slow axis, namely the ordinary beam, remains unaffected. This difference in the perpendicular component's phase velocities introduces a relative phase difference between the two beams, γ , which is given by:

$$\gamma = \frac{2\pi\Delta n L}{\lambda_0} \quad (2.40)$$

where Δn and L refer to the birefringence and thickness of the wave plate medium, respectively, and λ_0 refers to the vacuum wavelength of the beam (Hecht, 2017).

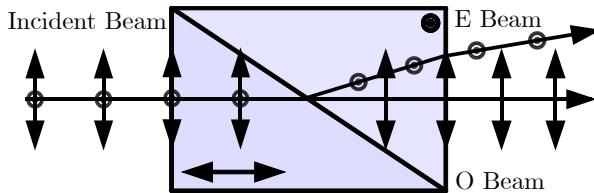


Figure 2.14: Diagram of a Rochon prism. Included in the diagram are the optical axes of the differing sections of the birefringent material as well as polarizing directions of the incident beam, denoted using the \leftrightarrow and \odot symbols, for the O - and E -beams, respectively. Figure adapted from ChrisHedgesUK, CC BY-SA 3.0, via Wikimedia Commons (2023).

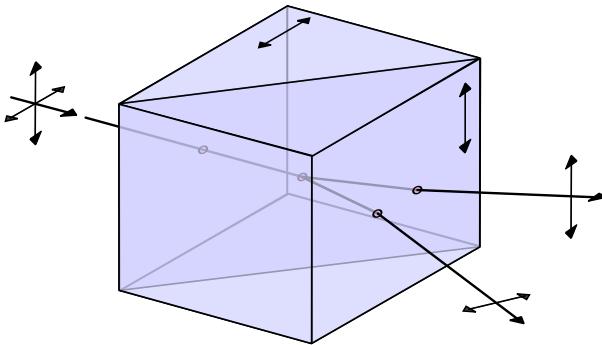


Figure 2.15: Diagram of a Wollaston prism. Included in the diagram are the optical axes of the differing sections of the birefringent material as well as polarizing directions of the incident beam, denoted using the \leftrightarrow and \ddagger symbols, for the O - and E -beams, respectively. Diagram adapted from fgalore, CC BY-SA 3.0, via Wikimedia Commons (2023).

This relative phase difference determines the name of the wave plate, such that the $\gamma = m(\pi/2)$ and $\gamma = m(\pi/4)$ phase differences, for $m \in \mathbb{Z}^+$, refer to the half- and quarter-wave plates (which are the most common wave plate phases), respectively. Phase differences with an integer multiple of one another relate to the same phase difference and are referred to as multiple-order wave plates, while wave plates with a phase difference less than an integer multiple are referred to as zero-order wave plates. Several multiple-order wave plates can be combined by alternatively aligning the fast axis of one to the slow axis of another to create a compound zero-order wave plate (Hale and Day, 1988).

Polarizers Polarizers are typically made from two prisms, of a birefringent material, cemented together with an optically transparent adhesive. The actual effect of separating the perpendicular polarization components is achieved using varying effects, namely through:

- absorption of one of the polarized components, such as in Polaroid polarizing filters,
- total internal reflection of a single polarized component, such as in a Nicol prism (Figure 2.10),
- Refraction of a single polarized component, such as in a Rochon prism (Figure 2.14), or
- Refraction of both polarization components in differing directions, such as in a Wollaston prism (Figure 2.15).

Wollaston Prisms The Wollaston prism consists of two right-angle prisms consisting of a birefringent monoaxial material, cemented together with an optically transparent adhesive along their hypotenuses with their optical axes orthogonal, as seen in Figure 2.15. The Wollaston prism is a common optical polarizing element in astrophysical polarimetry

which separates an incident beam into two linearly polarized *O*- and *E*-beams, orthogonal to one another, and deviated from their common axis equally. The deviation angle of the polarized beams is determined by the wedge angle which is defined as the angle from the common hypotenuse to that of the outer transmission face of either prism.

Wollaston prisms benefit over simpler elements (such as those listed in the polarizer paragraph) since a single frame allows for the observation of both orthogonal polarization components. This halves the observational time required to collect enough data to calculate the Stokes parameters, at the cost of an increase in calibration and reduction difficulty (Simon, 1986).

2.2.3 Polarimetric Calibrations

The raw science images acquired during polarimetric observations contain a combination of useful science data as well as noise, similar to § 2.1.8. Corrections and calibrations related to the detector remain unchanged from those described in § 2.1.8, while those related to correcting for the optical elements relate to corrections for spurious polarization effects.

Flat Fielding

Once the CCD calibrations have been completed, the polarization intrinsic to the optical elements needs to be accounted for such that the pixel-to-pixel response is made uniform. Flat-fielding is, once again, used to correct for this. The flats taken for polarimetry, however, introduce an additional challenge as the targets for conventional flats are polarized, such as twilight and dome flats which are polarized by light scattering in the atmosphere and the reflective surface of the dome, respectively.

If no unpolarized flat images can be taken for flat field calibrations then, when possible due to the polarimeter design, the wave plate may be constantly rotated to act as a depolarizing element; this is effective so long as the wave plate rotation period is much faster than the flat's exposure time. Alternatively, polarized flats may be taken at the same set of half-wave plate angles used for science observations and averaged together to achieve a similar depolarizing effect.

Observing additional ‘redundant’ exposures for the science and flat images increases the depolarizing effect up to the maximum of 16 half-wave plate positions, where exposures with a half-wave plate angle differing by $\pi/4$ from another are considered redundant due to the *O*- and *E*-beams swapping between the related exposures.

Increasing the amount of redundant observations proportionally increases the time needed to observe all the exposures, which in turn introduces time-dependent effects such as fringing or intensity variations of the flat source. As such, a middle ground must be found for the amount of redundant frames observed. (Patat and Romanielo, 2006; Peinado et al., 2010).

Dual-Beam Extraction and Alignment

After calibrations for the CCD and light path are accounted for, the O - and E -beams can be extracted and further reduced. The extraction depends heavily on the layout of the polarimeter but often a simple cropping of the differing sections is enough to separate the two images.

After extracting the O - and E -beams for a specific half-wave plate angle, the images need to be aligned such that the sources present in them overlap. The Wollaston prism needs to be corrected for as it introduces a beam deviation which differs across both images. The aligning of the O - and E -beams is crucial as the comparison of the dual images is what allows for the calculation of the polarization properties.

Sky Subtraction

The polarization introduced by the sky introduces a difference in the intensity of the background sky and needs to be removed as it will influence the polarization results of the target source. Thankfully, the background polarization is an additive type of noise and may be subtracted out across the frames. This subtraction is done independently for both beams in a frame and for each frame since the background intensity of all observed polarimetric beams will differ based on the observational parameters.

2.3 Spectropolarimetry

As the name suggests, spectropolarimetry is the measurement of the polarization of light for a chosen spectral range and provides polarimetric results as a function of wavelength. As spectropolarimetry is so closely reliant on both spectroscopy and polarimetry, advancements in spectropolarimeters have always been gated by the advancements of spectrometers and polarimeters (as described in § 2.1 and § 2.2).

The most notable historical contributions of spectropolarimetry are those of spectropolarimetric studies instead of instrumental developments. Spectropolarimetry provides further insights into a materials physical structure, chemical composition, and magnetic field, allowing spectropolarimetry to be useful across multiple disciplines. In astronomy in particular, spectropolarimetry has been used to study the magnetic field, chemical composition, and underlying structure and emission processes of multiple types of celestial objects (see for example Antonucci and Miller, 1985; Donati et al., 1997; Wang and Wheeler, 2008).

Along with common points of consideration when developing any instrumentation for observational astronomy, such as resolution and sensitivity, spectropolarimeters need also consider the spectral response of the polarimetric components as well as the polarization response of the spectroscopic components as both are simultaneously in the light-path during observations and have noticeable affects on one another. Time is another constraint for spectropolarimetry as the incident light is separated both by wavelength and by polarization states. This division of the incident light results in increased exposure times for both target observations and observations necessary for calibrations.

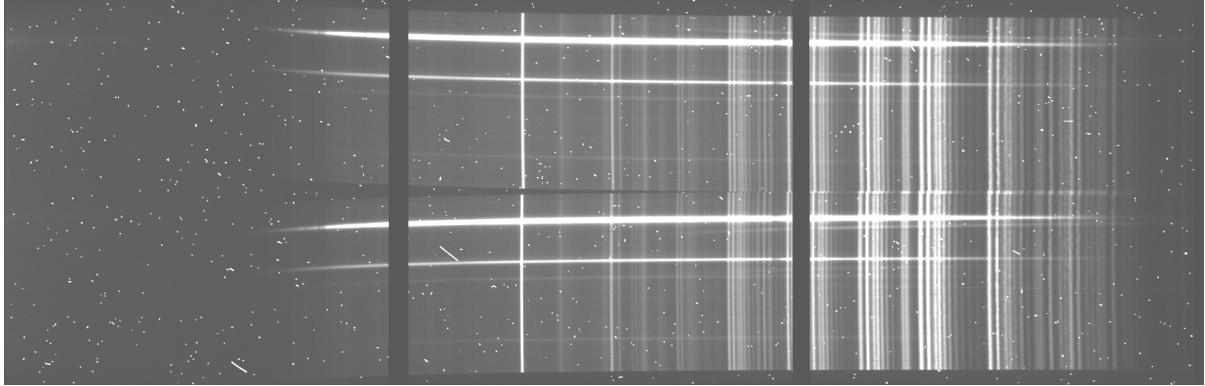


Figure 2.16: A spectropolarimetric target exposure as observed by the SALT RSS in spectropolarimetry mode.

Figure 2.16 illustrates a typical science image taken with a spectropolarimeter. The image contains the O - and E -beams which are both dispersed into their spectra. Spectropolarimetric results are acquired from measurements and calibrations of these images alongside any necessary calibration images.

2.3.1 Spectropolarimetric Measurement

The derived relations given in § 2.2.1, such as the Stokes parameters, describe polarization in general and are valid for both polarimetry and spectropolarimetry. Due to the time averaging of the observed light (Equation 2.28), any minor temporal variation, partial polarization, or monochromatic nature of the spectropolarimetric polarization parameters are accounted for.

For linear spectropolarimetry using a dual-beam polarizing element, an exposure measures the O - and E -beam wavelength dependent intensities, $f_{O,i}(\lambda)$ and $f_{E,i}(\lambda)$, for a given wave plate angle θ_i at angle i . These intensities thus relate to the wavelength dependent Stokes parameters as:

$$\begin{aligned} f_{O,i}(\lambda) &= \frac{1}{2}[I(\lambda) + Q(\lambda) \cos(4\theta_i) + U(\lambda) \sin(4\theta_i)], \text{ and} \\ f_{E,i}(\lambda) &= \frac{1}{2}[I(\lambda) - Q(\lambda) \cos(4\theta_i) - U(\lambda) \sin(4\theta_i)]. \end{aligned} \quad (2.41)$$

At least four linear equations are required to solve for three variables in a system of linear equations and thus at least two exposures must be taken to solve for the linear ($I(\lambda)$, $Q(\lambda)$, and $U(\lambda)$) polarization parameters (Degl’Innocenti et al., 2006; Keller, 2002).

The first Stokes parameter, $I(\lambda)$, may be recovered for each dual-beam exposure using

$$I_i(\lambda) = f_{O,i}(\lambda) + f_{E,i}(\lambda). \quad (2.42)$$

By calculating the $I_i(\lambda)$ Stokes parameter for each wave plate position i , the variation of the target over the course of observation may be corrected for, resulting in the $I(\lambda)$ Stokes parameter.

Next, the $Q(\lambda)$ and $U(\lambda)$ Stokes parameters are found by first defining the normalized

difference in relative intensities, $F_i(\lambda)$, as:

$$F_i(\lambda) \equiv \frac{f_{O,i}(\lambda) - f_{E,i}(\lambda)}{f_{O,i}(\lambda) + f_{E,i}(\lambda)}, \quad (2.43)$$

which allows Equation 2.41 to be written, as

$$F_i(\lambda) = \bar{Q}(\lambda) \cos(4\theta_i) + \bar{U}(\lambda) \sin(4\theta_i) = P \cos(4\theta_i - 2\chi), \quad (2.44)$$

in terms of the normalized Stokes parameters, or, alternatively, the degree of polarization, P , and polarization angle, χ (as described in Equation 2.33 and 2.34).

The optimal change in wave plate angle is $\Delta\theta_i = \pi/8$ as it allows the normalized Stokes polarization parameters to be calculated as:

$$\begin{aligned} \bar{Q}(\lambda) &= \frac{2}{N} \sum_{i=0}^{N-1} F_i(\lambda) \cos\left(\frac{\pi}{2}i\right), \text{ and} \\ \bar{U}(\lambda) &= \frac{2}{N} \sum_{i=0}^{N-1} F_i(\lambda) \sin\left(\frac{\pi}{2}i\right), \end{aligned} \quad (2.45)$$

where N is the number of exposures taken, limited such that $N \in [2, 16]$ (Patat and Romaniello, 2006).

2.3.2 Spectropolarimetric Calibrations

Just as the elements of a spectropolarimeter are an amalgamation of both a spectrometer and polarimeter, it naturally follows that the calibrations necessary to reduce spectropolarimetric data are a combination of the calibrations needed for spectroscopy and polarimetry, discussed further in § 2.1.8 and § 2.2.3. Even though the spectrometer and polarimeter components both have an effect on an incident beam following the light-path through the spectropolarimeter, the calibration procedures for both methods remain mostly independent of one another and as such need not be repeated here.

Spectropolarimetric calibrations are, however, more involved when compared to the same calibrations for either spectroscopy or polarimetry. Minor deviations in the calibrations across both the spectra and the polarized beam compound, especially when dealing with the wavelength calibration, resulting in poor Signal-to-Noise Ratio (S/N)'s. Generally, more exposures over longer timespans are required to acquire enough redundancy and signal for the calculation of the Stokes parameters on top of the time necessary for calibrations to be completed. It should therefore be noted just how important the calibrations are when dealing with spectropolarimetry.

2.4 The Southern African Large Telescope

Southern African Large Telescope (SALT) is a 10 m class optical/near-infrared telescope situated at the South African Astronomical Observatory (SAAO) field station near Sutherland, South Africa (Burgh et al., 2003). The operational design was based on the Hobby-Eberly Telescope (HET) situated at McDonald Observatory, Texas, which limits

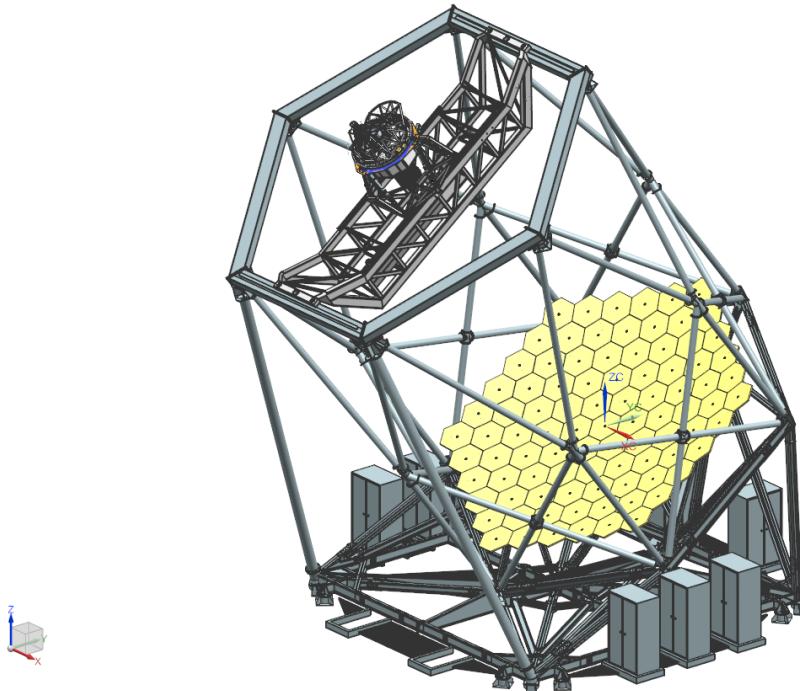


Figure 2.17: The tracker, supporting structure, and primary mirror of SALT. Figure adapted from the SALT call for proposals (2022).⁵

the pointing of the telescope’s primary mirror to a fixed elevation (37° from zenith in the case of SALT) while still allowing for full azimuthal rotation (Ramsey et al., 1998). Both SALT and HET utilize a spherical primary mirror which is stationary during observations and a tracker housing most of the instrumentation that tracks the primary mirrors spherically shaped focal path. Figure 2.17 depicts SALT’s tracker (top left), supporting structure, and primary mirror (bottom right).

2.4.1 The Primary Mirror

The primary mirror is composed of 91 individual 1 m hexagonal mirrors which together form an 11 m segmented spherical mirror. Each mirror segment can be adjusted by actuators allowing the individual mirrors to approximate a single monolithic spherical mirror. The fixed elevation means that SALT’s primary mirror has a fixed gravity vector allowing for a lighter, cost-effective supporting structure when compared to those of a more traditional altitude-azimuthal mount but with the trade-off that the control mechanism and tracking have increased complexity (Buckley et al., 2006).

2.4.2 Tracker and Tracking

During observations the primary mirror is stationary and the tracker tracks celestial objects across the sky by moving along the primary focus. The tracker is capable of 6 degrees of freedom with an accuracy of $5 \mu\text{m}$ and is capable of tracking $\pm 6^\circ$ from the optimal central track position. Targets at declinations from 10.5° to -75.3° , as shown in Figure 2.18 are accessible during windows of opportunity. As the tracker moves along the track the effective collecting area varies and thus SALT has a varying effective diameter

⁵http://pysalt.salt.ac.za/proposal_calls/current/ProposalCall.html

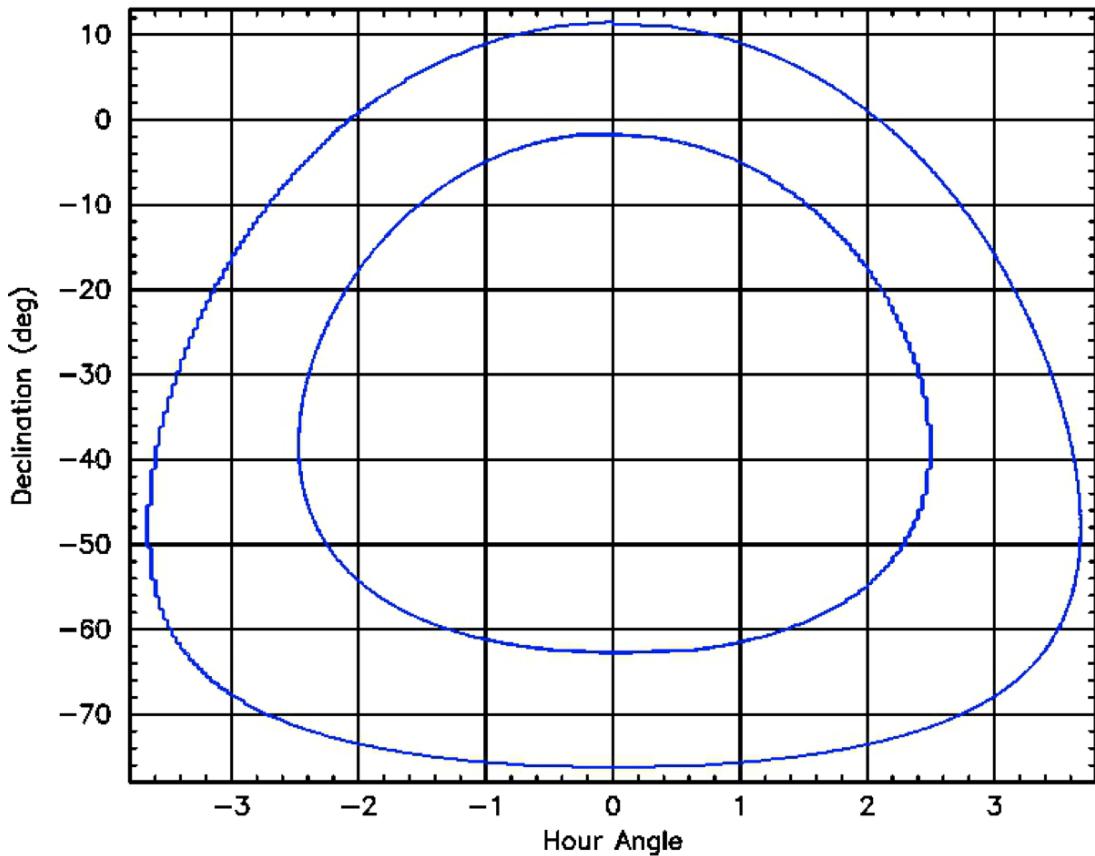


Figure 2.18: The visibility annulus of objects observable by SALT. Figure adapted from the SALT call for proposals (2013).⁶

of ~ 7 m to 9 m when the tracker is furthest and closest to the optimal central position, respectively.

The tracker is equipped with a spherical aberration corrector (O'Donoghue, 2000), and an atmospheric dispersion compensator (O'Donoghue, 2002), which corrects for the spherical aberration caused by the geometry of the primary mirror and allows access to wavelengths as short as 3200 Å. These return a corrected flat focal plane with an 8' diameter field of view at prime focus on to the science instruments, with a 1' annulus around it used by the Tracker in a closed-loop guidance system.

2.4.3 SALT Instrumentation

SALT is equipped with the SALT Imaging Camera (SALTICAM) and the RSS science instruments onboard the tracker, and the High Resolution Spectrograph (HRS) and Near Infra-Red Washburn Labs Spectrograph (NIRWALS) science instruments which are fibre-fed from the tracker to their own climate controlled rooms. The RSS is currently the only instrument used for spectropolarimetry.

⁶https://pysalt.salt.ac.za/proposal_calls/2013-2/

⁷https://pysalt.salt.ac.za/proposal_calls/current/ProposalCall.html

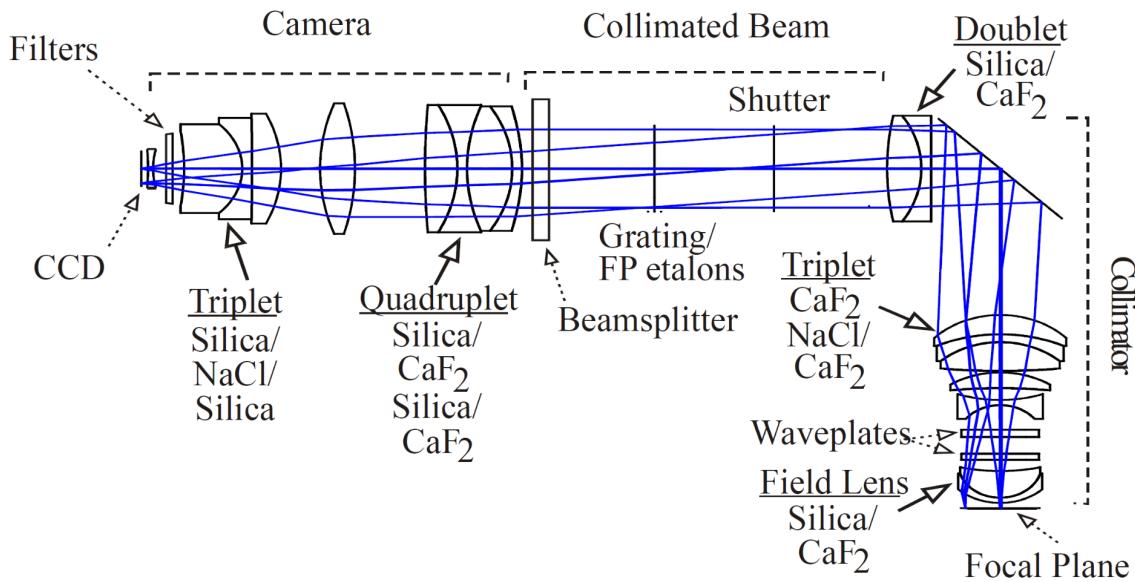


Figure 2.19: The optical path of the SALT RSS. Figure adapted from the SALT call for proposals (2023).⁷

NIRWALS

The Near Infra-Red Washburn Labs Spectrograph (NIRWALS) is currently being commissioned and will have a wavelength coverage of 8000 to 17000 Å, providing medium resolution spectroscopy at $R = 2000$ to 5000 over Near Infra-Red (NIR) wavelengths (Brink et al., 2022; Wolf et al., 2022). NIRWALS is fibre-fed from its integral field unit, containing 212 object fibers, along with a separate sky bundle, containing 36 fibers, housed in the SALT fibre instrument feed. It is ideally suited for studies of nearby galaxies.

HRS

The High Resolution Spectrograph (HRS) echelle spectrograph was designed for high resolution spectroscopy at $R = 37000$ - 67000 covering a wavelength range of 3700 - 8900 Å and consists of a dichroic beam splitter and two VPH gratings (Nordsieck et al., 2003). This instrument is capable of stellar atmospheric and radial velocity analysis.

SALTICAM

The SALT Imaging Camera (SALTICAM) functions as the acquisition camera and simple science imager with various imaging modes, such as full-mode and slot-mode imaging, and supports low exposure times, down to 50 ms (O'Donoghue et al., 2006). This enables photometry of faint objects, especially at fast exposure times.

RSS

The Robert Stobie Spectrograph (RSS) functions as the primary spectrograph on SALT and can operate in long-slit spectroscopy and spectropolarimetry modes, a narrowband imaging mode, and multi-object and high resolution spectroscopy modes (for an in-depth

Grating Name	Wavelength Coverage (Å)	Usable Angles (°)	Bandpass per tilt (Å)	Resolving Power (1.25'' slit)
PG0300 ⁸	3700 – 9000		3900/4400	250 – 600
PG0700 ⁸	3200 – 9000	3.0 – 7.5	4000 – 3200	400 – 1200
PG0900	3200 – 9000	12 – 20	~ 3000	600 – 2000
PG1300	3900 – 9000	19 – 32	~ 2000	1000 – 3200
PG1800	4500 – 9000	28.5 – 50	1500 – 1000	2000 – 5500
PG2300	3800 – 7000	30.5 – 50	1000 – 800	2200 – 5500
PG3000	3200 – 5400	32 – 50	800 – 600	2200 – 5500

Table 2.1: Gratings available for use with the RSS. Table adapted from the SALT call for proposals (2023).

discussion on operational modes see Kobulnicky et al., 2003, or the latest call for proposals).

The Detector The RSS detector consists of a mosaic of 3 CCD chips with a total pixel scale of $0.1267''$ per unbinned pixel with varying readout times depending on the binning and readout mode. The mosaicking results in a characteristic double ‘gap’ in the frames and resultant spectra taken with the RSS, as seen in Figure 2.16.

The Available Gratings The RSS is equipped with a rotatable magazine of six VPH gratings, as listed in Table 2.1. Observations may be planned using simulator tools provided by SALT and are performed in the first order only. The RSS has a clear filter, as well as three Ultraviolet (UV) (with differing lower filtering ranges) and one blue order blocking filter available, used in conjunction with the various gratings to block out contamination from the second order.

RSS Spectropolarimetry Spectropolarimetry using the RSS is currently commissioned for long-slit linear spectropolarimetry, (I, Q, U), where observations are taken following the waveplate pattern lists as in Table 2.2. Circular, (I, V), and all-Stokes, (I, Q, U, V), spectropolarimetry modes are in commissioning with observations including redundant half-wave plate pairs to be commissioned thereafter.⁹

⁸The PG0300 surface relief grating has been replaced with the PG0700 VPH grating as of November 2022 but has been included here as observations using the PG0300 are used in later sections.

⁹Commission status sighted from the latest ‘Polarimetry Observers Guide’ (2024).

Linear ($^{\circ}$)		Linear-Hi ($^{\circ}$)		Circular ($^{\circ}$)		Circular-Hi ($^{\circ}$)		All Stokes ($^{\circ}$)	
$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$
0	-	0	-	0	45	0	45	0	0
45	-	45	-	0	-45	0	-45	45	0
22.5	-	22.5	-			22.5	-45	22.5	0
67.5	-	67.5	-			22.5	45	67.5	0
	-	11.25	-			45	45	0	45
	-	56.25	-			45	-45	0	-45
	-	33.75	-			67.5	-45		
		78.75	-			67.5	45		

Table 2.2: Spectropolarimetry waveplate patterns defined for the RSS. The stated angles refer to the angle of the half ($\frac{1}{2}$ -) and quarter ($\frac{1}{4}$ -) waveplate's optical axis from the perpendicular of the dispersion axis. Table adapted from the SALT call for proposals (2023).

Chapter 3

Existing and Developed Software: An overview of Polarimetric reductions for SALT (POLSLT), Image Reduction and Analysis Facility (IRAF), and STOPS

This chapter contains an overview of POLSLT (§ 3.1) and the limitations faced during POLSLT wavelength calibrations (§ 3.1.8), a brief overview of the IRAF tasks relevant to spectropolarimetric wavelength calibrations (§ 3.2), and an overview of STOPS, the software developed to supplement the POLSLT reduction process (§ 3.3). Finally, a discussion of the updated reduction process, an example of which may be found in Appendix I, is included (§ 3.4).

3.1 POLSLT - Polarimetric reductions for SALT

Polarimetric reductions for SALT (POLSLT) is developed by SALT and is the official reduction pipeline for spectropolarimetric data taken using the SALT RSS.¹ The newest version of the software, aptly named the ‘beta version’ (‘version’ 23 January 2020), includes a GUI as well as limited interactivity during key steps in the reduction process and was the version adapted in this study.²

The steps that make up the POLSLT reduction pipeline include basic CCD reductions, wavelength calibrations, background subtraction and spectral extraction, raw Stokes calculations, final Stokes calculations, and visualization of the results. Accurate reductions in each step are crucial for accurate results and thus briefly discussed below. Further details for the reduction process may be found at the POLSLT GitHub wiki.³

¹ POLSLT is made freely available via the POLSLT GitHub repository, available at <https://github.com/saltastro/polsalt>. It is strongly advised to follow the wiki for installation instructions.

² Installation files and instructions for the ‘beta version’ utilizing the GUI are available at <http://www.saao.ac.za/~ejk/polsalt/code/> in a TAR GZIP file.

³ The GitHub wiki for POLSLT is available at <https://github.com/saltastro/polsalt/wiki>.

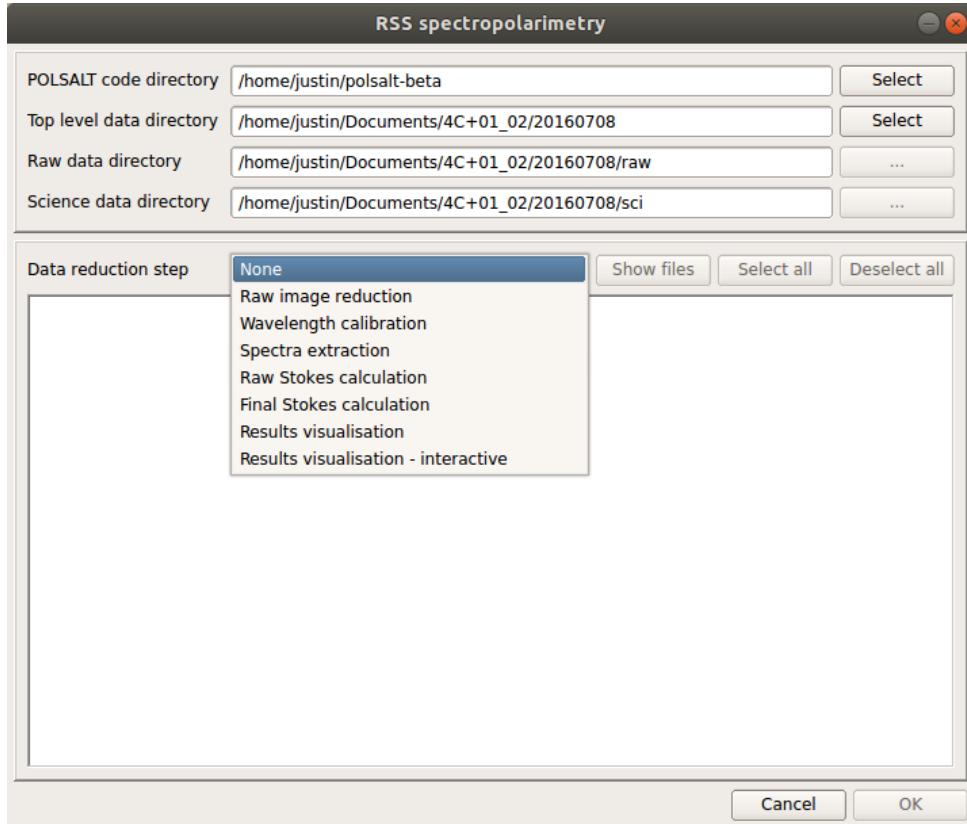


Figure 3.1: The layout of the `POLSALT` Graphical User Interface (GUI), including the contents of the reduction steps accessible via the dropdown menu. Note that there is no trailing forward slash after the ‘Top level data directory’. Figure created from local instance of the `POLSALT` GUI.

3.1.1 Basic CCD Reductions

Basic CCD reductions are run via `imred.py` and apply the necessary basic reductions to the raw data before any calibrations are applied. These reductions include overscan subtractions, gain corrections, crosstalk corrections, and mosaicking as well as attaching the bad pixel maps and pixel variance information. Files with basic reductions performed have “`mxgbp`” prepended to their names. As of February 2022, basic CCD reductions are automatically run for all RSS spectropolarimetric observations as part of the default SALT basic reduction pipeline that is run daily.

3.1.2 Wavelength Calibrations

Wavelength calibration and cosmic-ray rejection is performed via `specpolwavmap.py` and separately calibrates the *O*- and *E*-beams, based on the arc frames, and applies a simple cosmic-ray rejection for all science frames. This step is interactive and allows the user to individually fit wavelength calibration maps to each beam. The importance of an accurate correlation between both beams has been touched on previously (§ 2.3.2) and will be further discussed in § 3.1.8. The wavelength calibrated results are saved as an additional extension to each science FITS file, which are prefixed with a “`w`”, and the *O*- and *E*-beams of the extensions are split into their own sub-extensions.

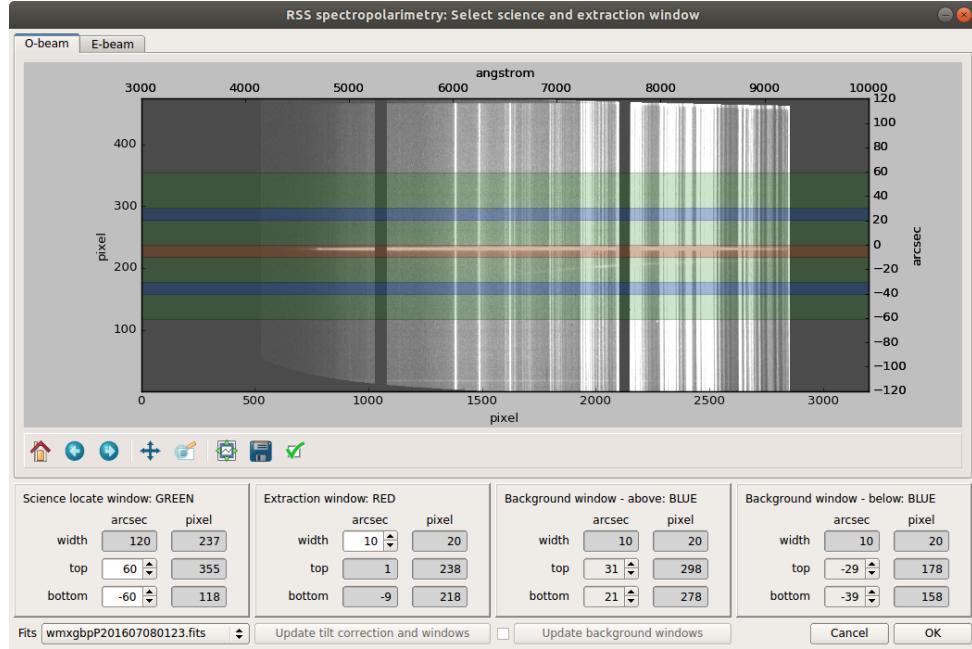


Figure 3.2: The layout of the interactive POLSALT spectra extraction GUI after selecting the ‘update tilt correction and windows’ button along the bottom border of the window. Figure created from local instance of the POLSALT GUI.

3.1.3 Spectral Extraction

Background subtraction and spectral extraction is run via `specpoleextract_dev.py` which corrects for the beam-splitter distortion and tilt, performs sky subtraction, and extracts a one dimensional wavelength dependent spectrum for each beam sub-extension. This step is interactive and, using the brightest trace in the images, allows the user to define regions which span the wavelength axis and which define the background and trace regions for the sky subtraction and spectral extraction. Files with corrections applied are saved with “c” prepended to their names and files which contain the extracted one dimensional spectrum have “e” further prepended to their names.

3.1.4 Raw Stokes Calculations

Raw Stokes calculations are performed via `specpolrawstokes_dev.py` and identify waveplate pairs for which the intensity, I , and a ‘raw Stokes’ signal, S , are calculated as:

$$I = \frac{1}{2}(O_1 + O_2 + E_1 + E_2), \text{ and} \quad (3.1)$$

$$S = \frac{1}{2} \left[\left(\frac{O_1 - O_2}{O_1 + O_2} \right) - \left(\frac{E_1 - E_2}{E_1 + E_2} \right) \right]. \quad (3.2)$$

The raw Stokes signal is calculated as the normalized difference of the O - and E -beams, for a waveplate pair, taken perpendicular to one another. The files generated containing the raw Stokes information have a very specific naming style, with most notably the pair of frames being used included in the file names.

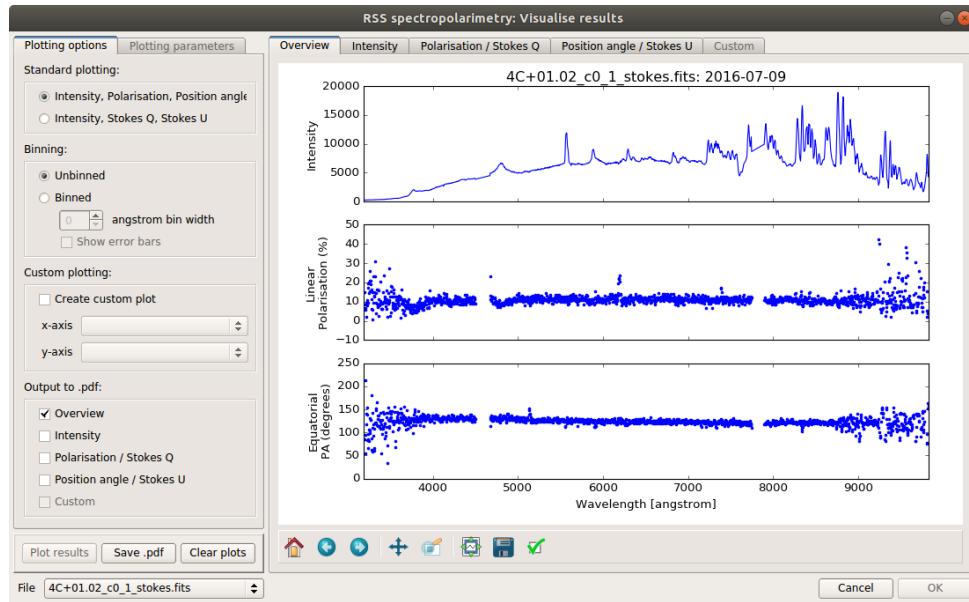


Figure 3.3: The layout of the interactive POLSALT visualization GUI after selecting the ‘Plot results’ button along the bottom border of the window. Figure created from local instance of the POLSALT GUI.

3.1.5 Final Stokes Calculations

The Final Stokes calculations are performed via `specpolfinalstokes.py` and, using the waveplate pattern along with the raw Stokes signals, calibrates for the polarimetric zero-point and waveplate efficiency, and calculates the final Stokes parameters. Before the final Stokes calculations are performed and when a sufficient amount of redundant exposures are taken, the raw Stokes signals are culled to eliminate outlier signals which may arise due to, for example, temporary atmospheric conditions affecting the signal. The data culling compares observation cycles against one another, compares the deviation of the signal means which estimate the baseline systematic polarization fluctuations (due to imperfections in repeatability), and performs a χ^2 analysis to eliminate outliers.

3.1.6 Visualization

Plotting the results of the spectropolarimetric reduction process uses `specpolview.py` and generates a plot of the Intensity, Linear Polarization (%), and Equatorial Polarization Angle ($^\circ$) against a shared wavelength axis, as seen in Figure 3.4. This step is interactive and various options, such as the wavelength range, binning, etc., are available.

3.1.7 Post-Processing Analysis

Generally, the plot of the spectropolarimetric results is the stopping point for most reduction procedures as it contains or creates the desired results. However, additional tools exist which may be used after the polarization reductions, and which are not represented in the GUI, namely, flux calibration and synthetic filtering.

Flux-calibrations are performed via `specpolflux.py` and are only intended for shape corrections of the spectrum. Additionally, a flux database file must exist for the observed standard and must be included in the working science directory.

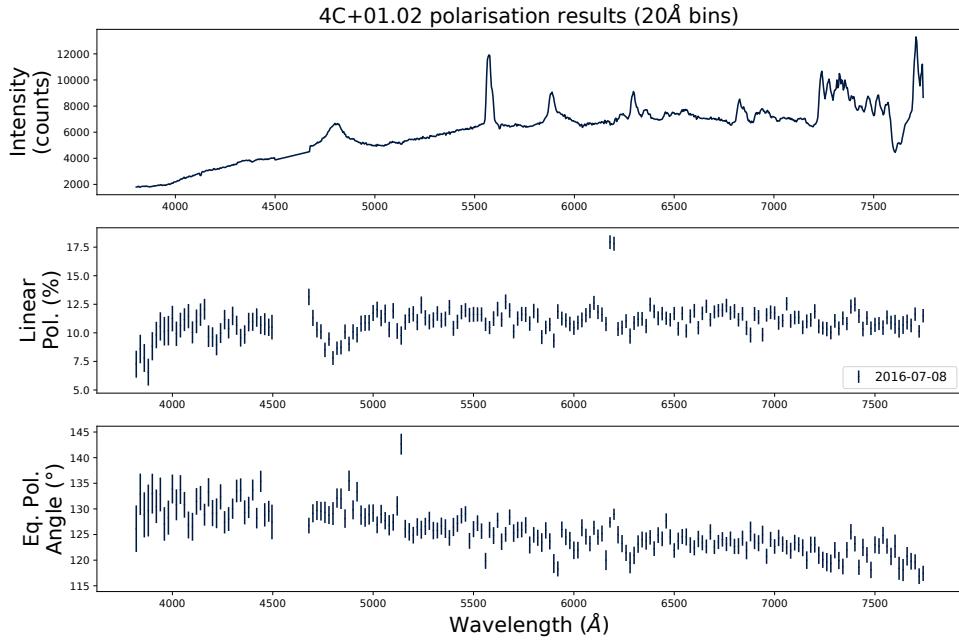


Figure 3.4: A typical plot resulting from the reduction process. Figure adapted from (Cooper et al., 2022).

Synthetic filtering is calculated via `specpolfilter.py` and computes the synthetically filtered polarization results. The filters which can be synthesized are the Johnson U , B , and V filter curves from the SALTICAM filters, as well as the Cousins R and I filter curves, along with any user defined wavelength dependent throughput filter curves.

3.1.8 POLSALT Limitations and the Need for Supplementary Tools

The creation of supplementary tools for POLSALT spectropolarimetric reductions stemmed from the limitations of the wavelength calibration process and a need to compare wavelength solutions across the perpendicular O and E polarization beams. The process of calibrating wavelength solutions using the POLSALT pipeline is time-consuming for the average user, and often results in unexpected crashes when receiving erroneous inputs or key presses. Due to the time-consuming process of recalibrating the wavelength solutions it is not feasible to perform the wavelength calibrations time and time again for any amount of reductions larger than a handful of observations. This is particularly true for observations performed with the SALT PG0300 grating as the sparse spectral features of the Ar arc lamp are not handled well by the POLSALT pipeline.

Since PG0300 provided the widest wavelength range and highest throughput, it was almost exclusively used for observations of flaring blazars, resulting in a large backlog of unanalyzed data. The only arc available for the PG0300 grating with a close enough articulation and grating angle ($\sim 10.68^\circ$ and $\sim 5.38^\circ$, respectively), was the Argon arc lamp which displays sparse spectral features with large gaps over the wavelength range at these grating and articulation angles (Figure 3.5). This often leads the POLSALT pipeline to create inconsistent wavelength solutions, or to fail to create a wavelength solution altogether, since minor deviations of identified spectral features result in large deviations in regions with no spectral features. To only further compound the difficulty of the wavelength calibrations, the spectrum of the Ar arc lamp contains a partial overlap of a differing order at higher wavelengths (§ 2.1.7, Equation 2.5).

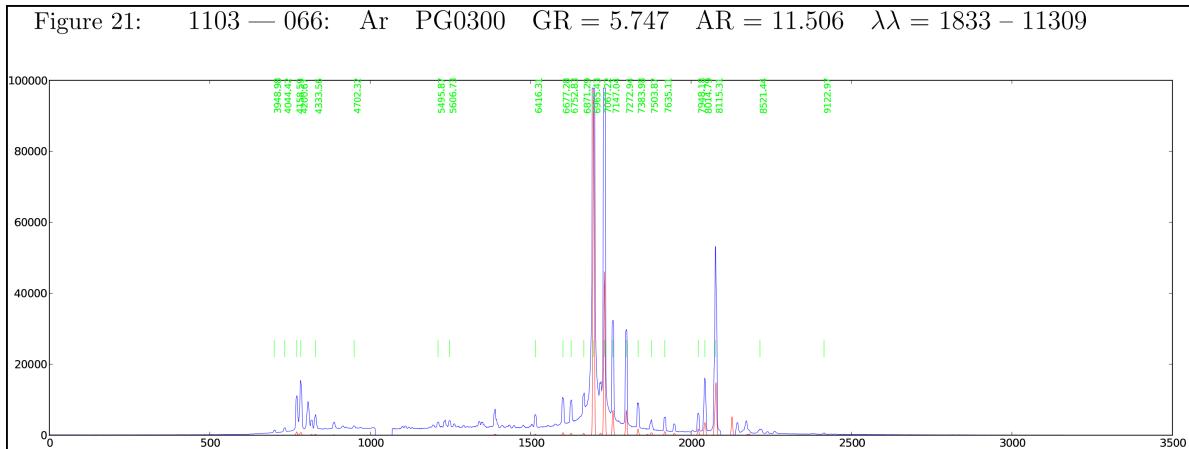


Figure 3.5: One of many Argon arc lamp spectra as provided by SALT for line identification. Plot adapted from SALT’s published Longslit Line Atlases (as of 2024), resized to fit within the document margins but otherwise unchanged.⁴

The chosen solution to overcome the limitations of the wavelength calibration process was to use well established wavelength calibration software which allows for rapid recalibrations and provides a familiar interface. IRAF provides this familiar environment and reliability, in part thanks to its continued community development.

Unfortunately, IRAF is unable to natively parse the data structure implemented by POLSALT ‘as is’ and so the files must be restructured. This restructuring works both ways as once the IRAF reductions are complete the data structure must be restructured to match that of the POLSALT `wavelength calibration` output such that the reduction process may be completed in POLSALT.

3.2 IRAF - Image Reduction and Analysis Facility

Image Reduction and Analysis Facility (IRAF) is a collection of software designed specifically for the reduction and analysis of astronomical images and spectra (Tody, 1986, 1993). The software consists of many tasks which perform specific operations and which are grouped into relevant packages. Only a brief overview of the tasks will be provided here. Help documentation for any of the IRAF tasks may be found online under <https://iraf.net/irafdocs/> or through the IRAF Command Line Interface (CLI) through the `?` or `:help` ‘cursor commands’ when running interactive tasks, with more specific help documentation provided in the relevant section.

Useful IRAF tasks that deserve a brief mention before the wavelength calibration related tasks are: the `mkscript` task in the `system` package which allows a user to create and save a task along with the defined parameters as a file which can later be called as a script,⁵ the `implot` task in the `plot` package which allows the rows or columns of an image to be interactively displayed,⁶ and the `eparam` task in the `language` package which

⁴The ‘low resolution’ Ar plot sourced from <https://astronomers.salt.ac.za/data/salt-longslit-line-atlas/>

⁵Help documentation for the `mkscript` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/system.mkscript.html.

⁶Help documentation for the `implot` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/plot.implot.html.

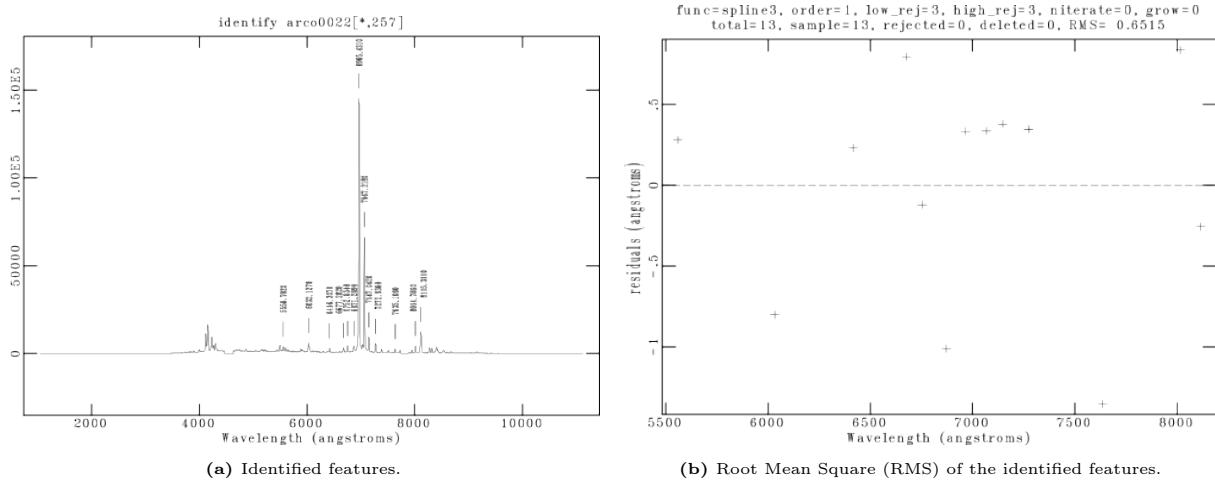


Figure 3.6: A plot and the RMS of the identified features found using the IRAF `identify` task. Figures created using the IRAF `identify` task.

allows the parameters of a task to be edited within the IRAF CLI.⁷

For wavelength calibrations taken with the SALT RSS, the relevant tasks, in order, are the `identify` and `reidentify` tasks located in the `noao.onedspec` package, and the `fitcoords` and optionally the `transform` tasks located under the `noao.twodspec.longslit` package. These tasks produce a two-dimensional wavelength solution which must be obtained separately for the *O*- and *E*-beam.

3.2.1 Identify

The `identify` task is used to interactively determine a one-dimensional wavelength function across a chosen row of an arc exposure by identifying features in the spectrum with known wavelengths.⁸ The task creates the first approximation of the wavelength solution as well as a local database in which the solution is saved. The initial identify solution is built on in subsequent tasks, and it is therefore imperative that the initial solution is well-fit to minimize errors further along the calibration process.

The process of using `identify` consists of identifying known features spanning the entire wavelength range and then removing identified features which negatively impact the wavelength solution. A balance must be found between the number of identified features and parameters of the fit against the deviation of the fit from the known features.

⁷Help documentation for the `eparam` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/language.eparam.html.

⁸Help documentation for the `identify` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.onedspec.identify.html.

⁹See also <https://iraf.net/irafdocs/formats/identify.php> for an explanation of the database contents.

Listing 3.1: An example of the identify database contents.⁹

```
# Thu 15:19:16 13-May-2021
begin    identify arc00057 [*,237]
id      arc00057
task    identify
image   arc00057 [*,237]
units   Angstroms
features 35
      53.61 5944.74989  5944.834  13.0 1 1 15257
     140.19 6029.9793  6029.997  13.0 1 1 4652
     185.30 6074.34644  6074.338  13.0 1 1 13396
     207.49 6096.15873  6096.161  13.0 1 1 21700
     255.23 6143.0493  6143.063  13.0 1 1 33330
     276.13 6163.56995  6163.594  13.0 1 1 11344
     330.89 6217.29293  6217.281  13.0 1 1 13705
     381.10 6266.51524  6266.495  13.0 1 1 21747
     420.21 6304.8113  6304.789  13.0 1 1 10226
     450.49 6334.45415  6334.428  13.0 1 1 36235
     500.18 6383.04826  6382.991  13.0 1 1 35824
     519.85 6402.26802  6402.248  13.0 1 1 70163
     626.70 6506.56147  6506.528  13.0 1 1 46165
     653.73 6532.91083  6532.882  13.0 1 1 21413
     721.60 6598.98642  6598.953  13.0 1 1 26396
     803.21 6678.31069  6678.277  13.0 1 1 51338
     843.15 6717.0732  6717.043  13.0 1 1 36780
     1099.95 6965.36335  6965.431  13.0 1 1 5618.4 ar
     1169.57 7032.38598  7032.413  13.0 1 1 100000
     1317.05 7173.89814  7173.938  13.0 1 1 5000 decrease
     1391.52 7245.11148  7245.167  13.0 1 1 73545
     1537.20 7383.93022  7383.981  13.0 1 1 5557.5 ar
     1595.02 7438.83545  7438.898  13.0 1 1 15000 decrease
     1663.64 7503.86263  7503.869  13.0 1 1 30000 ar; increase
     1697.46 7535.84584  7535.774  13.0 1 1 8000 increase
     1802.64 7635.07335  7635.106  13.0 1 1 20000 ar; decrease
     2209.19 8014.79559  8014.786  13.0 1 1 3000 ar; decrease
     2604.58 8377.66137  8377.607  13.0 1 1 14543
     2734.54 8495.41423  8495.359  13.0 1 1 8765
     2763.48 8521.52355  8521.442  13.0 1 1 4537.5 ar
     2840.92 8591.20799  8591.258  13.0 1 1 2000 decrease
     2889.39 8634.67334  8634.647  13.0 1 1 3059
     2911.42 8654.39264  8654.383  13.0 1 1 3000 decrease
     2926.56 8667.93501  8667.944  13.0 1 1 702.5 ar
     3135.72 8853.77575  8853.867  13.0 1 1 1820

function legendre
order 4
sample *
naverage 1
niterate 0
low_reject 3.
high_reject 3.
grow 0.
coefficients 8
 2.
 4.
53.60757446289061
3135.715576171875
7425.420339270724
1457.513831286474
-26.15751926622308
-3.000903509842187
```

3.2.2 Reidentify

The `reidentify` task is used to run the `identify` task autonomously and repeatedly across the entirety of the arc exposure at a defined interval.¹⁰ The task uses the one-dimensional wavelength solution stored in the database created by the initial `identify` call and refits the previously identified points to match the new positions of the relevant spectral features. The task may fail based on a number of conditions, most common of which is the loss of features as the task moves further from the row at which the user manually ran `identify`.

When running `reidentify` non-interactively, it is recommended to set the `verbose` parameter to ‘yes’ as this will provide immediate confirmation of if the task quit early. Regardless of whether or not the task quit successfully, the newly defined wavelength solutions are appended to the local database following the `identify` task database format (see Listing 3.1).

3.2.3 Fitcoords

The `fitcoords` task is used to combine the identified one-dimensional wavelength solutions in the database directory into a two-dimensional surface function.¹¹ The usage of `fitcoords` is similar to that of `identify` and consists of examining the distribution of identified points and eliminating any points that `reidentify` may have misidentified.

By eliminating outliers with bad residuals and modifying the two-dimensional surface function’s type and degree, the overall error of the fit is decreased, aligning more closely to what the ‘true’ wavelength solution is. This surface function is the final two-dimensional wavelength solution and is what is needed to convert the IRAF formatted wavelength calibrated Flexible Image Transport System (FITS) files back into the POLSALT format. The solution is stored in the local IRAF database and is the solution used by the STOPS `join` method.

3.2.4 Transform

The `transform` task is the optional final step in the IRAF wavelength calibration process.¹³ Simply put, `transform` converts the (pixel, pixel) units of an exposure to (wavelength, pixel) units which allows for an immediate check whether the wavelength solution is consistent across the frame. Any general error in the wavelength solution may be spotted in the transformed images (see Figure 3.8); ranging from minor errors, such as the arc exposure’s arc lines or science exposure’s sky lines not being straight across the columns of the frame, to more major errors, such as an incorrect wavelength solution skewing the exposure beyond recognition.

¹⁰Help documentation for the `reidentify` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.onedspec.reidentify.html.

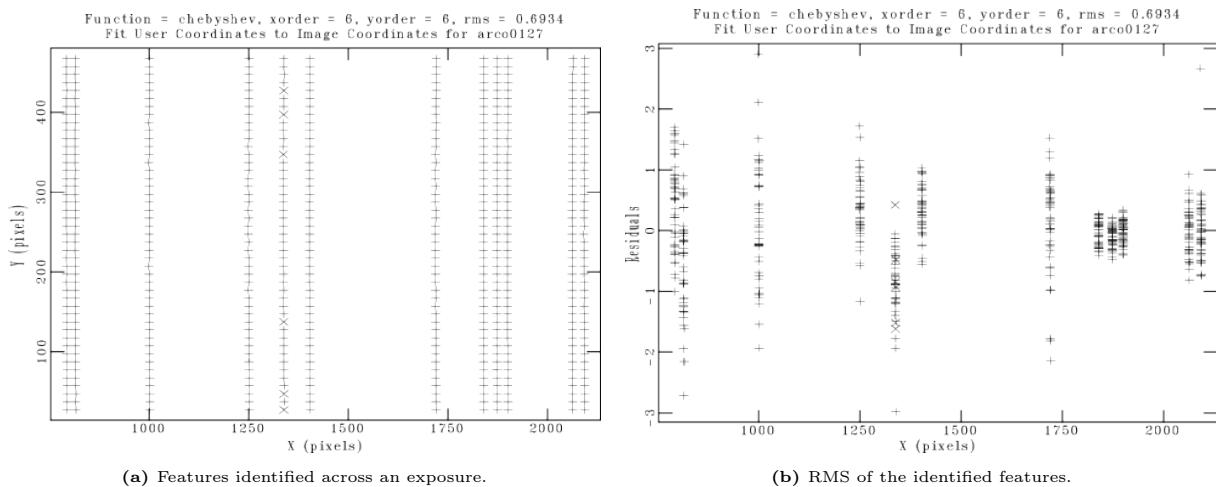
¹¹Help documentation for the `fitcoords` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.twodspec.longslit.fitcoords.html.

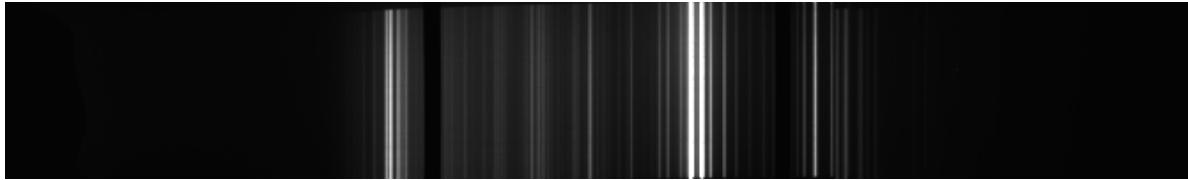
¹²See also <https://iraf.net/irafdocs/formats/fitcoords.php> for an explanation of the database contents.

¹³Help documentation for the `transform` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.twodspec.longslit.transform.html.

Listing 3.2: An example of the `fitcoords` database contents.¹²

```
# Thu 15:26:55 13-May-2021
begin    arc00057
task      fitcoords
axis      1
units     angstroms
surface   33
  1.
  5.
  5.
  1.
  1.
3199.
  1.
474.
7419.096745914063
1510.03933621895
-21.10886852752348
-2.079553916887794
0.06772631420528228
0.7720164913117386
-1.506773900054024
0.1341878190232142
-0.01659697703758917
0.0251087019569153
-3.318493303995171
-0.3612632489821799
0.003270665801371641
-0.0157962041414068
-0.003073690871589242
0.007533453962924031
0.02839687304474069
-0.003233465769521899
0.00174111456659807
0.00645177595090841
0.0105080093855621
-0.01157827440314294
-0.007789479002470706
-0.006562085282926231
-0.002321476801926803
```

**Figure 3.7:** A plot and the RMS of the features identified across the exposure using the IRAF `fitcoords` task. Figures created using the IRAF `fitcoords` task.



(a) A well-fit wavelength solution.



(b) A poorly fit wavelength solution with a region of no exposure (top of frame) displaying a terribly fit wavelength solution.

Figure 3.8: Examples of a well- and poor fit wavelength solution applied to the *O*- (a) and *E*-beams (b) of an arc image. The figures were scaled to best capture any deviation of the arc lines. Figures created by the `IRAF transform` task.

3.3 STOPS - Supplementary Tools for POLSALT Spectropolarimetry

Supplementary Tools for POLSALT Spectropolarimetry (STOPS) provides supplementary tools which convert the POLSALT and IRAF formats back and forth, allowing IRAF to be used for wavelength calibrations of SALT spectropolarimetric data. It also provides additional tools to check the accuracy of the wavelength calibration. STOPS is written in Python and requires Python 3.11+ to run, as well as `Astropy` (6.0.0+) (Astropy Collaboration et al., 2013, 2018, 2022), `ccdproc` (2.4.1+) (Craig et al., 2017), `Matplotlib` (3.5.2+) (Hunter, 2007), `NumPy` (1.26.4+) (Harris et al., 2020), and `SciPy` (1.13.0+) (Virtanen et al., 2020).

The parsing of POLSALT data into an IRAF usable format and the reformatting of the IRAF wavelength calibrated data back into a POLSALT usable format, referred to as *splitting* and *joining*, is performed by the STOPS `split` and `join` methods, respectively.

Methods to verify the validity of the alternate wavelength calibrations were also added to STOPS. The `skyline` method checks the sky line wavelength (*x*) positions across the frame as well as the variation of the sky lines across the positional (*y*) axis of the frame. The `correlate` method checks the correlation of the *O*- and *E*-beams either within a given FITS file or across multiple files (comparing only the *O*- and *E*-beams for each). With these two additional methods, a user is able to verify that the wavelength solutions do not conflict across the *O*- and *E*-beams and that no unexpected deviations are included in the wavelength solutions.

Help for the CLI commands for general STOPS usage or the specific modes may be found by running:

```
$ python ~/STOPS --help
# OR
$ python ~/STOPS [split|join|correlate|skylines] --help
```

or in Listing II.1 (in Appendix II). Finally, help documentation for the specific STOPS methods may be found within this section (Listing 3.3 to 3.6) or in Appendix II.

3.3.1 Splitting

Listing 3.3: The ‘docstring’ for `split.py`

```

26 """
27 The `Split` class allows for the splitting of `polsalt` FITS files
28 based on the polarization beam. The FITS files must have basic
29 `polsalt` pre-reductions already applied (`mzgbp...` FITS files).
30
31 Parameters
32 -----
33 data_dir : str
34     The path to the data to be split
35 fits_list : list[str], optional
36     A list of pre-reduced `polsalt` FITS files to be split within `data_dir`.
37     (The default is None, `Split` will search for `mzgbp*.fits` files)
38 split_row : int, optional
39     The row along which to split the data of each extension in the FITS file.
40     (The default is SPLIT_ROW (See Notes), the SALT RSS CCD's middle row)
41 no_arc : bool, optional
42     Decides whether the arc frames should be recombined.
43     (The default is False, `polsalt` has no use for the arc after wavelength calibrations)
44 save_prefix : dict[str, list[str]], optional
45     The prefix with which to save the O & E beams.
46     Setting `save_prefix` = ``None`` does not save the split O & E beams.
47     (The default is SAVE_PREFIX (See Notes))
48
49 Attributes
50 -----
51 arc : str
52     Name of arc FITS file within `data_dir`.
53     `arc` = `""` if `no_arc` or not detected in `data_dir`.
54 o_files, e_files : list[str]
55     A list of the 'O' - and 'E' -beam FITS file names.
56     The first entry is the arc file if `arc` defined.
57 data_dir
58 fits_list
59 split_row
60 save_prefix
61
62 Methods
63 -----
64 split_file(file: os.PathLike)
65     -> tuple[astropy.io.fits.HDUList]
66     Handles creation and saving the separated FITS files
67 split_ext(hdulist: astropy.io.fits.HDUList, ext: str = 'SCI')
68     -> astropy.io.fits.HDUList
69     Splits the data in the `ext` extension along the `split_row`
70 crop_file(hdulist: astropy.io.fits.HDUList, crop: int = CROP_DEFAULT (See Notes))
71     -> tuple[numumpy.ndarray]
72     Crops the data along the edge of the frame, that is,
73     'O'-beam cropped as [crop:], and
74     'E'-beam cropped as [:crop].
75 update_beam_lists(o_name: str, e_name: str)
76     -> None
77     Updates `o_files` and `e_files`.
78 save_beam_lists(file_suffix: str = 'frames')
79     -> None
80     Creates (Overwrites if exists) and writes the `o_files` and `e_files` to files named
81     `o_{file_suffix}` and `e_{file_suffix}`, respectively.
82 process()
83     -> None
84     Calls `split_file` and `save_beam_lists` on each file in `fits_list` for automation.
85
86 Other Parameters
87 -----
88 **kwargs : dict
89     keyword arguments. Allows for passing unpacked dictionary to the class constructor.
90
91 Notes
92 -----
93 Constants Imported (See utils.Constants):
94     SAVE_PREFIX
95     CROP_DEFAULT
96     SPLIT_ROW
97
98 """

```

As mentioned previously, the format of the FITS file created by POLSALT after basic CCD reductions and the format expected by IRAF to be used for the wavelength calibrations are incompatible. Basic POLSALT CCD reductions return FITS files which contain a primary header along with extensions for the science, variance, and Bad Pixel Map (BPM) images. These extensions carry the image of the trace for both polarimetry beams (see Figure 3.9), the variance of the image, and a map of the pixels to be masked out, respectively.

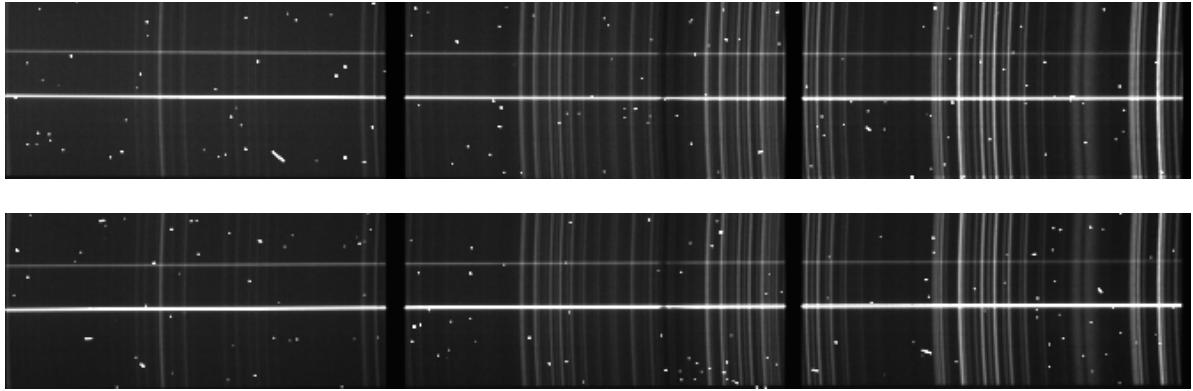


Figure 3.9: The split *O*- and *E*-beams as handed to IRAF. Figure created from the `STOPS split` method output.

IRAF is capable of dealing with multiple traces in an extension or lists of input files but is not as capable when dealing with multiple wavelength solutions contained in a single extension (as expected by the `POLSALT wavelength calibration`) or extensions containing sub-extensions (as expected by the `POLSALT spectral extraction`). To simplify the IRAF reduction procedure it was decided to separate the perpendicular polarization beams into their own files.

The files with POLSALT pre-reductions applied, namely FITS files with an ‘mxgbp’ prefix (§ 3.1), are used as the starting point for the supplementary tool’s `split` method. Running `split` finds all the FITS files for wavelength calibration within the working directory, creates two empty Header Data Unit (HDU) structures for each sub-extension of the FITS file, and appends all science and header data necessary for wavelength calibration to the relevant HDU structure.

As the intent was always to parse the wavelength function back into POLSALT it was decided to keep these temporary FITS files as small as possible. This is especially necessary when considering the amount of exposures that are taken for a single spectropolarimetric observation run, and how the number of observations increases for long term studies.

To aid the scripting of the IRAF wavelength calibration process, the `split` method also performs row cropping to exclude CCD regions with no exposure and creates files listing the split *O*- and *E*-beam FITS files to simplify the IRAF task inputs.¹⁴ Otherwise, defaults, such as which row to split the beams along, were kept as close to the POLSALT pipeline as possible.

¹⁴Row cropping was decided on as IRAF does not handle rows with no exposure well, specifically when it comes to the `reidentify` task.

3.3.2 Joining

As mentioned previously, the FITS file formats created by IRAF after wavelength calibrations versus that expected by the POLSALT `spectra extraction` are incompatible. The STOPS `join` method is used at this point since all pieces necessary to recreate the POLSALT wavelength calibrated FITS files exist once `fitcoords` has been successfully run. A typical FITS file expected by the POLSALT `spectra extraction` contains a primary header along with the various image extensions, with most importantly a newly created wavelength extension.

Running `join` finds all the relevant FITS and local IRAF database files, creates an empty HDU structure for each pair of matching spectropolarimetric beams, copies over the extensions and their respective image and header information, appends a new extension and parses the database wavelength solutions into the POLSALT intensity-wavelength format, performs cosmic ray cleaning, and masks the BPM to reflect the wavelength calibrated region.

Firstly, `join` parses the wavelength database file, described in § 3.2.3, for specifically either ‘Chebyshev’ or ‘Legendre’ solutions, and creates a function to convert a (*pixel*, *pixel*) position to a wavelength value. This is used to fill the pixels of the wavelength extension with their respective wavelength, as seen in Figure 3.10.

Next, the `join` method cleans the science extension of cosmic rays using the `lacosmic` python package which uses the L.A. Cosmic algorithm, based on Laplacian edge detection. The read noise and gain parameters used for cosmic ray cleaning were chosen based on the properties of the RSS, while the rest of the parameters were left as the default, following the publication and suggestions¹⁵ by the algorithm’s creator, as well as the implementation of the algorithm in the python `ccdproc` package (McCully et al., 2018; van Dokkum, 2001). The chosen parameters work well for most cosmic rays, as can be seen when comparing Figure 3.9 to Figure 3.11, but may be modified as needed.

Thereafter, `join` updates the headers to be near-identical to those created by the POLSALT `wavelength calibration`, most notably updating the data shape, ‘CTYPE3’, and data type, ‘BITPIX’, keywords. The only difference in the header is the ‘NAXIS2’ keyword, due to the cropping performed by `split`. The cropped region could be reintroduced but would be masked out and further discarded in the following POLSALT `spectra extraction` process, making it redundant.

Finally, the wavelength extension is masked to remove any uncalibrated wavelength regions as well as masked for the skewing of the trace introduced by the wollaston element. The masking of the wollaston skewing is necessary since POLSALT introduces a wollaston correction in the `spectra extraction` process. The BPM extension is masked to reflect the valid wavelength calibrated region, and the files are saved with the POLSALT wavelength calibrated ‘wmxgbp’ prefix.

¹⁵Suggested parameters for the `lacosmic` algorithm may be found at <http://www.astro.yale.edu/dokkum/lacosmic/pars.html>.

Listing 3.4: The ‘docstring’ for join.py

```

32 """
33
34 The `Join` class allows for the joining of previously split files and the
35 appending of an external wavelength solution in the `polsalt` FITS file format.
36
37 Parameters
38 -----
39 data_dir : str
40     The path to the data to be joined
41 database : str, optional
42     The name of the `IRAF` database folder.
43     (The default is "database")
44 fits_list : list[str], optional
45     A list of pre-reduced `polsalt` FITS files to be joined within `data_dir`.
46     (The default is ``None``, `Join` will search for `m*gbp*.fits` files)
47 solutions_list: list[str], optional
48     A list of solution filenames from which the wavelength solution is created.
49     (The default is ``None``, `Join` will search for `fc*` files within the `database` directory)
50 split_row : int, optional
51     The row along which the data of each extension in the FITS file was split.
52     Necessary when Joining cropped files.
53     (The default is 517, the SALT RSS CCD's middle row)
54 save_prefix : dict[str, list[str]], optional
55     The prefix with which the previously split `O`- & `E`-beams were saved.
56     Used for detecting if cropping was applied during the splitting procedure.
57     (The default is SAVE_PREFIX (See Notes))
58 verbose : int, optional
59     The level of verbosity to use for the Cosmic ray rejection
60     (The default is 30, I.E. logging.INFO)
61
62 Attributes
63 -----
64 fc_files : list[str]
65     Valid solutions found from `solutions_list`.
66 custom : bool
67     Internal flag for whether `solutions_list` uses the `IRAF` or a custom format.
68     See Notes for custom solution formatting.
69     (Default (inherited from `solutions_list`) is False)
70 arc : str
71     Deprecated. Name of arc FITS file within `data_dir`.
72 data_dir
73 database
74 fits_list
75 split_row
76 save_prefix
77
78 Methods
79 -----
80 get_solutions(wavlist: list / None, prefix: str = "fc") -> (fc_files, custom): tuple[list[str], bool]
81     Parse `solutions_list` and return valid solution files and if they are non-`IRAF` solutions.
82 parse_solution(fc_file: str, xshape: int, yshape: int) -> tuple[dict[str, int], np.ndarray]
83     Loads the wavelength solution file and parses keywords necessary for creating the wavelength extension.
84 join_file(file: os.PathLike) -> None
85     Joins the files,
86     attaches the wavelength solutions,
87     performs cosmic ray cleaning,
88     masks the extension,
89     and checks cropping performed in `Split`.
90     Writes the FITS file in a `polsalt` valid format.
91 check_crop(hdu: pyfits.HDUList, o_file: str, e_file: str) -> int
92     Opens the split `O`- and `E`-beam FITS files and returns the amount of cropping that was performed.
93 process() -> None
94     Calls `join_file` on each file in `fits_list` for automation.
95
96
97 Other Parameters
98 -----
99 no_arc : bool, optional
100     Deprecated. Decides whether the arc frames should be processed.
101     (The default is False, `polsalt` has no use for the arc after wavelength calibrations)
102 **kwargs : dict
103     keyword arguments. Allows for passing unpacked dictionary to the class constructor.
104
105 Notes
106 -----
107 Constants Imported (See utils.Constants):
108     DATADIR, SAVE_PREFIX, SPLIT_ROW, CR_PARAMS
109
110 Custom wavelength solutions must be formatted containing:
111     `x`, `y`, *coefficients...
112 where a solution are of order ('x' by 'y') and must contain x*y coefficients,
113 all separated by newlines. The name of the custom wavelength solution file
114 must contain either "cheb" or "leg" for Chebychev or Legendre
115 wavelength solutions, respectively.
116
117 Cosmic ray rejection is performed using lacosmic [1]_ implemented in ccdproc via astroscreappy [2]_.
118
119 References
120 -----
121 .. [1] van Dokkum 2001, PASP, 113, 789, 1420 (article : https://adsabs.harvard.edu/abs/2001PASP..113.1420V)
122 .. [2] https://zenodo.org/records/1482019
123
124 """
125

```

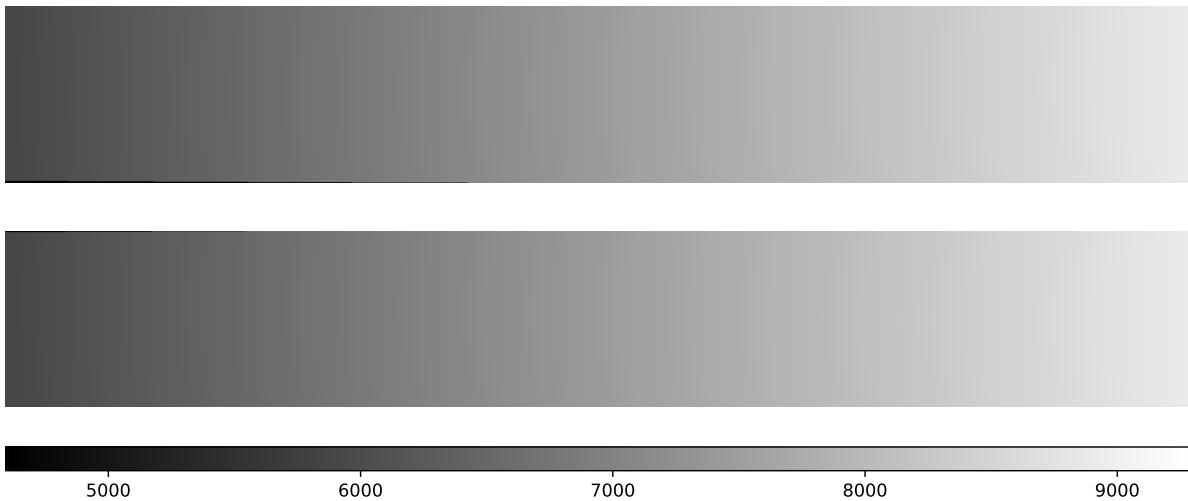


Figure 3.10: The wavelength extension of a FITS file ready to be handed back to the `POLSALT` pipeline. The color bar displays the wavelength in Å as displayed by the *O*- and *E*-beam sub-extensions. Note that regions which fall outside the exposed region are masked by setting the corresponding pixel values of the wavelength and BPM extensions to 0. Figure created from the `STOPS join` method output.

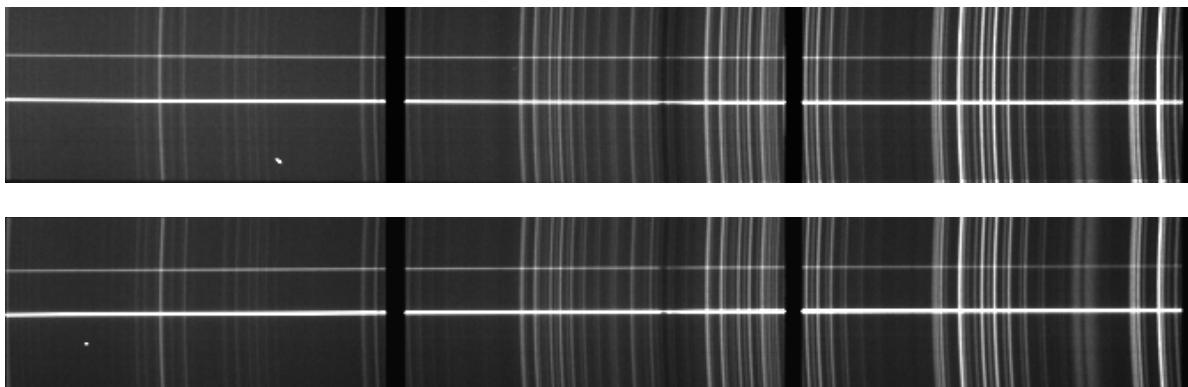


Figure 3.11: A representative science extension of a FITS file capable of being parsed by the `POLSALT` pipeline. The intensity of the *O*- and *E*-beam sub-extensions are displayed via the grayscale value at each pixel. Note the inclusion of regions of: solid black demarcating the chip gaps, horizontal stripes of high intensity demarcating the trace, and (curved) vertical stripes of high intensity demarcating the sky lines. Figure created from the `STOPS STOPSSjoin` method output.

3.3.3 Sky Line Checks

Sky line comparisons allow the user to confirm the accuracy of the wavelength solution across both the rows and columns of the frame. The `skyline` method naively transforms the wavelength calibrated files,¹⁶ allowing the deviation of a skyline spanning multiple rows to be measured, and compares the observed sky line wavelength positions to those measured by SALT, allowing the wavelength deviation of the skylines to be measured.¹⁷

The file used for sky line comparisons may either be the IRAF `transform` FITS file or the ‘wmxgbp’ FITS files created by `join`. The `skyline` method loads the wavelength calibrated files, transforms the frames if the frame was not transformed by `transform`, removes the continuum, compares the width of the sky lines before and after transforma-

¹⁶The transformation applied by the `skyline` method uses linear interpolation and is thus less accurate at flux conservation than the transformation applied by the `transform` method.

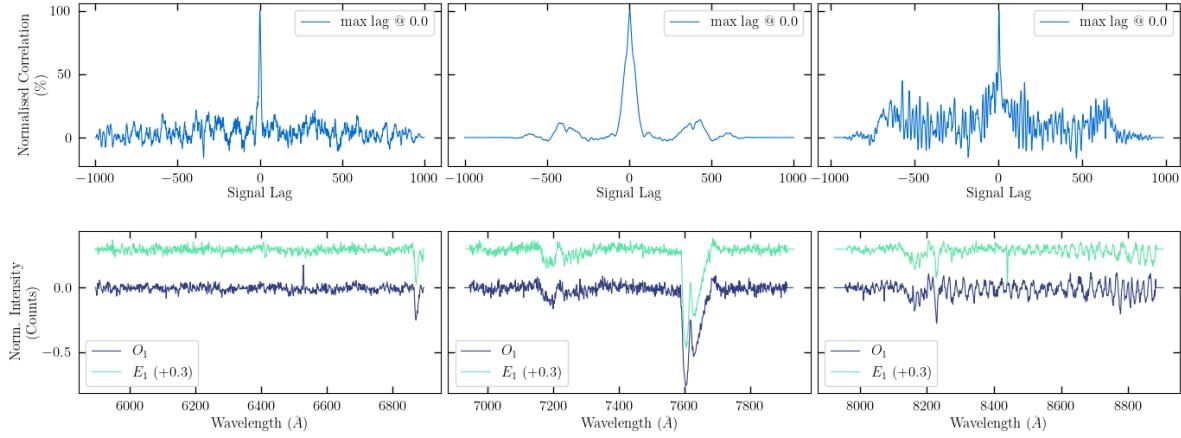
¹⁷The first iteration of a sky line atlas is available at <https://astronomers.salt.ac.za/data/salt-longslit-line-atlas/>

Listing 3.5: The ‘docstring’ for `skylines.py`

```

30
31 """
32 Class representing the Skylines object.
33
34 Parameters
35 -----
36 data_dir : Path
37     The directory containing the data files.
38 filenames : list[str]
39     The list of filenames to be processed.
40 beam : str, optional
41     The beam mode, by default "OE".
42 plot : bool, optional
43     Flag indicating whether to plot the continuum, by default False.
44 save_prefix : Path / None, optional
45     The prefix for saving the data, by default None.
46 **kwargs
47     Additional keyword arguments.
48
49 Attributes
50 -----
51 data_dir : Path
52     The directory containing the data files.
53 fits_list : list[str]
54     The list of fits file paths.
55 beam : str
56     The beam mode.
57 can_plot : bool
58     Flag indicating whether to plot the continuum.
59 save_prefix : Path / None
60     The prefix for saving the data.
61 wav_unit : str
62     The unit of wavelength.
63 rawWav : np.ndarray
64     The raw wavelength data.
65 rawSpec : np.ndarray
66     The raw spectral data.
67 rawBpm : np.ndarray
68     The raw bad pixel mask data.
69 corrWav : np.ndarray
70     The corrected wavelength data.
71 corrSpec : np.ndarray
72     The corrected spectral data.
73 spec : np.ndarray
74     The median spectrum.
75 normSpec : np.ndarray
76     The normalized spectrum.
77
78 Methods
79 -----
80 checkLoad(self, path1: str) -> np.ndarray:
81     Checks and loads the data from the given path.
82 transform(self, wav_sol: np.ndarray, spec: np.ndarray) -> np.ndarray:
83     Transforms the input wavelength and spectral data based on the given wavelength solution.
84 rmvCont(self) -> np.ndarray:
85     Removes the continuum from the spectrum.
86 skylines(self) -> None:
87     Placeholder method for processing skylines.
88 process(self) -> None:
89     Placeholder method for processing the data.
90 """

```



TODO: Include example of skyline result

Figure 3.12: The resultant output plot of the `STOPS skyline` method. Figure created via the `STOPS skyline` method.

tion, and compares the wavelength position of the sky lines to the reference sky lines as measured by SALT.

Firstly, determining if there is any inaccuracy in the wavelength solution in the spatial (y , or vertical) axis is relatively straightforward as a perfect wavelength solution will remove any horizontal variation of a sky line spanning multiple rows. The variation may be seen in the transformed frame, as mentioned in § 3.2.4, but is more accurately measured by the `skyline` method which compares the averaged sky line width before and after transformation. A wavelength solution exhibiting a poor fit across the spatial axis will display broader averaged sky lines than those of a relatively good fit.

Lastly, determining if there is any inaccuracy in the wavelength solution in the wavelength (x , or horizontal) axis is more challenging as no features, other than the trace of the observed sources, are exposed across a frame. Thankfully, SALT has published a sky line atlas which may be used to verify and measure the deviation of the observed sky line wavelength positions. Minor variations in the comparison of the sky lines are expected, but any uniform trends indicate an underlying poor fit across the horizontal axis of the wavelength solution. A poor horizontal fit is difficult to spot without supplementary tools and has adverse effect on the final polarization results.

3.3.4 Cross Correlation

The `skyline` method allows for confirmation of a single wavelength solution, but has no means for comparing how the wavelength solutions of two polarization beams differ from each other. As the Stokes results, and thus final polarization results, are determined and are heavily influenced by the differences in the spectra of the different O - and E -beams, a direct comparison is not appropriate. Any observed unpolarized light, however, will reflect equally in both polarization beams and so the general trend of the two spectra may reasonably be expected to follow one another. The `correlate` method was created to allow for comparisons between the wavelength solutions of the O - and E -beams of a single exposure or the O - or E -beams of differing exposures by cross correlating the spectra.

Listing 3.6: The ‘docstring’ for cross_correlate.py

```

34 """
35 Cross correlate allows for comparing the extensions of multiple
36 FITS files, or comparing the O and E beams of a single FITS file.
37
38 Parameters
39 -----
40 data_dir : str
41     The path to the data to be cross correlated
42 filenames : list[str]
43     The ecwmagbp*.fits files to be cross correlated.
44     If only one filename is defined, correlation is done against the two polarization beams.
45 split_ccd : bool, optional
46     Decides whether the CCD regions should each be individually cross correlated.
47     (The default is True, which splits the spectrum up into its separate CCD regions)
48 cont_ord : int, optional
49     The degree of a chebyshev to fit to the continuum.
50     (The default is 11)
51 plot : bool, optional
52     Decides whether or not the continuum fitting should be plotted
53     (The default is False, so no continua plots are displayed)
54 save_prefix : str, optional
55     The name or directory to save the figure produced to.
56     "" saves a default name to the current working. A default name is also used when save_prefix is a directory.
57     (The default is None, I.E. The figure is not saved, only displayed)
58
59 Attributes
60 -----
61 data_dir
62 fits_list
63 beams : str
64     The mode of correlation.
65     'OE' for same file, and 'O' or 'E' for different files but same ext's.
66 ccds : int
67     The number of CCD's in the data. Used to split the CCD's if split_ccd is True.
68 cont_ord : int
69     The degree of the chebyshev to fit to the continuum.
70 can_plot : bool
71     Decides whether or not the continuum fitting should be plotted
72 offset : int
73     The amount the spectrum is shifted, mainly to test the effect of the cross correlation
74     (The default is 0, I.E. no offset introduced)
75 save_prefix
76 wav_unit : str
77     The units of the wavelength axis.
78     (The default is Angstroms)
79 wav_cdel : int
80     The wavelength increment.
81     (The default is 1)
82 alt : Callable
83     An alternate method of cross correlating the data.
84     (The default is None)
85
86 Methods
87 -----
88 load_file(filename: Path) -> tuple[np.ndarray, np.ndarray, np.ndarray]
89     Loads the data from a FITS file.
90 get_bounds(bpm: np.ndarray) -> np.ndarray
91     Finds the bounds for the CCD regions.
92 remove_cont(spec: list, wav: list, bpm: list, plot_cont: bool) -> None
93     Removes the continuum from the data.
94 correlate(filename1: Path, filename2: Path | None = None) -> None
95     Cross correlates the data.
96 FTCS(filename1: Path, filename2: Path | None = None) -> None
97     Cross correlates the data using the Fourier Transform.
98 plot(spec, wav, bpm, corrdb, lagsdb) -> None
99     Plots the data.
100 process() -> None
101     Processes the data.
102
103 Other Parameters
104 -----
105 offset : int, optional
106     The amount the spectrum is shifted, mainly to test the effect of the cross correlation
107     (The default is 0, I.E. no offset introduced)
108 **kwargs : dict
109     keyword arguments. Allows for passing unpacked dictionary to the class constructor.
110 FTCS : bool, optional
111     Decides whether the Fourier Transform should be used for cross correlation.
112
113 See Also
114 -----
115 scipy
116     https://docs.scipy.org/doc/scipy/reference/generated/scipy.signal.correlate.html
117
118 Notes
119 -----
120 Constants Imported (See utils.Constants):
121     SAVE_CORR
122
123 """

```

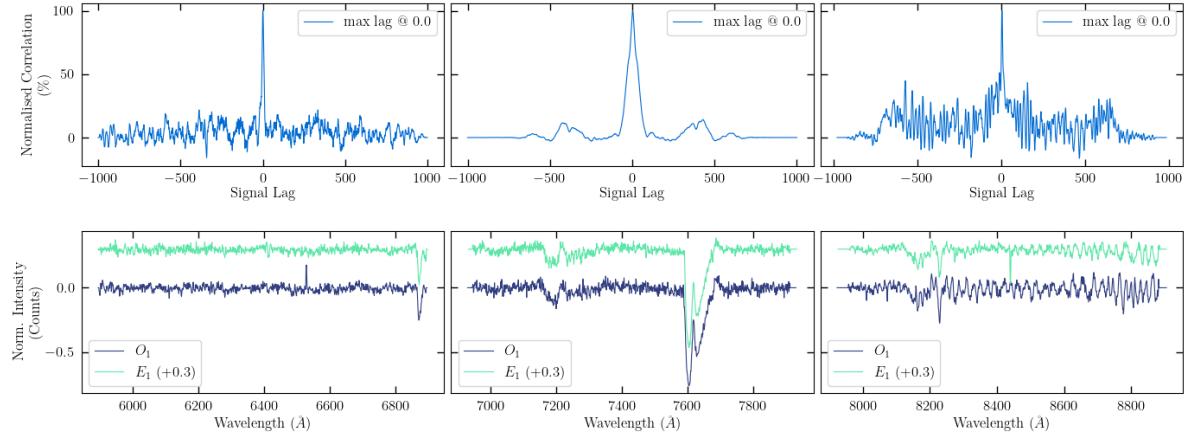


Figure 3.13: The resultant output plot of the `STOPS correlate` method. Figure created via the `STOPS correlate` method.

The `correlate` method loads the `POLSALT spectra extraction` FITS files, removes the continuum and separates the CCD regions. The relevant CCD regions are cross correlated and the correlation peak is plotted and specified in the plot legend, as seen in Figure 3.13.

Sources under spectropolarimetric observation are generally expected to vary over time and, as such, the ratio of polarized to unpolarized light is also expected to vary. The accuracy of correlation may decrease as features with differences in the polarized component of the polarization beams change, and it is up to the user to determine the validity of the correlation result taking into consideration the two spectra being correlated. The differences in the features of the different spectra are often negligible when compared to the overall continuum of the spectra and are generally only reflected in a change in the intensity of said features when the continuum is removed.

3.4 General Reduction Procedure

This section aims to provide a comprehensive discussion of the modified reduction procedure, an example of which is provided in Appendix I. As users all employ a variety of operating systems, language environments, and software setups, not much emphasis will be placed on how to get the software running or the managing of files: instead, the commands necessary to complete each step of the reduction process are discussed, assuming that the software is running as intended.

3.4.1 Initial Setup

It is important to note that while `POLSALT` was developed in Python 2.7, the `STOPS` supplementary tools were developed in, and require, Python 3.11+, as well as other requirements mentioned in § 3.3. While managing multiple versions of Python introduces some extra complication, it would not have been reasonable to develop `STOPS` in Python 2, as it is no longer supported, nor would it have been reasonable to update `POLSALT` to Python 3.

It is therefore recommended that the different versions of Python are managed using separate virtual environments. While the `anaconda` package manager was used in this

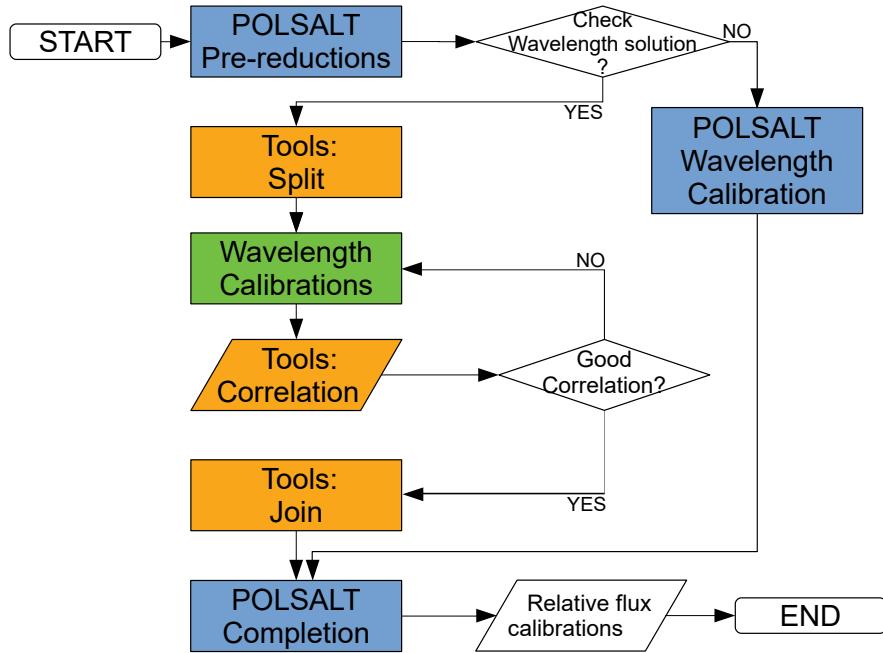


Figure 3.14: A general workflow for data reductions using a combination of POLSALT, IRAF, and the developed supplementary tools. Diagram adapted from Cooper et al. (2022).

study and is recommended, any package manager may be used. The `anaconda` environments are aliased ‘`salt`’ for Python 2.7 and ‘`stops`’ for Python 3.11. When Listings are provided (see for example Listing I.1 or the Listing in § 3.4.2 below), the `anaconda` environment is activated at the start of the Listing, otherwise it is assumed the previously specified environment is still active.

It is recommended to use POLSALT through the GUI as it provides a user-friendly environment while also sequentially listing each step of the reduction process in a dropdown menu, as seen in Figure 3.1. Reductions are possible, however, purely through the CLI using the POLSALT ‘beta’ scripts.

3.4.2 POLSALT Pre-Reductions

The POLSALT reduction process requires a file structure such that the raw data received from SALT is located in a folder named using the observing date with a sub-folder named `raw`, following the format `YYYYMMDD/raw/`. This directory structure allows POLSALT to create a ‘working’ directory following the format `YYYYMMDD/sci/` which contains all the files modified during the reduction process. Multiple reduction procedures using the same data may therefore be separated by simply renaming the `sci/` sub-folder.

The POLSALT GUI may be launched by opening a CLI and running the commands given in Listing I.1. Once the window, depicted in Figure 3.1, has launched, ensure that the first two paths at the top of the window point to the POLSALT and working directories, as seen in Figure 3.1. The ‘raw image reduction’ entry may then be selected from the dropdown menu and the pre-reductions run.

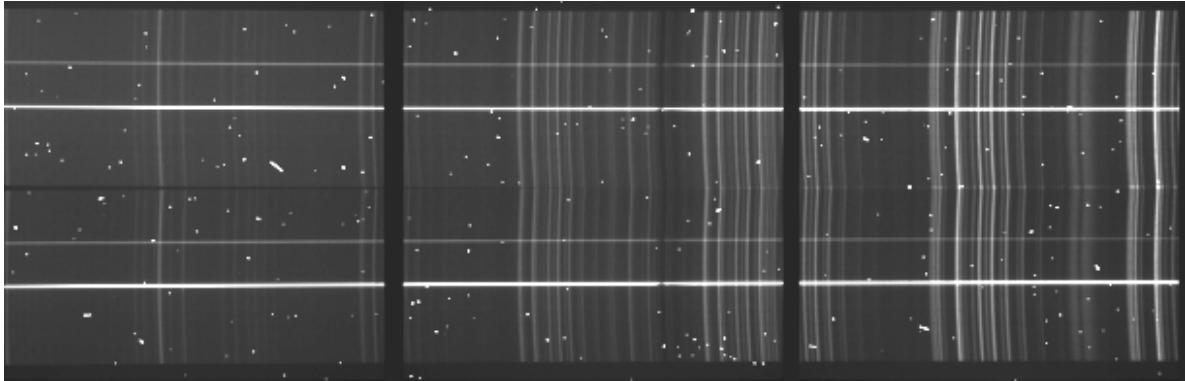


Figure 3.15: The science extension of a typical spectropolarimetric FITS file taken with the SALT RSS, after basic POLSALT CCD reductions have been completed. Figure created from the `STOPS split` output.

Alternatively, if the data already includes ‘mxgbp’ FITS files in the `YYYYMMDD/sci/` working directory, a CLI may be used to complete the initial pre-reductions using

```
$ cd <OBSDATE>/sci
$ conda activate salt
$ python ~/polsalt/scripts/reducepoldata_sc.py <OBSDATE>
```

which will start the full POLSALT reduction process. This process is quit once the POLSALT `wavelength calibration` GUI opens, and the alternate wavelength calibration procedure is followed.

3.4.3 Wavelength Calibration

The wavelength calibrations may now be completed in IRAF. This section concerns the procedure for parsing the FITS files to and from both IRAF and POLSALT, as well as the relevant task names and methods to be run to complete the calibrations. A base working case of each of the tasks and methods are presented in Listing I.2 to I.8, but it should be noted that the art of wavelength calibration consists of modifying the parameters to achieve a well-fit calibration function. This process depends heavily, and varies greatly, based on the user and as such not all use cases can be discussed.

Preparing the Data for IRAF

Splitting the data is presented in Listing I.2. The `STOPS split` method may take multiple parameters, as seen in § 3.3, but default parameters should be used wherever possible. The most notable parameters are the directory, which defaults to the current working directory of the CLI, the split row, which defaults to POLSALT’s default center row, and the save prefix, which defaults to ‘`obeam`’ and ‘`ebeam`’.

IRAF Wavelength Calibrations

The IRAF wavelength calibrations are performed using the tasks described in § 3.2, namely `identify`, `reidentify`, `fitcoords`, and optionally `transform`. In general, these tasks are run directly in the IRAF terminal using:¹⁸

¹⁸Please see the IRAF help docs, available at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/iraf.html, on the relevant tasks for a comprehensive discussion of the parameters available.

```
cl> identify arc_files
cl> reidentify arc_ref arc_files
cl> fitcoords arc_files fit_2d
cl> transform files tr_file fit_2d
```

where ‘arc_files’ refers to a list or file containing the FITS files relevant to the task, ‘arc_ref’ refers to the FITS file previously identified, ‘fit_2d’ refers to the name to be used for the final two-dimensional wavelength solution, and ‘tr_file’ refers to the new name for the transformed input ‘files’.

The interactive tasks take up the bulk of the reduction time as this is where the fine-tuning of the reduction is done, through the use of cursor (or colon) commands, which allow modification of the parameters mid-reduction. Task parameters may, however, be edited beforehand within the IRAF terminal using the `eparam` task, and optionally saved, and quit or run using a combination of `:w`, and `:q` or `:go` cursor commands, respectively.

The reduction process in Appendix I, namely Listing I.4 to I.7, describes how to script the tasks for posterity. It is recommended to create an IRAF Command Language (cl) script for each task to keep track of which parameters were used and for simple recalibrations. The scripts are created using the `mkscrip` task which interactively asks for a task to script and parameters to use. Multiple tasks may be appended to an IRAF script, allowing for the parameters of both beams to be tracked. Running an IRAF script may be done by running:

```
cl> cl < script_name.cl
```

but is not suggested for interactive scripts, which run best when simply copied from the `<...>/sci/script_name.cl` file to the IRAF terminal.

Preparing the Data for POLSALT

After the wavelength calibrations have been completed, the wavelength solution is parsed back into the format expected by POLSALT. Joining the separate beams with their respective wavelength solutions is performed in the CLI following Listing I.8.

Similar to the `split` procedure, the `join` procedure has the same defaults defined. The onus of keeping track of any previously changed default parameters falls to the user, but logging is implemented in STOPS see § 3.3, which allows for later reference of any changed parameters.

Sky Line Checks

The optional IRAF `transform` task and STOPS `skylines` method are used to confirm the wavelength solution across the frame (see § 3.3.3) by transforming and comparing known and observed sky line wavelength positions, respectively.

The `skyline` method is run in the CLI following Listing I.9. The difference in the flux conservation when `skyline` transforms the frames is discussed in § 3.3.3. Otherwise, as with the rest of STOPS, default parameters describe the overplotting behavior for the *O*- and *E*-beams, the skylines provided by SALT, and the calculated variation of the wavelength axis of a frame.

Cross Correlation Checks

The `correlate` method is run in the CLI following Listing I.11. The input of the `correlate` method takes the output of the POLSALT `spectra extraction` and is thus only run thereafter, but is mentioned here as the completion of the POLSALT reductions is not discussed in much depth. If the user wishes to compare the *O*- and *E*-beams of a single file then only that image name is to be provided, otherwise it is assumed that the user wishes to compare the same polarization beam across each file provided.

Cleaning Up the IRAF and STOPS Output

Before the final POLSALT reductions, it is recommended that the user ‘clean up’ the `sci/` directory of all IRAF and STOPS files since the ‘wmxgbp’ FITS files are all that is expected by POLSALT. The POLSALT methods use wildcard file collection and as such any errant detections of files added by the user will result in unexpected crashes. It is suggested to move any additional files to a new subfolder following Listing I.10, but a remove command may also be used, for example, following:

```
$ rm beam0* beamE* arc0* arcE*
```

3.4.4 POLSALT Reduction Completion

Reductions may now be completed using POLSALT. The reduction process consists of correcting for the wollaston tilt, extracting the spectra, creating the Stokes files, and displaying the results. The ‘beta’ version of POLSALT provides access to a GUI but may also be handled entirely through a CLI as scripts.

POLSALT Beta in the GUI

The reduction process using the POLSALT GUI is completed by selecting and, when applicable, interactively modifying the reduction step through the interactive windows, one-by-one, from the GUI’s dropdown menu, as explained in Appendix I (p. 67 onwards).¹⁹

POLSALT Beta through a CLI

Both GUI and CLI implementations of the POLSALT beta pipeline access the same script files. Although the GUI is more user-friendly, the CLI offers a more streamlined approach to the reduction process, allowing the reduction process to be automated once the IRAF wavelength solution is known and parsed into the ‘wmxgbp’ FITS file format. A modified version of the POLSALT beta `reducepoldata_sc.py` script (see Listing 3.7) is used to run the entire reduction process without needing to select which process to run next, using:

```
$ python reducepoldata_sc.py YYYYMMDD
```

where the only modification made to the `reducepoldata_sc.py` script file is the removal of a call to the `specpolwavmap` method.

¹⁹See the official POLSALT wiki or alternative online resources such as the SALT workshop slides.

Listing 3.7: The modified `reducepoldata_sc.py` script file.

```

import os, sys, glob, shutil
poldir = '/home/justin/polsalt-beta/'                                     # Will differ according to user
reddir=poldir+'polsalt/'
scrdir=poldir+'scripts/'
sys.path.extend((reddir,scrdir,poldir))

datadir = reddir+'data/'
import numpy as np
from astropy.io import fits as pyfits
from specpolview import printstokes
from imred import imred
from specpolwvmap import specpolwvmap
from specpolextract_sc import specpolextract_sc
from specpolrawstokes import specpolrawstokes
from specpolfinalstokes import specpolfinalstokes

print sys.argv
obsdate = sys.argv[1]
print obsdate
os.chdir(obsdate)
if not os.path.isdir('sci'): os.mkdir('sci')
shutil.copy(scrdir+'script.py','sci')
os.chdir('sci')

# basic image reductions
infilelist = sorted(glob.glob('../raw/P*fits'))
imred(infilelist, './', datadir+'bpm_rss_11.fits', crthresh=False, cleanup=True)

# basic polarimetric reductions
logfile='specpol'+obsdate+'.log'                                         # The following lines may be removed or commented out as below

# wavelength map
# infilelist = sorted(glob.glob('m*fits'))
# linelistlib=""
# specpolwvmap(infilelist, linelistlib=linelistlib, logfile=logfile)

#background subtraction and extraction
infilelist = sorted(glob.glob('wm*fits'))
extract = 10.    # star +/-5, bkg=+/- (25-35) arcsec: 2nd order is 9-20 arcsec away
locate = (-120.,120.)      # science target is brightest target in whole slit
#locate = (-20.,20.)

specpolextract_sc(infilelist,logfile=logfile,locate=locate,extract=extract)
#specpolextract_sc(infilelist,logfile=logfile,locate=locate,extract=extract, docomp=True, useoldc=True)

# raw Stokes
infilelist = sorted(glob.glob('e*fits'))
specpolrawstokes(infilelist, logfile=logfile)

# final Stokes
infilelist = sorted(glob.glob('*_h*.fits'))
specpolfinalstokes(infilelist, logfile=logfile)

```

The POLSALT beta `reducepoldata_sc.py` copies a `script.py` file into the science working directory, ‘YYYYMMDD/sci/’, which provides analysis scripts for analysis and modification of the POLSALT beta results. These tools consist of data culling for the final Stokes calculations, text and plot output, relative flux calibration corrections, and synthetic filtering of polarization results. The POLSALT analysis scripts may be run using:

```
$ python script.py
```

followed by `specpolfinalstokes.py`, `specpolview.py`, `specpolflux.py`, or `specpolfilter.py`, for the different analysis modes, respectively.²⁰

²⁰Please see <https://github.com/saltastro/polsalt/wiki/Linear-Polarization-Reduction>.
--Beta-version for a comprehensive discussion of the POLSALT beta analysis scripts.

Chapter 4

Testing and Application

Short intro to chapter contents.

- No POLSALT or data tests
 - POLSALT is trusted to be accurate. See ... (reference tests of POLSALT)
- Testing `split`
 - POLSALT to IRAF file structure conversion.
 - Show changes to data files are intended (I.E. only splitting the data, no changes to the data itself)
 - Tested over multiple grating/articulation angles to ensure robustness.
 - Mention any header updates skipped specific to POLSALT (if any)
 - Figure showing split fits file contents difference (cropped rows shown, etc.)
- Testing IRAF wavelength solution
 - IRAF is trusted to be accurate. See ... (reference tests of IRAF)
 - The `skylines` and `correlate` outputs are tests of the wavelength calibration.
 - * Testing correlate functionality using ‘offset’, comparisons of arcs, FSRQ’s and BLLac’s.
 - * Any figures showing correlation tests?
 - * Testing skylines using known spectral sky lines.
 - * Any figures showing skyline tests?
- Testing `join`
 - IRAF to POLSALT file structure conversion
 - Show changes to data files are intended (I.E. only joining the data, and ‘WAV’ appended. No changes to the data itself)
 - Wollaston correction of wavelength and bpm extensions
 - update to python 3 of ‘polsalt’ functions
 - Mention any header differences (if any)
 - Figure showing joined fits file contents difference (cropped rows shown once again, bpm differences due to CRR and NO wollaston bpm differences, etc.)
- Testing reduction results not negatively impacted by STOPS.
 - General discussion of testing (I.E. not this test was done specifically this source, more along the lines of these tests were done to check this issue, seen here using this source for example.)

- Wavelength solution validation from correlate and skylines results.
 - * Figures showing Correlate and Skyline results.
 - * RMS comparisons between POLSALT and IRAF to quantify differences.
 - * Any Figures for RMS comparisons or wavelength validation?
- Polarization parameters validation from known sources.
 - * Polarization tested using 3C 279, 4C+01.02, and preliminary testing data provided by David.
 - * Polarization tested using spectropolarimetric standards (4 highly polarized, 2 non-polarized).
 - * Tabulate sources used, with their properties.
 - * Figures showing comparison plots of polarization parameters from POLSALT and STOPS.
- Background information on each object.
- Detailed reductions steps performed on each object.
- Comparison of POLSALT results to those obtained using the STOPS pipeline.
- Application to Spectropolarimetric Standards
 - Science results, what the results can tell us and why it is useful, also comparison of results to FORS1/2 published data, focus on the polarization results.
- Application in Publications
 - Summarize the results of the publications appended to appendix.

Chapter 5

Science Applications

TODO: Short introduction to chapter contents

5.1 Application to Spectropolarimetric Standards

TODO: Spectropolarimetric standards (4 highly polarized, 2 non-polarized)

- (Same as ch04 with science results)
- Background on objects
- Reductions
- Actual results - comparison of polsalt results to supplementary pipeline results
- Science results, what the results can tell us and why it is useful, also comparison of results to FORS1/2 published data, focus on the polarization results

5.2 Application in Publications

TODO: Summary of results from papers in appendix.

- Hester paper(s)
- Joleen proceedings and work
- My proceedings

TODO: 3C 279 and 4C+01.02

- Give Background on objects, Reduction steps, and Science results (what the results can tell us and why it is useful)
- (comparison of polsalt results to supplementary pipeline results will be in testing)

Chapter 6

Conclusions

TODO: A summary of the dissertation, main focus on the results and that the supplementary pipeline is a success since it allows an alternate method using IRAF to wavelength calibrate the polsalt data.

6.1 Future Work

TODO: Edit paragraph below to mention python wavelength solutions implemented to ‘future-proof’ the pipeline.

Another option to perform the wavelength calibration is Python which allows for a more modern and flexible approach, but is not discussed here. What will be discussed, however, is the structure of the wavelength solutions created through Python to be later reintroduced to the POLSALT pipeline. The solutions must be stored such that the ‘ x ’ and ‘ y ’ orders of the solution, as well as all the coefficients (C_{00} to C_{xy}) making up the solution, separated by new lines, are included. The only limitations to the names of the solution files is that they must make mention of the specific O - or E -beam as well as the wavelength solution type (e.g. ‘Chebyshev’, ‘Legendre’, etc.).

Appendix I

The Modified Reduction Process

This section of the Appendix aims to provide a minimum working example of the commands necessary to reduce POLSALT data using STOPS and IRAF. It contains the commands necessary to activate all software and run through the reduction process but makes no attempt at discussion.

Both POLSALT and IRAF are launched from the default CLI but use independent interfaces during the reduction process. To distinguish which window is in focus, the ‘\$’ token is used for default CLI commands while the ‘c1>’ and ‘>>>’ tokens are used for IRAF’s ‘xgterm’ single- and multi-line commands, respectively.

General instructions for the reduction process which might not necessarily be line-fed commands passed to a CLI may either be discussed outside a ‘Listing’ environment or included as part of the ‘Listing’ environment with a preceding ‘#’ token. Finally, POLSALT implements a GUI and thus takes no line-fed commands. As such, the instructions when using the POLSALT GUI follow those of the general instructions with the added exception that they relate to the GUI.

As a final note, some parameters are distinguished using an ‘<angle brackets>’ notation. They signify necessary parameters that may vary from reduction to reduction. Notable uses of this notation include the date of observation, $\langle OBSDATE \rangle$ (formatted ‘YYYYMMDD’), the split science FITS files, $\langle O\text{-beam FILES} \rangle$ or $\langle E\text{-beam FILES} \rangle$, the split arc FITS files, $\langle O\text{-beam ARC} \rangle$ or $\langle E\text{-beam ARC} \rangle$, and a wildcard symbol, $\langle * \rangle$.

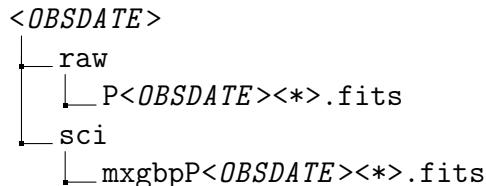


Figure I.1: The typical minimal file structure of data provided by SALT.

Ensure the data is formatted in a file structure similar to that in Figure I.1. Data located in the ‘sci’ folder is often provided by SALT but is not strictly necessary to begin the reduction process. If ‘mxgbp’ prefixed data is available, the reductions may be begun starting at Listing I.2. The POLSALT GUI is launched from the default CLI running the commands in Listing I.1.

Listing I.1: Launching the POLSALT GUI

```
$ cd ~/polsalt
$ conda activate salt
$ python -W ignore reducepoldataGUI.py &
```

Refer to Figure 3.1 for a depiction of the POLSALT GUI. To complete the POLSALT pre-calibrations, and with the GUI in focus:

- Ensure that the ‘POLSALT code directory’ is correct.
- Set the ‘Top level data directory’ to $\langle OBSDATE \rangle$.
- Ensure ‘Raw data directory’ is correct.
- Ensure ‘Science data directory’ is correct.
- Select ‘Raw image reduction’ from the ‘Data reduction step’ drop down menu.
- Check the tick boxes of all raw images to be processed (include the arc) in the display box covering the lower half of the GUI.
- Proceed with the reductions by clicking the ‘OK’ button.

The pre-calibrated ‘mxgbp’ FITS files are now available in the ‘sci’ folder. The files may be split using STOPS by running the commands in Listing I.2.

Listing I.2: Splitting data using STOPS

```
$ cd <OBSDATE>/sci
$ conda activate stops
$ python ~/STOPS . split
```

The split *O*- and *E*-beam FITS files are now available. The IRAF wavelength calibrations are now run. The IRAF xgterm CLI is launched using Listing I.3.

Listing I.3: Launching IRAF in xgterm

```
$ cd ~/iraf
$ xgterm -sb &
cl> conda activate salt
cl> cl
cl> noao
cl> twodspec
cl> longslit
cl> unlearn longslit
cl> longslit.dispaxis=1
```

The IRAF `identify` task requires an average feature width, ‘fwidth’, as a parameter. The width of a feature may be found in IRAF using the `implot` task¹ along with cursor

¹See https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/plot.implot.html for documentation on the `implot` task.

commands, but may also be found using FITS viewing software, such as `ds9`.² The `identify` task may be run using the commands in Listing I.4.

Listing I.4: Running the IRAF `identify` task

```
cl> mkscript 01_identify.cl
cl> # Add identify to 01_identify.cl twice, for both beams
cl> # Edit the parameters of 01_identify.cl in a text editor
cl> # Paste an identify script into the CLI, resulting in:
cl>
cl> identify ("<O-beam ARC>",
>>> "", "", section="middle line", database="database",
>>> coordlist="linelists$idheneare.dat", units="", nsum="10", match=-3.,
>>> maxfeatures=50, zwidth=100., ftype="emission", fwidth=8.,
>>> cradius=5., threshold=0., minsep=2., function="spline3", order=2,
>>> sample="*", niterate=0, low_reject=3., high_reject=3., grow=0.,
>>> autowrite=no, graphics="stdgraph", cursor="", aidpars="")
```

The `identify` task will launch an interactive window. Cursor commands refer to keys that provide unique functionality to the interactive IRAF tasks. The cursor commands for `identify` allow the arc lines to be identified using ‘m’ (and typing the relevant wavelength), while ‘d’ and ‘i’ will delete a single and all identified arc lines, respectively. The ‘f’ cursor command will perform a preliminary fit which can be quit using the ‘q’ cursor command. The ‘l’ cursor command will attempt to identify any unidentified arc lines. Once complete, a figure of the identified lines may be saved using ‘:labels coord’ and ‘:.snap eps’, and the task safely quit with the ‘q’ cursor command.³ The `identify` procedure is repeated, replacing `<O-beam ARC>` with `<E-beam ARC>`.

The `reidentify` task may be run using the commands in Listing I.5.

Listing I.5: Running the IRAF `reidentify` task

```
cl> mkscript 02_reidentify.cl
cl> # Add reidentify to 02_reidentify.cl twice, for both beams
cl> # Edit the parameters of 02_reidentify.cl in a text editor
cl> # Paste a reidentify script into the CLI, resulting in:
cl>
cl> reidentify ("<O-beam ARC>",
>>> "<O-beam ARC>", "yes", "", "", interactive="no", section="middle
>>> line", newaps=yes, override=no, refit=yes, trace=yes, step="10",
>>> nsum="10", shift="0.", search=0., nlost=0, cradius=5.,
>>> threshold=0., addfeatures=no, coordlist="linelists$idheneare.dat",
>>> match=-3., maxfeatures=50, minsep=2., database="database",
>>> logfiles="logfile", plotfile="", verbose=yes, graphics="stdgraph",
>>> cursor="", aidpars="")
```

The `reidentify` task will run autonomously so long as the `interactive` parameter is set to “no”.⁴ Repeat the `reidentify` procedure, replacing `<O-beam ARC>` with `<E-beam ARC>` at both the ‘reference’ and ‘image’ parameter locations.

²See <https://sites.google.com/cfa.harvard.edu/saoimageds9> for documentation on the `ds9` software.

³See https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.onedspec.identify.html for documentation on the `identify` task.

⁴See https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.onedspec.reidentify.html for documentation on the `reidentify` task.

The `fitcoords` task may be run using the commands in Listing I.6.

Listing I.6: Running the `IRAF fitcoords` task

```
cl> mkscript 03_fitcoords.cl
cl> # Add fitcoords to 03_fitcoords.cl twice, for both beams
cl> # Edit the parameters of 03_fitcoords.cl in a text editor
cl> # Paste a fitcoords script into the CLI, resulting in:
cl>
cl> fitcoords ("<O-beam ARC> (exclude the file extension)",
>>> fitname="", interactive=yes, combine=no, database="database",
>>> deletions="deletions.db", function="chebyshev", xorder=6, yorder=6,
>>> logfiles="STDOUT,logfile", plotfile="plotfile",
>>> graphics="stdgraph", cursor="")
```

The `fitcoords` task will launch an interactive window. The x- and y-axis being plotted may be changed using the ‘x’ or ‘y’ cursor commands followed by the desired data axis (‘x’ for the x-axis, ‘y’ for the y-axis, or ‘r’ for the residuals).⁵ Repeat the `fitcoords` procedure, replacing $<O\text{-beam } ARC>$ with $<E\text{-beam } ARC>$.

The `transform` task may be run using the commands in Listing I.7.

Listing I.7: Running the `IRAF transform` task

```
cl> mkscript 04_transform.cl
cl> # Add transform to 04_transform.cl twice, for both beams
cl> # Edit the parameters of 04_transform.cl in a text editor
cl> # Paste a transform script into the CLI, resulting in:
cl>
cl> transform ("@<O-beam FILES>",
>>> "t//@<O-beam FILES>", "<O-beam ARC> (exclude the file extension)",
>>> minput="", moutput="", database="database", interptype="linear",
>>> x1="INDEF", x2="INDEF", dx="INDEF", nx="INDEF", xlog="no",
>>> y1="INDEF", y2="INDEF", dy="INDEF", ny="INDEF", ylog="no",
>>> flux="yes", blank="INDEF", logfiles="STDOUT,logfile")
```

Inspect the transformed images, most notably the arc images, using any FITS viewer as a cursory check that the wavelength calibrations were completed without error.⁶

The ‘gain’ and ‘read noise’ are now needed as the cosmic-ray rejection of the STOPS `join` method accepts them as parameters. These parameters may be found using the ‘*GAINSET*’ and ‘*ROSPEED*’ keywords in the FITS headers. The cosmic ray rejection defaults to *GAINSET*=‘FAINT’, and *ROSPEED*=‘SLOW’. If the gain and read noise values differ from the defaults, the parameters should be updated when running `join`.⁷

⁵See https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.twodspec.longslit.fitcoords.html for documentation on the `fitcoords` task.

⁶See https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.twodspec.longslit.transform.html for documentation on the `transform` task.

⁷The read noise and gain may be determined from http://pysalt.salt.ac.za/proposal_calls/current/ProposalCall.html, specifically Table 6.1 and Table 6.2.

The STOPS `join` method may be run using the commands in Listing I.8.

Listing I.8: Joining the data using STOPS

```
$ cd <OBSDATE>/sci
$ conda activate stops
$ python ~/STOPS . join
```

The STOPS `skylines` method may be run on any ‘joined’ or transformed FITS files, $\langle FILE(S) \rangle$, using the commands in Listing I.9.

Listing I.9: Running the STOPS `skylines` method

```
$ cd <OBSDATE>/sci
$ conda activate stops
$ python ~/STOPS . skylines <FILE(S)>
```

The ‘`sci/`’ directory may now be slightly organized by running the commands in Listing I.10, moving all the files relevant to the wavelength calibrations into either the ‘`database`’ or ‘`split_files`’ directories.

Listing I.10: Directory cleanup for POLSALT

```
$ cd <OBSDATE>/sci
$ mkdir split_files
$ mv *beam0* *beamE* *arc0* *arcE* split_files/
$ mv *.eps *.cl *.db database/
```

The POLSALT `spectra extraction` is now run. If the POLSALT GUI was closed it should now be reopened using Listing I.1. With the GUI in focus:

- Ensure all directories are still correct.
- Select ‘Spectra extraction’ from the ‘Data reduction step’ drop down menu.
- Check the tick boxes of all wavelength calibrated images to be processed (exclude the arc) in the display box covering the lower half of the GUI.
- Proceed with the reductions by clicking ‘OK’.

The POLSALT `spectra extraction` is interactive and will launch a separate GUI for the background subtraction and spectral extraction (see Figure 3.2). The background and spectral regions to be extracted may be adjusted, noting that adjustments affect both *O*- and *E*-beams. Once both background regions contain no trace and the spectral region fully contains only the science trace, the reduction may be completed by clicking ‘OK’.

The STOPS `correlate` method may now be run on any ‘joined’ FITS files by running the commands in Listing I.11.

Listing I.11: Running the STOPS `correlate` method

```
$ cd <OBSDATE>/sci
$ conda activate stops
$ python ~/STOPS . correlate <FILE(S)>
```

The POLSALT **raw Stokes calculation**, **final Stokes calculation**, and **results visualisation** may now be completed. For the last time, if the POLSALT GUI was closed it should now be reopened using Listing I.1. With the GUI in focus:

- Ensure all directories are still correct.
- Select ‘Raw Stokes calculation’ from the ‘Data reduction step’ drop down menu.
- Check the tick boxes of all the extracted spectra images to be processed in the display box covering the lower half of the GUI.
- Proceed with the **raw Stokes calculation** by clicking ‘OK’.
- Select ‘Final Stokes calculation’ from the ‘Data reduction step’ drop down menu.
- Check the tick boxes of all the “raw Stokes” images to be processed in the display box covering the lower half of the GUI.
- Proceed with the **Final Stokes calculation** by clicking ‘OK’.
- Select ‘Results visualisation - interactive’ from the ‘Data reduction step’ drop down menu.
- Check the tick boxes of the “final Stokes” image to be visualized in the display box covering the lower half of the GUI.
- Proceed with the **visualisation** by clicking ‘OK’.

The POLSALT **visualisation** is interactive and will launch a separate GUI (See Figure 3.3). The GUI may be used to change the binning and parameters of the plot before saving the plot to a PDF file.

This concludes the minimum working example of the POLSALT reduction process when substituting the POLSALT **wavelength calibrations** with those done in IRAF. Aside from the final results, the file structure after reductions should resemble something akin to that provided in Figure I.2.

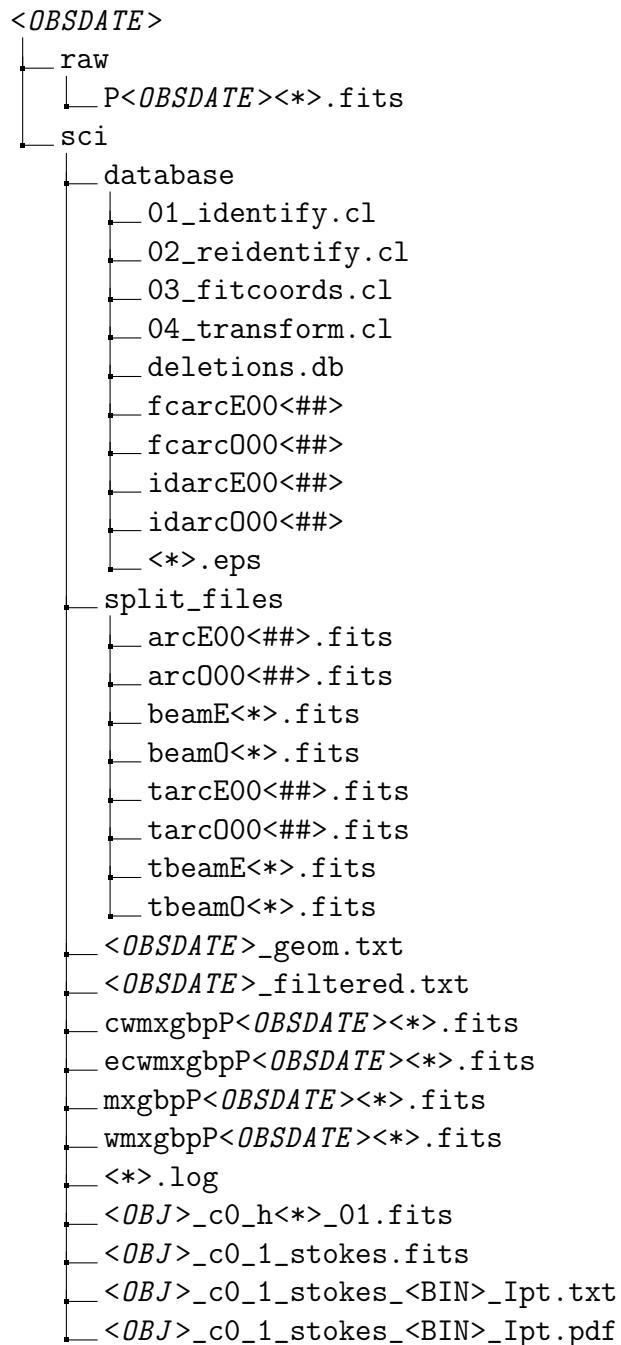


Figure I.2: The typical file structure after completing the reduction process.

Appendix II

STOPS Source Code

This section of Appendix includes all the major STOPS source code files related to the reduction process. Files such as those related to python initialization, testing directories, and other non-essential modules have been excluded for brevity and clarity.

Listing II.1: The source code for `__main__.py`

```
1 """Argument parser for STOPS."""
2
3 #!/usr/bin/env python3
4 # -*- coding: utf-8 -*-
5
6 from __init__ import __version__, __author__, __email__
7
8 # MARK: Imports
9 import os
10 import sys
11 import argparse
12 import logging
13 from pathlib import Path
14
15 from split import Split
16 from join import Join
17 from cross_correlate import CrossCorrelate
18 from skylines import Skylines
19
20 from utils import ParserUtils as pu
21 from utils.Constants import SPLIT_ROW, PREFIX, PARSE, SAVE_CORR,
22   ↪ SAVE_SKY
23
24 # MARK: Constants
25 PROG = "STOPS"
26 DESCRIPTION = """
27 Supplementary Tools for Polsalt Spectropolarimetry (STOPS) is a
28 collection of supplementary tools created for SALT's POLSALT pipeline,
29 allowing for wavelength calibrations with IRAF. The tools provide
30 support for splitting and joining polsalt formatted data as well as
31 cross correlating complementary polarimetric beams.
32 DOI: 10.22323/1.401.0056
```

```

33 """
34
35
36 # MARK: Universal Parser
37 parser = argparse.ArgumentParser(
38     prog=PROG,
39     description=DESCRIPTION,
40     formatter_class=argparse.RawDescriptionHelpFormatter,
41 )
42 parser.add_argument(
43     "-V",
44     "--version",
45     action="version",
46     version=f"%(prog)s as of {__version__}",
47 )
48 parser.add_argument(
49     "-v",
50     "--verbose",
51     action="count",
52     default=PARSE['VERBOSE'],
53     help=(
54         "Counter flag which enables and increases verbosity. "
55         "Use -v or -vv for greater verbosity levels."
56     ),
57 )
58 parser.add_argument(
59     "-l",
60     "--log",
61     action="store",
62     type=pu.parse_logfile,
63     help=(
64         "Filename of the logging file. "
65         "File is created if it does not exist. Defaults to None."
66     ),
67 )
68 parser.add_argument(
69     "data_dir",
70     action="store",
71     nargs="?",
72     default=PARSE['DATA_DIR'],
73     type=pu.parse_path,
74     help=(
75         "Path of the directory which contains the working data. "
76         f"Defaults to the cwd -> '{PARSE['DATA_DIR']}' (I.E. '.')."
77     ),
78 )
79
80
81 # MARK: Split\Join Parent
82 split_join_args = argparse.ArgumentParser(add_help=False)
83 split_join_args.add_argument(
84     "-n",
85     "--no_arc",
86     action="store_true",
87     help="Flag to exclude arc files from processing.",
88 )
89 split_join_args.add_argument(
90     "-s",

```

```

91     "--split_row",
92     default=SPLIT_ROW,
93     type=int,
94     help=(
95         "Row along which the O and E beams are split. "
96         f"Defaults to polsalt's default -> {SPLIT_ROW}.""
97     ),
98 )
99 split_join_args.add_argument(
100    "-p",
101    "--save_prefix",
102    nargs=2,
103    default=PREFIX,
104    help=(
105        "Prefix appended to the filenames, "
106        "with which the O and E beams are saved. "
107        f"Defaults to {PREFIX}.""
108    ),
109 )
110
111
112 # MARK: Correlate\Skylines Parent
113 corr_sky_args = argparse.ArgumentParser(add_help=False)
114 corr_sky_args.add_argument(
115    "filenames",
116    action="store",
117    nargs="+",
118    type=pu.parse_file,
119    help=(
120        "File name(s) of FITS file(s) to be processed."
121        "A minimum of one filename is required."
122    ),
123 )
124 corr_sky_args.add_argument(
125    "-b",
126    "--beams",
127    choices=["O", "E", "OE"],
128    type=str.upper,
129    default=PARSE['BEAMS'],
130    help=(
131        "Beams to process. "
132        f"Defaults to {PARSE['BEAMS']}, but "
133        "may be given 'O', 'E', or 'OE' to "
134        "determine which beams are processed."
135    ),
136 )
137 corr_sky_args.add_argument(
138    "-ccd",
139    "--split_ccd",
140    action="store_false",
141    help=(
142        "Flag to NOT split CCD's. "
143        "Recommended to leave off unless the chip gaps "
144        "have been removed from the data."
145    ),
146 )
147 corr_sky_args.add_argument(
148    "-c",

```

```

149     "--continuum_order",
150     type=int,
151     default=PARSE['CONT_ORD'],
152     dest="cont_ord",
153     help=(
154         "Order of continuum to remove from spectra. "
155         "Higher orders recommended to remove most variation, "
156         "leaving only significant features."
157     ),
158 )
159 corr_sky_args.add_argument(
160     "-p",
161     "--plot",
162     action="store_true",
163     help="Flag for additional plot outputs.",
164 )
165 corr_sky_args.add_argument(
166     "-s",
167     "--save_prefix",
168     action="store",
169     nargs="?",
170     type=lambda path: Path(path).expanduser().resolve(),
171     const=SAVE_CORR,
172     help=(
173         "Prefix used when saving plot. "
174         "Excluding flag does not save output plot, "
175         f"flag usage of option uses default prefix, "
176         "and a provided prefix overwrites default prefix."
177     ),
178 )
179
180
181 # MARK: Create subparser modes
182 subparsers = parser.add_subparsers(
183     dest="mode",
184     help="Operational mode of supplementary tools",
185 )
186
187
188 # MARK: Split Subparser
189 split_parser = subparsers.add_parser(
190     "split",
191     aliases=["s"],
192     help="Split mode",
193     parents=[split_join_args],
194 )
195 # 'children' split args here
196 # Change defaults here
197 split_parser.set_defaults(
198     mode="split",
199     func=Split,
200 )
201
202
203 # MARK: Join Subparser
204 join_parser = subparsers.add_parser(
205     "join",
206     aliases=["j"],

```

```

207     help="Join mode",
208     parents=[split_join_args],
209 )
210 # 'children' join args here
211 join_parser.add_argument(
212     "-c",
213     "--coefficients",
214     dest="solutions_list",
215     nargs='*',
216     type=pu.parse_file,
217     help=(
218         "Custom coefficients to use instead of the `IRAF` fitcoords "
219         "database. Use as either '-c <o_solution> <e_solution>' or "
220         "a regex descriptor '-c <*solution*extention>'."
221     ),
222 )
223 # Change defaults here
224 join_parser.set_defaults(
225     mode="join",
226     func=Join,
227 )
228
229
230 # MARK: Correlate Subparser
231 corr_parser = subparsers.add_parser(
232     "correlate",
233     aliases=["x"],
234     help="Cross correlation mode",
235     parents=[corr_sky_args],
236 )
237 # 'children' join args here
238 corr_parser.add_argument(
239     "-o",
240     "--offset",
241     type=int,
242     default=PARSE['OFFSET'],
243     help=(
244         "Introduces an offset when correcting for "
245         "known offset in spectra or for testing purposes. "
246         f"Defaults to {PARSE['OFFSET']}. "
247         "(For testing, not used during regular operation.)"
248     ),
249 )
250 # Change defaults here
251 corr_parser.set_defaults(
252     mode="correlate",
253     func=CrossCorrelate,
254 )
255
256
257 # MARK: Skyline Subparser
258 sky_parser = subparsers.add_parser(
259     "skylines",
260     aliases=["sky"],
261     help="Sky line check mode",
262     parents=[corr_sky_args],
263 )
264 # 'children' skyline args here

```

```

265 sky_parser.add_argument(
266     "-t",
267     "--transform",
268     action="store_false",
269     help=(
270         "Flag to force transform images. "
271         "Recommended to use only when input image(s) "
272         "are prefixed 't' but are not yet transformed."
273     ),
274 )
275 # Change defaults here
276 sky_parser.set_defaults(
277     mode="skyline",
278     func=Skylines,
279 )
280
281
282 # MARK: Keyword Clean Up
283 args = parser.parse_args()
284
285 if len(sys.argv) == 1:
286     parser.print_help(sys.stderr)
287     sys.exit(2)
288
289 args.verbose = pu.parse_loglevel(args.verbose)
290
291 if 'log' in args and args.log not in [None]:
292     args.log = args.data_dir / args.log
293
294 if "filenames" in args:
295     args.filenames = pu.flatten(args.filenames)
296
297 if "solutions_list" in args and type(args.solutions_list) == list:
298     args.solutions_list = pu.flatten(args.solutions_list)
299
300 # MARK: Begin logging
301 logging.basicConfig(
302     filename=args.log,
303     format"%(asctime)s - %(module)s - %(levelname)s - %(message)s",
304     datefmt="%Y-%m-%d %H:%M:%S",
305     level=args.verbose,
306 )
307
308 # MARK: Call Relevant Class(Args)
309 logging.debug(f"Argparse namespace: {args}")
310 logging.info(f"Mode:{args.mode}")
311 args.func(**vars(args)).process()
312
313
314 # Confirm all processes completed and exit without error
315 logging.info("All done! Come again!\n")

```

Listing II.2: The source code for `split.py`

```

51     -----
52     arc : str
53         Name of arc FITS file within `data_dir`.
54         `arc` = `""` if `no_arc` or not detected in `data_dir`.
55     o_files, e_files : list[str]
56         A list of the `O`- and `E`-beam FITS file names.
57         The first entry is the arc file if `arc` defined.
58     data_dir
59     fits_list
60     split_row
61     save_prefix
62
63     Methods
64     -----
65     split_file(file: os.PathLike)
66         -> tuple[astropy.io.fits.HDUList]
67             Handles creation and saving the separated FITS files
68     split_ext(hdulist: astropy.io.fits.HDUList, ext: str = 'SCI')
69         -> astropy.io.fits.HDUList
70             Splits the data in the `ext` extension along the `split_row`.
71     crop_file(hdulist: astropy.io.fits.HDUList, crop: int =
72         ↪ CROP_DEFAULT (See Notes))
73         -> tuple[numpy.ndarray]
74             Crops the data along the edge of the frame, that is,
75             `O`-beam cropped as [crop:], and
76             `E`-beam cropped as [: - crop].
77     update_beam_lists(o_name: str, e_name: str)
78         -> None
79             Updates `o_files` and `e_files`.
80     save_beam_lists(file_suffix: str = 'frames')
81         -> None
82             Creates (Overwrites if exists) and writes the `o_files` and `e_files` to files named
83             `o_{file_suffix}` and `e_{file_suffix}`, respectively.
84     process()
85         -> None
86             Calls `split_file` and `save_beam_lists` on each file in `fits_list` for automation.
87
88     Other Parameters
89     -----
90     **kwargs : dict
91         keyword arguments. Allows for passing unpacked dictionary to
92             ↪ the class constructor.
93
94     Notes
95     -----
96     Constants Imported (See utils.Constants):
97         SAVE_PREFIX
98         CROP_DEFAULT
99         SPLIT_ROW
100
101     """
102     # -----split1-----
103     # MARK: Split init
104     def __init__(


```

```

105     self,
106     data_dir: Path,
107     fits_list: list[str] = None,
108     split_row: int = SPLIT_ROW,
109     no_arc: bool = False,
110     save_prefix: Path | None = None,
111     **kwargs
112 ) -> None:
113     self.data_dir = data_dir
114     self.fits_list = find_files(
115         data_dir=data_dir,
116         filenames=fits_list,
117         prefix="mxgbp",
118         ext="fits"
119     )
120     self.split_row = split_row
121     self.save_prefix = SAVE_PREFIX
122     if type(save_prefix) == dict:
123         self.save_prefix = save_prefix
124
125     self.arc = "" if no_arc else find_arc(self.fits_list)
126     self.o_files = []
127     self.e_files = []
128
129     logging.debug(f"__init__ - \n{self.__dict__}")
130     return
131
132 # MARK: Split Files
133 def split_file(
134     self,
135     file: os.PathLike
136 ) -> tuple[pyfits.HDUList]:
137     """
138         Split the single FITS file into separated `O`- and `E`- FITS
139         files.
140
141     Parameters
142     -----
143     file : os.PathLike
144         The name of the FITS file to be split.
145
146     Returns
147     -----
148     tuple[astropy.io.fits.HDUList]
149         Tuple containing the split O and E beam HDULists.
150
151     """
152     # Create empty HDUList
153     O_beam = pyfits.HDUList()
154     E_beam = pyfits.HDUList()
155
156     # Open file and split O & E beams
157     with pyfits.open(file) as hdul:
158         O_beam.append(hdul["PRIMARY"].copy())
159         E_beam.append(hdul["PRIMARY"].copy())
160
161         # Split specific extention
162         raw_split = self.split_ext(hdul, "SCI")

```

```

162
163     # O_beam[0].data = raw_split['SCI'].data[1]
164     # E_beam[0].data = raw_split['SCI'].data[0]
165     O_beam[0].data, E_beam[0].data = self.crop_file(raw_split)
166
167     # Handle prefix and names
168     pref = "arc" if file == self.arc else "beam"
169     o_name = self.save_prefix[pref][0] + file.name[-9:]
170     e_name = self.save_prefix[pref][1] + file.name[-9:]
171
172     # Add split data to O & E beam lists
173     self.update_beam_lists(o_name, e_name, pref == "arc")
174
175     # Handle don't save case
176     if self.save_prefix == None:
177         return O_beam, E_beam
178
179     # Handle save case
180     O_beam.writeto(o_name, overwrite=True)
181     E_beam.writeto(e_name, overwrite=True)
182
183     return O_beam, E_beam
184
185     # MARK: Split extensions
186 def split_ext(
187     self,
188     hdulist: pyfits.HDUList,
189     ext: str = "SCI"
190 ) -> pyfits.HDUList:
191     """
192         Split the data of the specified extension of `hdulist` into its
193         → `O`- and `E`- beams.
194
195         Parameters
196         -----
197         hdulist : astropy.io.fits.HDUList
198             The FITS HDUList to be split.
199         ext : str, optional
200             The name of the extension to be split.
201             (Defaults to 'SCI')
202
203         Returns
204         -----
205         astropy.io.fits.HDUList
206             The HDUList with the split applied.
207
208         """
209         hdu = deepcopy(hdulist)
210         rows, cols = hdu[ext].data.shape
211
212         # if odd number of rows, strip off the last one
213         rows = int(rows / 2) * 2
214
215         # how far split is from center of detector
216         offset = int(self.split_row - rows / 2)
217
218         # split arc into o/e images
219         ind_rc = np.indices((rows, cols))[0]

```

```

219     padbins = (ind_rc < offset) | (ind_rc > rows + offset)
220
221     # Roll split_row to be centre row
222     image_rc = np.roll(hdu[ext].data[:rows, :], -offset, axis=0)
223     image_rc[padbins] = 0.0
224
225     # Split columns equally
226     hdu[ext].data = image_rc.reshape((2, int(rows / 2), cols))
227
228     return hdu
229
230 # MARK: Crop files
231 def crop_file(
232     self,
233     hdulist: pyfits.HDUList,
234     crop: int = CROP_DEFAULT
235 ) -> tuple[np.ndarray]:
236     """
237         Crop the data with respect to the `O`/`E` beam.
238
239     Parameters
240     -----
241     hdulist : astropy.io.fits.HDUList
242         The HDUList containing the data to be cropped.
243     crop : int, optional
244         The number of rows to be cropped from the bottom and top
245         of the `O` and `E` beam, respectively.
246         (Defaults to 40)
247
248     Returns
249     -----
250     tuple[numpy.ndarray]
251         Tuple containing the cropped O and E beam data arrays.
252
253     """
254     o_data = hdulist["SCI"].data[1, 0:-crop]
255     e_data = hdulist["SCI"].data[0, crop:]
256
257     return o_data, e_data
258
259 # MARK: Update beam lists
260 def update_beam_lists(
261     self,
262     o_name,
263     e_name,
264     arc: bool = True
265 ) -> None:
266     """
267         Update the `o_files` and `e_files` attributes.
268
269     Parameters
270     -----
271     o_name : str
272         The filename of the O beam.
273     e_name : str
274         The filename of the E beam.
275     arc : bool, optional
276         Indicates whether the first entry should be the arc frame.

```

```

277             (Defaults to True)
278
279         Returns
280         -----
281         None
282
283         """
284         if arc:
285             self.o_files.insert(0, o_name)
286             self.e_files.insert(0, e_name)
287         else:
288             self.o_files.append(o_name)
289             self.e_files.append(e_name)
290
291     return
292
293 # MARK: Save beam lists
294 def save_beam_lists(self, file_suffix: str = 'frames') -> None:
295     with open(f"o_{file_suffix}", "w+") as f_o, \
296         open(f"e_{file_suffix}", "w+") as f_e:
297         for i, j in zip(self.o_files, self.e_files):
298             f_o.write(i + "\n")
299             f_e.write(j + "\n")
300
301     return
302
303 # MARK: Process all Listed Images
304 def process(self) -> None:
305     """
306         Process all FITS images stored in the `fits_list` attribute
307
308     Returns
309     -----
310     None
311
312     """
313     for target in self.fits_list:
314         logging.debug(f"Processing {target}")
315         self.split_file(target)
316
317     self.save_beam_lists()
318
319     return
320
321 # MARK: Main function
322 def main(argv) -> None:
323     """Main function."""
324
325     return
326
327
328 if __name__ == "__main__":
329     main(sys.argv[1:])

```

Listing II.3: The source code for `join.py`

```

1 """Module for joining the split FITS files with an external wavelength
2      solution."""
3
4 #!/usr/bin/env python3
5 # -*- coding: utf-8 -*-
6
7 from __init__ import __author__, __email__, __version__
8
9 # MARK: Imports
10 import os
11 import sys
12 import logging
13 import re
14 from pathlib import Path
15
16 import numpy as np
17 from numpy.polynomial.chebyshev import chebgrid2d as chebgrid2d
18 from numpy.polynomial.legendre import leggrid2d as leggrid2d
19 from astropy.io import fits as pyfits
20
21 # from lacosmic import lacosmic # Replaced: ccdproc is ~6x faster
22 from ccdproc import cosmicray_lacosmic as lacosmic
23
24 from utils.specpolpy3 import read_wollaston, split_sci
25 from utils.SharedUtils import find_files, find_arc
26 from utils.Constants import DATADIR, SAVE_PREFIX, SPLIT_ROW, CR_PARAMS
27
28 # MARK: Join Class
29 class Join:
30
31     #-----join0-----
32
33     """
34     The `Join` class allows for the joining of previously split files
35     and the
36     appending of an external wavelength solution in the `polsalt` FITS
37     file format.
38
39     Parameters
40     -----
41     data_dir : str
42         The path to the data to be joined
43     database : str, optional
44         The name of the `IRAF` database folder.
45         (The default is "database")
46     fits_list : list[str], optional
47         A list of pre-reduced `polsalt` FITS files to be joined within `data_dir`.
48         (The default is ``None``, `Join` will search for `mxgbp*.fits` files)
49     solutions_list: list[str], optional
50         A list of solution filenames from which the wavelength solution
51         is created.
52         (The default is ``None``, `Join` will search for `fc*` files
53         within the `database` directory)

```



```

99      -----
100     no_arc : bool, optional
101         Deprecated. Decides whether the arc frames should be processed.
102         (The default is False, `polsalt` has no use for the arc after
103         ↪ wavelength calibrations)
104     **kwargs : dict
105         keyword arguments. Allows for passing unpacked dictionary to
106         ↪ the class constructor.
107
108     Notes
109     -----
110     Constants Imported (See utils.Constants):
111         DATADIR, SAVE_PREFIX, SPLIT_ROW, CR_PARAMS
112
113     Custom wavelength solutions must be formatted containing:
114         `x`, `y`, *coefficients...
115     where a solution are of order (`x` by `y`) and must contain x*y
116     ↪ coefficients,
117     all separated by newlines. The name of the custom wavelength
118     ↪ solution file
119     must contain either "cheb" or "leg" for Chebychev or Legendre
120     wavelength solutions, respectively.
121
122     Cosmic ray rejection is performed using lacosmic [1]_
123     ↪ in ccdproc via astroscrappy [2]_.
124
125     References
126     -----
127     .. [1] van Dokkum 2001, PASP, 113, 789, 1420 (article :
128         ↪ https://adsabs.harvard.edu/abs/2001PASP..113.1420V)
129     .. [2] https://zenodo.org/records/1482019
130
131     """
132
133     # -----join1-----
134
135     # MARK: Join init
136     def __init__(
137         self,
138         data_dir: Path,
139         database: str = "database",
140         fits_list: list[str] = None,
141         solutions_list: list[Path] = None,
142         split_row: int = SPLIT_ROW,
143         no_arc: bool = True,
144         save_prefix: Path | None = None,
145         verbose: int = 30,
146         **kwargs,
147     ) -> None:
148         self.data_dir = data_dir
149         self.database = Path(data_dir) / database
150         self.fits_list = find_files(
151             data_dir=self.data_dir,
152             filenames=fits_list,
153             prefix="mxgbp",
154             ext="fits",
155         )
156         self.fc_files, self.custom = self.get_solutions(solutions_list)

```

```

151     self.split_row = split_row
152     self.save_prefix = SAVE_PREFIX
153     if type(save_prefix) == dict:
154         self.save_prefix = save_prefix
155
156     self.no_arc = no_arc
157     self.arc = find_arc(self.fits_list)
158
159     self.verbose = verbose < 30
160
161     logging.debug("__init__ - \n", self.__dict__)
162     return
163
164 # MARK: Find 2D WAV Functions
165 def get_solutions(
166     self,
167     wavlist: list[str] | None,
168     prefix: str = "fc"
169 ) -> tuple[list[str], bool]:
170     """
171         Get the list of wavelength solution files.
172
173     Parameters
174     -----
175     wavlist : list[str] / None
176         A list of custom wavelength solutions files.
177         If ``None``, `Join` will search for wavelength solutions in
178         the `database` directory.
179     prefix : str, optional
180         The prefix of the wavelength solution files.
181         (Defaults to "fc")
182
183     Returns
184     -----
185     tuple[list[str], bool]
186         A tuple containing the list of wavelength solutions files
187         and
188         a boolean indicating whether custom solutions were provided.
189
190     """
191     # No custom solutions
192     if not wavlist:
193         # Handle finding solutions
194         ws = []
195         for fl in os.listdir(self.database):
196             if os.path.isfile(self.database / fl) and (prefix ==
197                 fl[0:len(prefix)]):
198                 ws.append(fl)
199
200         if len(ws) != 2:
201             # Handle incorrect number of solutions found
202             msg = (
203                 f"\"Incorrect amount of wavelength solutions "
204                 f"({len(ws)} fc... files) found in the solution "
205                 f"dir.: {self.database}\""
206             )
207             logging.error(msg)
208             raise FileNotFoundError(msg)

```

```

206         return (sorted(ws, reverse=True), False)
207
208
209     # Custom solution
210     if len(wavlist) >= 2:
211         if len(wavlist) > 2:
212             logging.warning(f" Too many solutions, only
213                             → {wavlist[:2]} are considered")
214             wavlist = wavlist[:2]
215
216         for fl in wavlist:
217             if not os.path.isfile(os.path.join(self.data_dir, fl)):
218                 msg = (
219                     f"{fl} not found in the "
220                     f"data directory {self.data_dir}"
221                 )
222                 logging.error(msg)
223                 raise FileNotFoundError(msg)
224
225
226     # MARK: Parse 2D WAV Function
227     def parse_solution(
228         self,
229         fc_file: str,
230         xshape: int,
231         yshape: int
232     ) -> tuple[dict[str, int], np.ndarray]:
233         """
234             Parse the 2D wavelength solution function from `fc_file`.
235
236             Parameters
237             -----
238             fc_file : str
239                 The filename of the wavelength solutions file.
240             xshape : int
241                 The x-order of the 2D solution.
242             yshape : int
243                 The y-order of the 2D solution.
244
245             Returns
246             -----
247             tuple[dict[str, int], np.ndarray]
248                 A tuple containing a dictionary of the parameters of the
249                 → solution function
250                 and the function coefficients.
251
252             """
253             fit_params = {}
254             coeff = []
255
256             if self.custom:
257                 # Load coefficients
258                 coeff = np.loadtxt(fc_file)
259
260                 fit_params["xorder"] = coeff[0].astype(int)
261                 fit_params["yorder"] = coeff[1].astype(int)
262                 coeff = coeff[2:]

```

```

262
263     f_type = 3
264     if "cheb" in str(fc_file): f_type = 1
265     elif "leg" in str(fc_file): f_type = 2
266     fit_params["function"] = f_type
267
268     fit_params["xmin"], fit_params["xmax"] = 1, xshape
269     fit_params["ymin"], fit_params["ymax"] = 1, yshape
270
271 else:
272     # Parse IRAF fc database files
273     file_contents = []
274     with open(self.database / fc_file) as fcfile:
275         for i in fcfile:
276             file_contents.append(re.sub(r"\n\t\s*", "", i))
277
278 if file_contents[9] != "1.": # xterms - Cross-term type
279     msg=(
280         "Cross-term not recognised (always 1 for "
281         "'FITCOORDS'), redo FITCOORDS or change manually."
282     )
283     raise Exception(msg)
284
285     fit_params["function"] = int(file_contents[6][:-1])
286
287     fit_params["xorder"] = int(file_contents[7][:-1])
288     fit_params["yorder"] = int(file_contents[8][:-1])
289
290     fit_params["xmin"] = int(file_contents[10][:-1])
291     fit_params["xmax"] = xshape
292     # int(file_contents[11][:-1])# stretch fit over x
293     fit_params["ymin"] = int(file_contents[12][:-1])
294     fit_params["ymax"] = yshape
295     # int(file_contents[13][:-1])# stretch fit over y
296
297     coeff = np.array(file_contents[14:], dtype=float)
298
299     coeff = np.reshape(
300         coeff,
301         (fit_params["xorder"], fit_params["yorder"])
302     )
303
304     return (fit_params, coeff)
305
306 # MARK: Join Files
307 def join_file(self, file: os.PathLike) -> None:
308     """
309         Join the `O`- and `E`-beams, attach the wavelength solutions,
310         perform cosmic ray cleaning, mask the extensions,
311         and checks cropping performed by `Split`.
312         Write the FITS file in a `polsalt` valid format.
313
314     Parameters
315     -----
316     file : os.PathLike
317         The path of the FITS file to be joined.
318
319     See Also

```

```

320      -----
321      IRAF - `fitcoords` task
322      https://iraf.net/irafdocs/formats/fitcoords.php,
323      numpy 2D grid functions
324      https://numpy.org/doc/stable/reference/generated/numpy
325      Chebyshev: + '.polynomial.chebyshev.chebgrid2d.html'
326      Legendre: + '.polynomial.legendre.leggrid2d.html'
327
328      """
329      # Create empty wavelength appended hdu list
330      whdu = pyfits.HDUList()
331      primary_ext = ""
332
333      # Handle prefix and names
334      pref = "arc" if file == self.arc else "beam"
335      o_file = self.save_prefix[pref][0] + file.name[-9:]
336      e_file = self.save_prefix[pref][1] + file.name[-9:]
337
338      # Open file
339      with pyfits.open(file) as hdu:
340          # Check if file has been cropped
341          cropsize = self.check_crop(hdu, o_file, e_file)
342
343          y_shape = int(hdu["SCI"].data.shape[0] / 2) - cropsize
344          x_shape = hdu["SCI"].data.shape[1]
345
346          # No differences in "PRIMARY" extention header
347          primary_ext = hdu["PRIMARY"]
348          whdu.append(primary_ext)
349
350          for ext in ["SCI", "VAR", "BPM"]:
351              whdu.append(pyfits.ImageHDU(name=ext))
352              whdu[ext].header = hdu[ext].header.copy()
353              whdu[ext].header["CTYPE3"] = "O,E"
354
355          # Create empty extention with correct order and format
356          if ext == "BPM":
357              whdu[ext].data = np.zeros(
358                  (2, y_shape, x_shape),
359                  dtype="uint8")
360
361              whdu[ext].header["BITPIX"] = "-uint8"
362          else:
363              whdu[ext].data = np.zeros(
364                  (2, y_shape, x_shape),
365                  dtype=">f4")
366
367              whdu[ext].header["BITPIX"] = "-32"
368
369          # Fill in empty extentions
370          if cropsize:
371              temp_split = split_sci(
372                  hdu,
373                  self.split_row,
374                  ext=ext
375              )[ext].data
376              whdu[ext].data[0] = temp_split[0, cropsize:]
377              whdu[ext].data[1] = temp_split[1, 0:-cropsize]

```

```

378
379         else:
380             whdu[ext].data = split_sci(
381                 hdu,
382                 self.split_row,
383                 ext=ext
384             )[ext].data
385 # End of hdu calls, close hdu
386
387 # MARK: Join (Wav. Ext.)
388 whdu.append(pyfits.ImageHDU(name="WAV"))
389 wav_header = whdu["SCI"].header.copy()
390 wav_header["EXTNAME"] = "WAV"
391 wav_header["CTYPE3"] = "O,E"
392 whdu["WAV"].header = wav_header
393
394 whdu["WAV"].data = np.zeros(
395     whdu["SCI"].data.shape,
396     dtype=">f4"
397 )
398
399 for num, fname in enumerate(self.fc_files):
400     pars, chebvals = self.parse_solution(
401         fname,
402         x_shape,
403         y_shape
404     )
405
406     if pars["function"] == 1: # Function type (1 = chebyshev)
407         # Set wavelength extention values to function
408         whdu["WAV"].data[num] = chebgrid2d(
409             x=np.linspace(-1, 1, pars["ymax"]),
410             y=np.linspace(-1, 1, pars["xmax"]),
411             c=chebvals,
412         )
413
414     elif pars["function"] == 2: # Function type (2 = legendre)
415         # Set wavelength extention values to function
416         whdu["WAV"].data[num] = leggrid2d(
417             x=np.linspace(-1, 1, pars["ymax"]),
418             y=np.linspace(-1, 1, pars["xmax"]),
419             c=chebvals,
420         )
421
422     else:
423         msg = (
424             "Function type not recognised, please wavelength "
425             "calibrate using either chebychev or legendre."
426         )
427         raise Exception(msg)
428
429 # MARK: Cosmic Ray Cleaning
430 # See utils.Constants for `CR_PARAMS` discussion
431 whdu["SCI"].data[num] = lacosmic(
432     whdu["SCI"].data[num],
433     # contrast=CR_PARAMS['CR_CONTRAST'],
434     # threshold=CR_PARAMS['CR_THRESHOLD'],
435     # neighbor_threshold=CR_PARAMS['CR_NEIGH_THRESH'],

```

```

436         # effective_gain=CR_PARAMS['GAIN'],
437         # background=CR_PARAMS['BACKGROUND'],
438         readnoise=CR_PARAMS['READNOISE'],
439         gain=CR_PARAMS['GAIN'],
440         verbose=self.verbose,
441     )[0]
442
443     # MARK: WAV masking
444     # Left & Right Crop
445     whdu["WAV"].data[whdu["WAV"].data[:] < 3_000] = 0.0
446     whdu["WAV"].data[whdu["WAV"].data[:] >= 10_000] = 0.0
447
448     # Top & Bottom Crop (shift\tilt)
449     rpix_oc, cols, rbin, lam_c = read_wollaston(
450         whdu,
451         DATADIR + "wollaston.txt"
452     )
453
454     drow_oc = (rpix_oc - rpix_oc[:, int(cols / 2)][:, None]) / rbin
455
456     ## Cropping as suggested
457     for c, col in enumerate(drow_oc[0]):
458         if np.isnan(col):
459             continue
460
461         if int(col) < 0:
462             whdu["WAV"].data[0, int(col) :, c] = 0.0
463         elif int(col) > cropsize:
464             whdu["WAV"].data[0, 0 : int(col) - cropsize, c] = 0.0
465
466     for c, col in enumerate(drow_oc[1]):
467         if np.isnan(col):
468             continue
469
470         if int(col) > 0:
471             whdu["WAV"].data[1, 0 : int(col), c] = 0.0
472         elif (int(col) < 0) & (abs(int(col)) > cropsize):
473             whdu["WAV"].data[1, int(col) + cropsize :, c] = 0.0
474
475     # MARK: BPM masking
476     whdu["BPM"].data[0] = np.where(
477         whdu["WAV"].data[0] == 0,
478         1,
479         whdu["BPM"].data[0]
480     )
481     whdu["BPM"].data[1] = np.where(
482         whdu["WAV"].data[1] == 0,
483         1,
484         whdu["BPM"].data[1]
485     )
486
487     whdu.writeto(f"w{os.path.basename(file)}", overwrite="True")
488
489     return
490
491     # MARK: Check Crop
492     def check_crop(
493         self,

```

```

494     hdu: pyfits.HDUList,
495     o_file: str,
496     e_file: str
497 ) -> int:
498     """
499     Check if cropping is necessary when joining `O`- and `E`-beams.
500
501     Parameters
502     -----
503     hdu : astropy.io.fits.HDUList
504         The HDUList to check for cropping.
505     o_file : str
506         The name of the previously split `O`-beam FITS file.
507     e_file : str
508         The name of the previously split `E`-beam FITS file.
509
510     Returns
511     -----
512     int
513         The number of rows which were cropped by `Split`.
514
515     """
516     cropsize = 0
517     o_y = 0
518     e_y = 0
519
520     with pyfits.open(o_file) as o, \
521         pyfits.open(e_file) as e:
522         o_y = o[0].data.shape[0]
523         e_y = e[0].data.shape[0]
524
525     if hdu["SCI"].data.shape[0] != (o_y + e_y):
526         # Get crop size, assuming crop same on both sides
527         cropsize = int((hdu["SCI"].data.shape[0] - o_y - e_y) / 2)
528
529     return cropsize
530
531     # MARK: Process all Listed Images
532 def process(self) -> None:
533     """Process all FITS images stored in the `fits_list`  

534     ↳ attribute"""
535     for target in self.fits_list:
536         logging.debug(f"Processing {target}")
537         self.join_file(target)
538
539     return
540
541 def main(argv) -> None:
542     """Main function."""
543
544     return
545
546
547 if __name__ == "__main__":
548     main(sys.argv[1:])

```

Listing II.4: The source code for `cross_correlate.py`

```

1 """Module for cross correlating polarization beams."""
2
3 #!/usr/bin/env python3
4 # -*- coding: utf-8 -*-
5
6 from __init__ import __author__, __email__, __version__
7
8 # MARK: Imports
9 import os
10 import sys
11 import logging
12 import itertools as iters
13 from pathlib import Path
14 from typing import Callable
15
16 import numpy as np
17 from numpy.polynomial import chebyshev
18 import matplotlib.pyplot as plt
19 from astropy.io import fits as pyfits
20 from scipy import signal
21
22 from utils.SharedUtils import find_files, continuum
23 from utils.Constants import SAVE_CORR
24
25 OFFSET = 0.3
26
27 mpl_logger = logging.getLogger('matplotlib')
28 mpl_logger.setLevel(logging.INFO)
29
30 # MARK: Correlate class
31 class CrossCorrelate:
32
33     #-----corr0-----
34
35     """
36     Cross correlate allows for comparing the extensions of multiple
37     FITS files, or comparing the O and E beams of a single FITS file.
38
39     Parameters
40     -----
41     data_dir : str
42         The path to the data to be cross correlated
43     filenames : list[str]
44         The ecwmxgbp*.fits files to be cross correlated.
45         If only one filename is defined, correlation is done against
46         ↪ the two polarization beams.
47     split_ccd : bool, optional
48         Decides whether the CCD regions should each be individually
49         ↪ cross correlated.
50         (The default is True, which splits the spectrum up into its
51         ↪ separate CCD regions)
52     cont_ord : int, optional
53         The degree of a chebyshev to fit to the continuum.
54         (The default is 11)
55     plot : bool, optional
56         Decides whether or not the continuum fitting should be plotted

```

```

54     (The default is False, so no continua plots are displayed)
55     save_prefix : str, optional
56         The name or directory to save the figure produced to.
57         "." saves a default name to the current working. A default name
58         ↪ is also used when save_prefix is a directory.
59         (The default is None, I.E. The figure is not saved, only
60         ↪ displayed)

61     Attributes
62     -----
63     data_dir
64     fits_list
65     beams : str
66         The mode of correlation.
67         '0E' for same file, and '0' or 'E' for different files but same
68         ↪ ext's.
69     ccds : int
70         The number of CCD's in the data. Used to split the CCD's if
71         ↪ split_ccd is True.
72     cont_ord : int
73         The degree of the chebyshev to fit to the continuum.
74     can_plot : bool
75         Decides whether or not the continuum fitting should be plotted
76     offset : int
77         The amount the spectrum is shifted, mainly to test the effect
78         ↪ of the cross correlation
79         (The default is 0, I.E. no offset introduced)
80     save_prefix
81     wav_unit : str
82         The units of the wavelength axis.
83         (The default is Angstroms)
84     wav_cdelt : int
85         The wavelength increment.
86         (The default is 1)
87     alt : Callable
88         An alternate method of cross correlating the data.
89         (The default is None)

90     Methods
91     -----
92     load_file(filename: Path) -> tuple[np.ndarray, np.ndarray,
93         ↪ np.ndarray]
94         Loads the data from a FITS file.
95     get_bounds(bpm: np.ndarray) -> np.ndarray
96         Finds the bounds for the CCD regions.
97     remove_cont(spec: list, wav: list, bpm: list, plot_cont: bool) ->
98         ↪ None
99         Removes the continuum from the data.
100    correlate(filename1: Path, filename2: Path | None = None) -> None
101        Cross correlates the data.
102    FTCS(filename1: Path, filename2: Path | None = None) -> None
103        Cross correlates the data using the Fourier Transform.
104    plot(spec, wav, bpm, corrdbs, lagsdb) -> None
105        Plots the data.
106    process() -> None
107        Processes the data.

108    Other Parameters

```

```

105 -----
106 offset : int, optional
107     The amount the spectrum is shifted, mainly to test the effect
108     ↗ of the cross correlation
109     (The default is 0, I.E. no offset introduced)
110 **kwargs : dict
111     keyword arguments. Allows for passing unpacked dictionary to
112     ↗ the class constructor.
113 FTCS : bool, optional
114     Decides whether the Fourier Transform should be used for
115     ↗ cross correlation.
116
117 See Also
118 -----
119
120 Notes
121 -----
122 Constants Imported (See utils.Constants):
123     SAVE_CORR
124
125 """
126
127 #-----corr1-----
128
129 # MARK: Correlate init
130 def __init__(
131     self,
132     data_dir: Path,
133     filenames: list[str],
134     beams: str = "OE",
135     split_ccd: bool = True,
136     cont_ord: int = 11,
137     plot: bool = False,
138     offset: int = 0,
139     save_prefix: Path | None = None,
140     **kwargs
141 ) -> None:
142     self.data_dir = data_dir
143     self.fits_list = find_files(
144         data_dir=self.data_dir,
145         filenames=filenames,
146         prefix="ecwmxgbp",
147         ext="fits",
148     )
149     self._beams = None
150     self.beams = beams
151     self.ccds = 1
152     if split_ccd:
153         # BPM == 2 near center of CCD if CCD count varies
154         with pyfits.open(self.fits_list[0]) as hdu:
155             self.ccds = sum(hdu["BPM"].data.sum(axis=1)[0] == 2)
156
157     self.cont_ord = cont_ord
158     self.can_plot = plot

```

```

160     self.offset = offset
161     if offset != 0:
162         logging.warning("'offset' is only for testing.")
163
164         errMsg = "Offset removed after finalizing testing."
165         logging.error(errMsg)
166         raise ValueError(errMsg)
167         # # Add an offset to the spectra to test cross correlation
168         # self.spec1 = np.insert(
169         #     self.spec1, [0] * offset, self.spec1[:, :offset],
170         #     ↪ axis=-1
171         # )[ :, : self.spec1.shape[-1]]
172
172     self.save_prefix = save_prefix
173     # Handle directory save name
174     if self.save_prefix and self.save_prefix.is_dir():
175         self.save_prefix /= SAVE_CORR
176         logging.warning((
177             f"Correlation save name resolves to a directory. "
178             f"Saving under {self.save_prefix}"
179         ))
180
181     self.wav_unit = "$\AA$"
182     self.wav_cdelt = 1
183
184     self.alt = self.FTCS if kwargs.get("FTCS") else None
185
186     logging.debug("__init__ - \n", self.__dict__)
187     return
188
189 # MARK: Beams property
190 @property
191 def beams(self) -> str:
192     return self._beams
193
194 @beams.setter
195 def beams(self, mode: str) -> None:
196     if mode not in ['O', 'E', 'OE']:
197         errMsg = f"Correlation mode '{mode}' not recognized."
198         logging.error(errMsg)
199         raise ValueError(errMsg)
200
201     self._beams = mode
202
203     return
204
205 # MARK: Load file
206 def load_file(
207     self,
208     filename: Path
209 ) -> tuple[np.ndarray, np.ndarray, np.ndarray]:
210     """
211     Load the data from a FITS file.
212
213     Parameters
214     -----
215     filename : Path
216         The name of the FITS file to load.

```



```

275             min(mid + bpm.shape[-1] // CCDs, bpm.shape[-1])
276         )
277
278     return bounds.astype(int)
279
280     # MARK: Remove Continua
281 def remove_cont(
282     self,
283     spec: list,
284     wav: list,
285     bpm: list,
286     plot_cont: bool
287 ) -> np.ndarray:
288     """
289     Remove the continuum from the data.
290
291     Parameters
292     -----
293     spec : list
294         The spectrum to remove the continuum from.
295     wav : list
296         The wavelength of the spectrum.
297     bpm : list
298         The bad pixel mask.
299     plot_cont : bool
300         Decides whether or not the continuum fitting should be
301         ↪ plotted
302
303     Returns
304     -----
305     None
306
307     """
308     # Mask out the bad pixels for fitting continua
309     okwav = np.where(bpm != 1)
310
311     # Define continua
312     ctm = continuum(
313         wav[okwav],
314         spec[okwav],
315         deg=self.cont_ord,
316         plot=plot_cont,
317     )
318
319     # Normalise spectra
320     spec /= chebyshev.chebval(wav, ctm)
321     spec -= 1
322
323     return spec
324
325     # MARK: Correlate
326 def correlate(
327     self,
328     filename1: Path,
329     filename2: Path | None = None,
330     alt: Callable = None
331 ) -> None:
332     """

```

```

332     Cross correlates the data.
333
334     Parameters
335     -----
336     filename1 : Path
337         The name of the first FITS file to cross correlate.
338     filename2 : Path, optional
339         The name of the second FITS file to cross correlate.
340         (Defaults to None)
341     alt : Callable, optional
342         An alternate method of cross correlating the data.
343         (Defaults to None)
344
345     Returns
346     -----
347     None
348
349     """
350     # mode: O_E -> '01' & 'E1', O -> '01' & '02', E -> 'E1' & 'E2',
351     # Load data
352     spec, wav, bpm = self.load_file(filename1)
353     if filename2 and self.beams != 'O_E':
354         unpack = lambda ext, *args: [arr[ext] for arr in args]
355
356     if self.beams == 'O':
357         spec[-1], wav[-1], bpm[-1] = unpack(
358             0, *self.load_file(filename2))
359     )
360
361     else:
362         spec[0], wav[0], bpm[0] = spec[-1], wav[-1], bpm[-1]
363         spec[-1], wav[-1], bpm[-1] = unpack(
364             -1, *self.load_file(filename2))
365     )
366
367     bounds = self.get_bounds(bpm)
368
369     logging.debug(
370         f"correlate - data shape:\n{tspec/wav/bpm: {spec.shape}}"
371     )
372
373     corrdb = [[] for _ in range(self.ccdb)]
374     lagsdb = [[] for _ in range(self.ccdb)]
375     for ccd in range(self.ccdb):
376         sig = []
377         for ext in range(2):
378             lb, ub = bounds[ext, ccd]
379
380             if self.cont_ord > 0:
381                 spec[ext, lb:ub] = self.remove_cont(
382                     spec[ext, lb:ub],
383                     wav[ext, lb:ub],
384                     bpm[ext, lb:ub],
385                     self.can_plot
386                 )
387
388             # Invert BPM (and account for 2); zero bad pixels
389             sig.append((

```

```

390             spec[ext, lb:ub]
391             * abs(bpm[ext, lb:ub] * -1 + 1)
392         ))
393
394     # Finally!!!! cross correlate signals and scale max -> 1
395     corrdb[ccd] = signal.correlate(*sig) if not alt else
396     ↪ alt(*sig)
397     corrdb[ccd] /= np.max(corrdb[ccd])
398     lagsdb[ccd] = signal.correlation_lags(
399         sig[0].shape[-1],
400         sig[1].shape[-1]
401     ) * self.wav_cdel
402
403     return (spec, wav, bpm), (corrdb, lagsdb)
404
405 # MARK: FTCS alternate
406 def FTCS(
407     self,
408     signal1: np.ndarray,
409     signal2: np.ndarray
410 ) -> None:
411     """
412         Cross correlates the data using the Fourier Transform.
413
414     Parameters
415     -----
416     signal1 : np.ndarray
417         The first signal to cross correlate.
418     signal2 : np.ndarray
419         The second signal to cross correlate.
420
421     Returns
422     -----
423     np.ndarray
424         The correlation data using the Fourier Transform.
425
426     """
427     logging.debug(
428         f"FTCS - data shape:\n{tspec/wav/bpm: {signal1.shape}}"
429     )
430
431     # Invert BPM (and account for 2); zero bad pixels
432     ft_spec1 = np.fft.fft(signal1)
433     ft_spec2 = np.fft.fft(signal2)
434
435     if self.can_plot:
436         plt.plot(ft_spec1)
437         plt.plot(ft_spec2)
438         plt.show()
439
440     # Cross correlate signals
441     # ft_spectrum1 * np.conj(ft_spectrum2)
442     corr_entry = signal.correlate(ft_spec1, ft_spec2)
443
444     return np.fft.ifft(corr_entry)
445
446 # MARK: Plot
447 def plot(self, spec, wav, bpm, corrdb, lagsdb) -> None:

```

```

447 """
448 Plot the data.
449
450 Parameters
451 -----
452 spec : np.ndarray
453     The spectrum.
454 wav : np.ndarray
455     The wavelength.
456 bpm : np.ndarray
457     The bad pixel mask.
458 corrdb : np.ndarray
459     The cross correlation data.
460 lagsdb : np.ndarray
461     The lags data.
462
463 Returns
464 -----
465 None
466
467 """
468 plt.style.use(Path(__file__).parent.resolve() /
469             'utils/STOPS.mplstyle')
470 bounds = self.get_bounds(bpm)
471
472 fig, axs = plt.subplots(2, self.ccds, sharey="row")
473
474 if self.ccds == 1:
475     # Convert axes to a 2D array
476     axs = np.swapaxes(np.atleast_2d(axs), 0, 1)
477
478 # for ext, ccd in iters.product(range(2), range(self.ccds)):
479
480 for ccd in range(self.ccds):
481     axs[0, ccd].plot(
482         lagsdb[ccd],
483         corrdb[ccd] * 100,
484         color='C4',
485         label=f"max lag @ {lagsdb[ccd][corrdb[ccd].argmax()]} - "
486             f"(bounds[1, ccd, 0] - bounds[0, ccd, 0])",
487     )
488
489     for ext in range(2):
490         lb, ub = bounds[ext, ccd]
491         logging.debug(f"fl-{ext}: {wav[ext, lb]}:{wav[ext, ub - "
492             f"1]}")
493
494         axs[1, ccd].plot(
495             wav[ext, lb:ub],
496             spec[ext, lb:ub] * abs(bpm[ext, lb:ub] * -1 + 1) +
497             OFFSET * ext,
498             label=(
499                 f"${self.beams} if self.beams != 'OE' else "
500                 f"self.beams[{ext}]"
501                 f"_{ext + 1} if self.beams != 'OE' else 1${}"
502                 f"{{'({} + str(OFFSET * ext) + ')')} if ext > 0 "
503                 f"else ''"
504             ),
505             )

```

```

499
500
501     )
502
503     axs[0, 0].set_ylabel("Normalised Correlation\n(\%)")
504     for ax in axs[0, :]:
505         ax.set_xlabel("Signal Lag")
506     for ax in axs[1:, 0]:
507         ax.set_ylabel("Norm. Intensity\n(Counts)")
508     for ax in axs[-1, :]:
509         ax.set_xlabel(f"Wavelength ({self.wav_unit})")
510     for ax in axs.flatten():
511         ax.legend()
512
513     # plt.tight_layout()
514     # fig1 = plt.gcf()
515     # DPI = fig1.get_dpi()
516     # fig1.set_size_inches(700.0/float(DPI), 250.0/float(DPI))
517     plt.show()
518
519     # Handle do not save
520     if not self.save_prefix:
521         return
522
523     # Handle save
524     fig.savefig(fname=self.save_prefix)
525
526     return
527
528     # MARK: Process all listed images
529     def process(self) -> None:
530         """
531             Process the data.
532
533             Returns
534             -----
535             None
536
537             """
538
539         if self.beams != 'OE' and len(self.fits_list) == 1:
540             # change mode to OE with warning
541             logging.warning((
542                 f"`{self.beams}` correlation not possible for "
543                 "a single file. correlation `mode` changed to 'OE'."
544             ))
545             self.beams = 'OE'
546
547         # OE `mode` (same file, diff. ext.)
548         if self.beams == 'OE':
549             for fl in self.fits_list:
550                 logging.info(f"'OE' correlation of {fl}.")
551                 (spec, wav, bpm), (corr, lags) = self.correlate(fl,
552                     ↪ alt=self.alt)
553                 self.plot(spec, wav, bpm, corr, lags)
554
555         return
556
557         # O/E `mode` (diff. files, same ext.)
558         for fl1, fl2 in iters.combinations(self.fits_list, 2):
559             logging.info(f"{self.beams} correlation of {fl1} vs {fl2}.")

```

```
556         (spec, wav, bpm), (corr, lags) = self.correlate(f11, f12,
557         ↪ alt=self.alt)
558         self.plot(spec, wav, bpm, corr, lags)
559     return
560
561
562 # MARK: Main function
563 def main(argv) -> None:
564     return
565
566 if __name__ == "__main__":
567     main(sys.argv[1:])
```

Listing II.5: The source code for `skylines.py`

```

1 """Module for analyzing the sky lines of a wavelength calibrated
2    ↪ image."""
3
4 #!/usr/bin/env python3
5 # -*- coding: utf-8 -*-
6
7 from __init__ import __author__, __email__, __version__
8
9 # MARK: Imports
10 import os
11 import sys
12 import logging
13 from pathlib import Path
14
15 import numpy as np
16 import matplotlib.pyplot as plt
17 from astropy.io import fits as pyfits
18 from scipy import signal, stats, interpolate
19
20 from utils.SharedUtils import find_files, continuum
21 from utils.Constants import SAVE_SKY
22
23 mpl_logger = logging.getLogger('matplotlib')
24 mpl_logger.setLevel(logging.INFO)
25 # plt.rcParams['figure.figsize'] = (20, 4)
26
27 # MARK: Skylines Class
28 class Skylines:
29
30     #-----sky0-----
31
32     """
33         Class representing the Skylines object.
34
35     Parameters
36     -----
37     data_dir : Path
38         The directory containing the data files.
39     filenames : list[str]
40         The list of filenames to be processed.
41     beam : str, optional
42         The beam mode, by default "OE".
43     plot : bool, optional
44         Flag indicating whether to plot the continuum, by default False.
45     save_prefix : Path / None, optional
46         The prefix for saving the data, by default None.
47     **kwargs
48         Additional keyword arguments.
49
50     Attributes
51     -----
52     data_dir : Path
53         The directory containing the data files.
54     fits_list : list[str]
55         The list of fits file paths.
      beam : str

```

```

56     The beam mode.
57     can_plot : bool
58         Flag indicating whether to plot the continuum.
59     save_prefix : Path | None
60         The prefix for saving the data.
61     wav_unit : str
62         The unit of wavelength.
63     rawWav : np.ndarray
64         The raw wavelength data.
65     rawSpec : np.ndarray
66         The raw spectral data.
67     rawBpm : np.ndarray
68         The raw bad pixel mask data.
69     corrWav : np.ndarray
70         The corrected wavelength data.
71     corrSpec : np.ndarray
72         The corrected spectral data.
73     spec : np.ndarray
74         The median spectrum.
75     normSpec : np.ndarray
76         The normalized spectrum.

77
78     Methods
79     -----
80     checkLoad(self, path1: str) -> np.ndarray:
81         Checks and loads the data from the given path.
82     transform(self, wav_sol: np.ndarray, spec: np.ndarray) ->
83         np.ndarray:
84         Transforms the input wavelength and spectral data based on the
85         given wavelength solution.
86     rmvCont(self) -> np.ndarray:
87         Removes the continuum from the spectrum.
88     skylines(self) -> None:
89         Placeholder method for processing skylines.
90     process(self) -> None:
91         Placeholder method for processing the data.
92     """
93
94     # -----sky1-----
95
96     # MARK: Skylines init
97     def __init__(
98         self,
99         data_dir: Path,
100        filenames : list[str],
101        beams: str = "OE",
102        split_ccd: bool = False,
103        cont_ord: int = 11,
104        plot: bool = False,
105        transform: bool = True,
106        save_prefix: Path | None = None,
107        **kwargs,
108    ) -> None:
109         self.data_dir = data_dir
110         self.fits_list = find_files(
111             data_dir=self.data_dir,
112             filenames=filenames,
113             prefix="wmxgbp", # t[o/e]beam

```

```

112         ext="fits",
113     )
114     self._beams = None
115     self.beams = beams
116     self.ccds = 1
117     if split_ccd:
118         # See cross_correlate for initial implementation
119         self.ccds = 3
120
121     self.cont_ord = cont_ord
122     self.can_plot = plot
123     self.must_transform = transform
124
125     self.save_prefix = save_prefix
126     # Handle directory save name
127     if self.save_prefix and self.save_prefix.is_dir():
128         self.save_prefix /= SAVE_SKY
129         logging.warning((
130             f"Skylines save name resolves to a directory. "
131             f"Saving under {self.save_prefix}"
132         ))
133
134     self.wav_unit = "$\AA"
135
136     # self.rawWav, self.rawSpec, self.rawBpm = self.checkLoad(
137     #     self.fits_list
138     # )
139     # self.corrWav, self.corrSpec = self.transform(
140     #     self.rawWav,
141     #     self.rawSpec
142     # )
143     # self.spec = np.median(self.corrSpec, axis=1)
144     # self.normSpec = self.rmvCont(self.spec)
145
146     logging.debug("__init__ - \n", self.__dict__)
147     return
148
149     # MARK: Beams property
150     @property
151     def beams(self) -> str:
152         return self._beams
153
154     @beams.setter
155     def beams(self, mode: str) -> None:
156         if mode not in ['O', 'E', 'OE']:
157             errMsg = f"Correlation mode '{mode}' not recognized."
158             logging.error(errMsg)
159             raise ValueError(errMsg)
160
161         self._beams = mode
162
163     return
164
165     # MARK: Load Sky lines
166     def load_sky_lines(self, filename: Path | None = None) ->
167         np.ndarray:
168             """
169             Loads the sky lines from the given file.

```

```

169
170     Parameters
171     -----
172     filename : Path / None, optional
173         The path to the file to be loaded.
174         Defaults to loading the skylines from utils/sky.salt
175
176     Returns
177     -----
178     sky_lines : np.ndarray
179         The sky lines from the file.
180
181     """
182     if not filename:
183         filename = Path(__file__).parent.resolve() /
184             'utils/sky.salt'
185
186     dtype = [('wav', float), ('flux', float)]
187     skylines = np.genfromtxt(filename, dtype=dtype, skip_header=3,
188                             skip_footer=1)
189
190     if self.can_plot:
191         plt.plot(skylines['wav'], skylines['flux'], 'x',
192                   label="Model peaks")
193         plt.xlabel(f'Wavelength {self.wav_unit}')
194         plt.ylabel('Relative intensities')
195         plt.title('Known sky lines')
196         plt.legend()
197         plt.show()
198
199     return skylines
200
201
202     # MARK: Transform spectra
203     @staticmethod
204     def transform(wav_sol: np.ndarray, spec: np.ndarray, resPlot: bool
205                   = False) -> np.ndarray:
206         """
207             Transforms the input wavelength and spectral data based on the
208             given wavelength solution.
209
210         Parameters
211         -----
212         wav_sol : np.ndarray
213             The wavelength solution.
214         spec : np.ndarray
215             The spectral data.
216         resPlot : bool, optional
217             Flag indicating whether to plot the results, by default
218             False.
219
220         Returns
221         -----
222         wav, spec : np.ndarray
223             The transformed wavelength and spectral data.
224
225         """
226         # Create arrays to return
227         cw = np.zeros_like(wav_sol)

```

```

221     cs = np.zeros_like(wav_sol)
222
223     exts = cw.shape[0]
224     rows = cw.shape[1]
225
226     for ext in range(exts):
227         # Get middle row (to interpolate the rest of the rows to)
228         avg_max = [np.where(spec[ext, :, col] == spec[ext, :, col].max())[0][0] for col in range(spec[ext].shape[1])]
229         avg_max = np.sum(avg_max) // spec[ext].shape[1]
230
231         # Get wavelength values at row with most trace
232         wav = wav_sol[ext, avg_max, :]
233
234         # Correct extensions based on wavelength
235         # Wavelength ext
236         cw[ext, :, :] = wav
237
238         # Spec ext
239         # for row in range(rows):
240         #     f_2d = interpolate.interp2d(
241         #         wav_sol[ext, row],
242         #         np.arange(rows),
243         #         spec[ext],
244         #     )
245         #     cs[ext] = f_2d(cw[ext, row], np.arange(rows))
246         for row in range(rows):
247             cs[ext][row, :] = np.interp(
248                 wav,
249                 wav_sol[ext][row, :],
250                 spec[ext][row, :]
251             )
252
253         # Plot results
254         if resPlot:
255             fig, ax1 = plt.subplots(figsize=[20, 4])
256             ax1.imshow(cs[ext],
257                         vmax=cs[0].mean() + 2*cs[0].std(),
258                         vmin=cs[0].mean() - 2*cs[0].std()
259                     )
260             print(f"Average continuum of {'E' if ext else 'O'} at"
261                  f"\n{np.median(np.median(cs[ext], axis=0)):4.3f}")
262             ax2 = ax1.twinx()
263             ax2.hlines(np.median(np.median(cs[ext], axis=0)), 0,
264                         cs[ext].shape[-1], colors='black')
265             ax2.plot(cs[ext].mean(axis=0), "k", label=f"mean {'E' if ext else 'O'}")
266             ax2.plot(np.median(cs[ext], axis=0), "r",
267                         label=f"median {'E' if ext else 'O'}")
268             ax2.legend()
269             plt.show()
270
271         return cw, cs
272
# MARK: Remove continuum
def remove_cont(self, spec: np.ndarray, wav: np.ndarray) ->
    np.ndarray:
    ctm = continuum(wav, spec, deg=self.cont_ord,

```

```

    ↵ plot=self.can_plot)

273     return self.spec / ctm - 1

275

276 # MARK: Skylines
277 def skylines(self, filename) -> None:
278     # raise error if arc image
279     with pyfits.open(filename) as hdul:
280         if hdul[0].header['OBSTYPE'] == 'ARC':
281             logging.warning(f"ARC images, {filename}, contain no
282             ↵ sky lines. File skipped.")
283             return

284     # Load data
285     spec2D = hdul["SCI"].data
286     wav2D = hdul["WAV"].data
287     bpm2D = hdul["BPM"].data

288     spec2D *= ~bpm2D

290

291     logging.debug(f"skylines - {filename.name} - spec:
292     ↵ {spec2D.shape}")

293     # Mask trace
294     # TODO@JustinoanotherGitter: Add trace masking if median is
295     ↵ insufficient

296     # Save initial feature widths
297     # Mean to not filter out skewed features
298     spec1D_init = np.mean(spec2D, axis=1)
299     # Median to sort for most common wavelength
300     wav1D_init = np.median(wav2D, axis=1)

301

302     peaks = [[] for _ in range(2)]
303     properties = [[] for _ in range(2)]

304

305     if self.can_plot: fig, axs = plt.subplots(2, 1)
306     for ext in range(2):
307         peaks[ext], properties[ext] = signal.find_peaks(
308             spec1D_init[ext],
309             prominence=0.5 * np.std(spec1D_init[ext]),
310             width=[1, 1000],
311             rel_height=0.3
312         )
313         peak_width = [properties[ext]['widths'],
314             ↵ properties[ext]['width_heights'],
315             ↵ properties[ext]['left_ips'],
316             ↵ properties[ext]['right_ips']]

317

318         logging.debug(f"skylines - initial features {'E' if ext
319             ↵ else 'O'}: {len(peaks[ext])}")
320         logging.debug(f"skylines - props: {properties[ext]}")

321

322         if self.can_plot:
323             axs[ext].plot(spec1D_init[ext], label=f'{0 if ext
324                 ↵ else 1} initial')
325             axs[ext].vlines(peaks[ext], 0,
326                 ↵ np.mean(spec1D_init[ext]), color='r', label='Feature'

```

```

    ↪ positions')
    axs[ext].hlines(*peak_width[1:], color='g',
    ↪ label='Initial widths')
    axs[ext].errorbar(
        peaks[ext],
        properties[ext]['prominences'],
        xerr=np.array([
            peaks[ext] - properties[ext]['left_ips'],
            properties[ext]['right_ips'] - peaks[ext]
        ]),
        fmt='x',
        label='Prominences'
    )

332
333     if self.can_plot:
334         for ax in axs: ax.legend()
335         plt.show()

336
337     # Transform data, skip if filename starts with 't'
338     if self.must_transform or not filename.name.startswith('t'):
339         wav2D, spec2D = self.transform(wav2D, spec2D, self.can_plot)

340
341     # Convert to 1D spectra
342     wav1D = np.median(wav2D, axis=1)
343     spec1D = np.median(spec2D, axis=1)

344
345     # Remove continuum
346     if self.cont_ord > 0:
347         for ext in range(2):
348             # spec1D_init[ext] = self.remove_cont(spec1D_init[ext],
349             ↪ wav1D[ext])
350             # spec1D[ext] = self.remove_cont(spec1D[ext],
351             ↪ wav1D[ext])
352             pass

353
354     if self.can_plot:
355         # Plot transformed & normalized feature widths
356         plt.plot(spec1D_init[0], label="O, initial")
357         plt.plot(spec1D_init[1], label="E, initial")
358         plt.plot(spec1D[0], label="O spec")
359         plt.plot(spec1D[1], label="E spec")
360         plt.legend()
361         plt.show()

362     # Find observed skylines
363     # skyline_cols, properties = find_peaks(sky_norm,
364     ↪ prominence=0.2) # 1000
365     # prominence is basically the ylimit above which peaks should
366     ↪ be found
367     skyline_cols, skyline_wavs, properties = [], [], []
368     for ext in range(2):
369         cols, prop = signal.find_peaks(wav1D[ext], spec1D[ext],
370         ↪ prominence=1)
371         skyline_cols.append(cols)
372         properties.append(prop)
373         skyline_wavs.append(wav1D[ext, cols]) # col_to_wav(coeff2,
374         ↪ skyline_cols)

```

```

371     plt.plot(wav1D[ext, cols], cols, label='Observed')
372     plt.xlabel('Wavelength ($\AA$)')
373     plt.ylabel('Counts')
374     plt.legend()
375     plt.show()
376
377     for ext in range(2):
378         for i in range(len(skyline_cols[ext])):
379             logging.debug(("skylines - found features:\n"
380                           f"{properties[ext]['right_bases'][i] - "
381                           f"properties[ext]['left_bases'][i]:4d}\t"
382                           f"{skyline_cols[ext][i]:4d} - "
383                           f" {skyline_wavs[ext][i]:.1f} - "
384                           f" {properties[ext]['prominences'][i]:.2f}"
385                         ))
386
387
388     # Return results
389     return
390
391
392     # MARK: Plot
393     def plot(self, ) -> None:
394         plt.style.use(Path(__file__).parent.resolve() /
395                       'utils/STOPSS.mplstyle')
396
397         # Find deviation of observed skylines from known skylines
398
399         # Find feature / initial feature widths
400
401         # Load known skylines
402         skylines = self.load_sky_lines()
403
404         # Plot results
405         fig, axs = plt.subplots(3, self.ccds, sharex='row')
406
407         if self.ccds == 1:
408             # Convert axs to a 2D array
409             axs = np.swapaxes(np.atleast_2d(axs), 0, 1)
410
411         # Split skylines into ccds
412         split_sky = np.array_split(skylines, self.ccds)
413
414         for ccd in range(self.ccds):
415             # spectrum
416             axs[0, ccd].plot(
417                 split_sky[ccd]['wav'],
418                 split_sky[ccd]['flux'] / np.max(skylines['flux']),
419                 color='C4',
420                 label="\text{salt} sky lines",
421             )
422
423             # # OE intensity
424             # if self.beams == 'OE':
425             #     for ext in range(2):
426             #         axs[0, ccd].plot(
427             #             split_sky[ccd]['wav'],
428             #             split_sky[ccd]['flux'] /
429             #             np.max(skylines['flux']) + 0.5 * (ext + 1),

```

```

424         #           # color='C4',
425         #           label=f"E' if ext else 'O'", 
426         )
427
428     # # O or E intensity
429     # else:
430     #     for i, im in enumerate(images):
431     #         axs[0, ccd].plot(
432     #             im[ccd]['wav'],
433     #             im[ccd]['flux'] / np.max(im['flux']) + 0.5,
434     #             # color='C4',
435     #             label=f"${self.beams}_{i + 1}",
436     #         )
437
438
439     # for ext in range(2):
440     #     logging.debug(f"fl-{ext}: {wav[ext, lb]}:{wav[ext, ub
441     # - 1]}")
442
443     #     axs[1, ccd].plot(
444     #         wav[ext, lb:ub],
445     #         spec[ext, lb:ub] * abs(bpm[ext, lb:ub] * -1 + 1)
446     #         + OFFSET * ext,
447     #         label=(
448     #             f"${self.beams} if self.beams != 'OE' else
449     #             self.beams[ext]}"
450     #             f"-{ext + 1 if self.beams != 'OE' else 1}"
451     #             f"{{({} + str(OFFSET * ext) + {})}} if ext >
452     #             0 else ''}"
453     #             ),
454     #         )
455
456     axs[0, 0].set_ylabel("Norm. Intensity\n(Counts)")
457     axs[1, 0].set_ylabel("Closest Deviation\n($\sigma$)")
458     axs[2, 0].set_ylabel("$W / W_{i}$")
459     for ax in axs[-1, :]:
460         ax.set_xlabel(f"Wavelength ({self.wav_unit})")
461     for ax in axs[:, -1]:
462         ax.legend()
463
464     # plt.tight_layout()
465     # fig1 = plt.gcf()
466     # DPI = fig1.get_dpi()
467     # fig1.set_size_inches(700.0/float(DPI), 250.0/float(DPI))
468     plt.show()
469
470
471     # Save results
472     fig.savefig(fname=self.save_prefix)
473
474
475     return
476
477 def show_frame(self, frame: np.ndarray, title: str = None, label:
478     str = None, std: int = 1) -> None:
479     if not self.can_plot:
480         return
481
482     fig, axs = plt.subplots(2, 1)
483     axs[0].set_title(title)

```

```

477     axs[0].imshow(
478         frame[0],
479         label=f"O beam - {label}",
480         vmin=frame[0].mean() - std * frame[0].std(),
481         vmax=frame[0].mean() + std * frame[0].std()
482     )
483     axs[1].imshow(
484         frame[1],
485         label=f"E beam - {label}",
486         vmin=frame[1].mean() - std * frame[0].std(),
487         vmax=frame[1].mean() + std * frame[0].std()
488     )
489     for ax in axs: ax.legend()
490     plt.show()
491
492     return
493
494
495 # MARK: Process all listed images
496 def process(self,) -> None:
497     if self.beams == 'OE':
498         for fl in self.fits_list:
499             logging.info(f"'OE' skyline of {fl}.")
500             self.skylines(fl)
501             self.plot()
502
503     if self.beams in ['O', 'E']:
504         for fl in self.fits_list:
505             logging.info(f'{self.beams} skyline of {fl}.')
506             self.skylines(fl)
507             self.plot()
508
509     return
510
511
512 # MARK: Main function
513 def main(argv) -> None:
514     return
515
516 if __name__ == "__main__":
517     main(sys.argv[1:])

```


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List of Acronyms

IRAF	Image Reduction and Analysis Facility
POLSLAT	Polarimetric reductions for SALT
STOPS	Supplementary Tools for POLSLAT Spectro-polarimetry
ADC	Analog-to-Digital Converter
BPM	Bad Pixel Map
CCD	Charged-Coupled Device
CLI	Command Line Interface
CMOS	Complementary Metal-Oxide-Semiconductor
FITS	Flexible Image Transport System
FWHM	Full Width at Half Maximum
GUI	Graphical User Interface
HDU	Header Data Unit
HET	Hobby-Eberly Telescope
HRS	High Resolution Spectrograph
L+45°	Linear +45° Polarized
L-45°	Linear -45° Polarized
LCP	Left Circularly Polarized
LHP	Linear Horizontally Polarized
LVP	Linear Vertically Polarized
NIR	Near Infra-Red
NIRWALS	Near Infra-Red Washburn Labs Spectrograph
RCP	Right Circularly Polarized
RMS	Root Mean Square
RSS	Robert Stobie Spectrograph
S/N	Signal-to-Noise Ratio
SAAO	South African Astronomical Observatory
SALT	Southern African Large Telescope
SALTICAM	SALT Imaging Camera
UV	Ultraviolet
VPH	Volume Phase Holographic