

Supplementary wavelength calibration methods for SALT/RSS spectropolarimetric observations

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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.

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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.

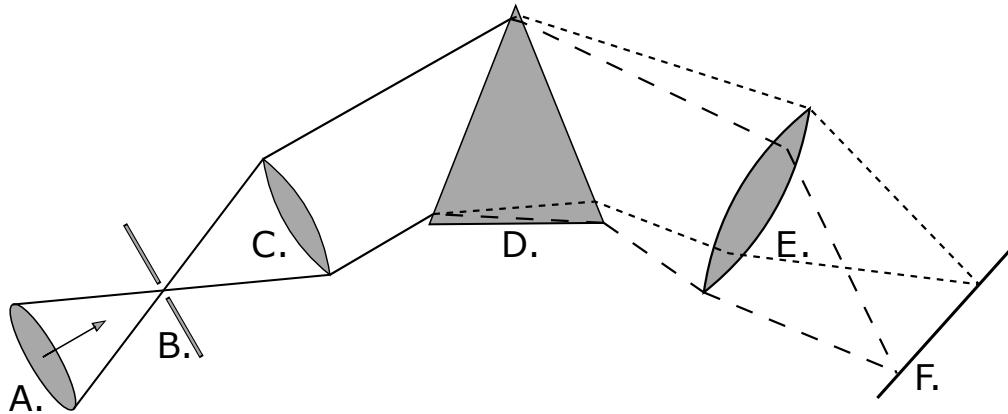


Figure 2.1: Layout depicting the light path through a spectrometer. Diagram adapted from Birney et al. (2006).

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

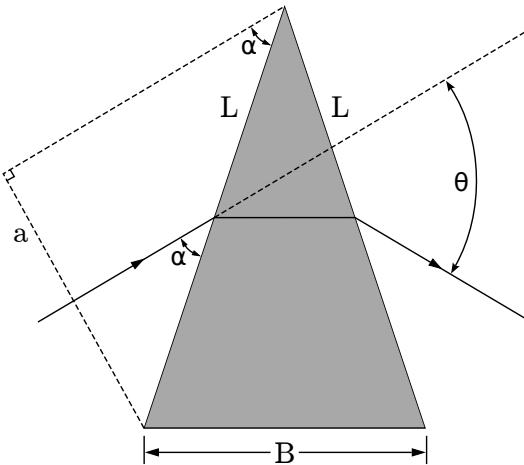


Figure 2.2: Geometry of a prism refracting an incident monochromatic beam at a minimum deviation angle. Diagram adapted from Birney et al. (2006).

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.

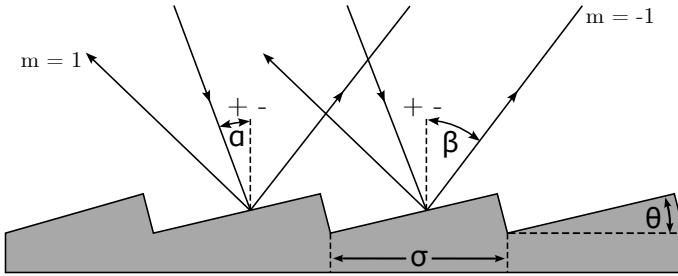


Figure 2.3: Geometry of a reflective blazed grating refracting an incident monochromatic beam. Diagram adapted from Birney et al. (2006).

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,

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

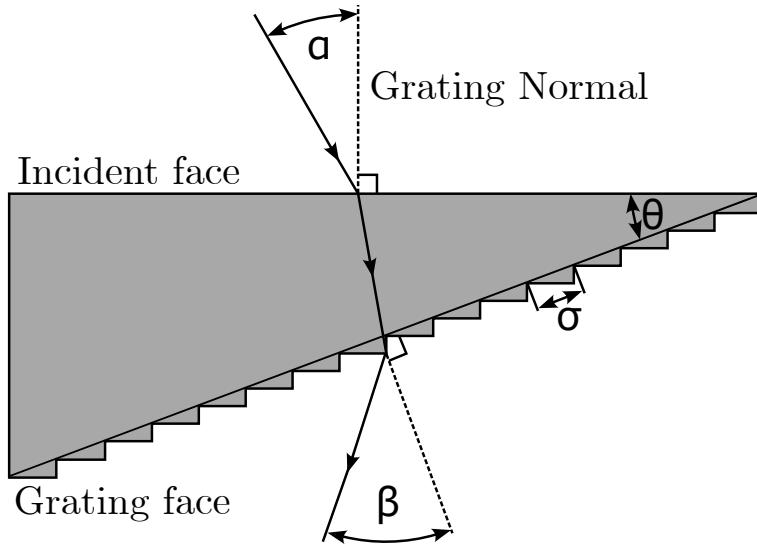


Figure 2.4: Diagram of a grism for an incident monochromatic beam of light and a diffracted beam of order $m = 1$. Diagram adapted from Birney et al. (2006).

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

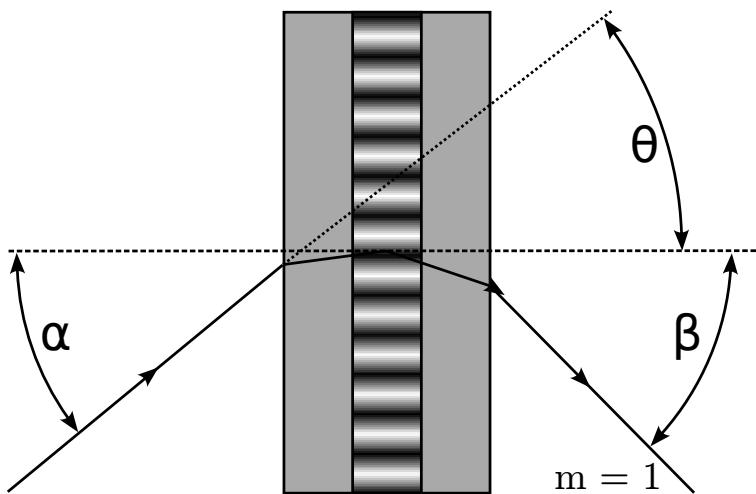


Figure 2.5: Diagram of a VPH grating for an incident monochromatic beam of light. Diagram adapted from Birney et al. (2006).

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

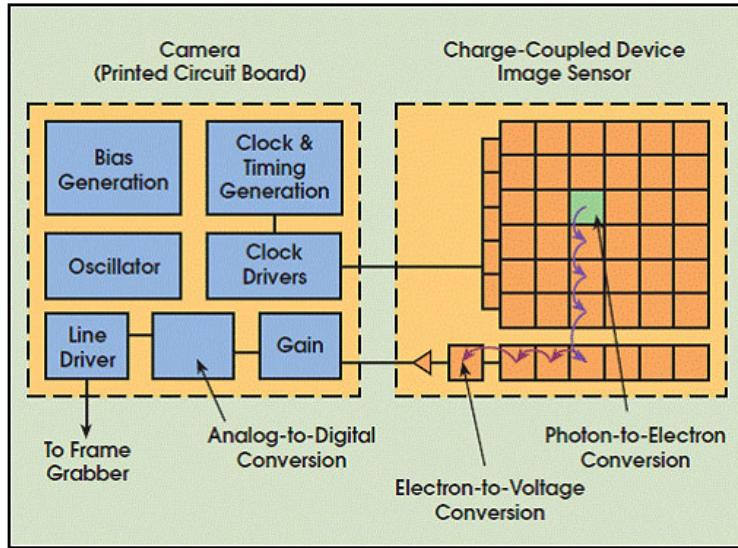


Figure 2.6: Diagram of the inner logic of a CCD. Figure adapted from Litwiller (2001).

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.

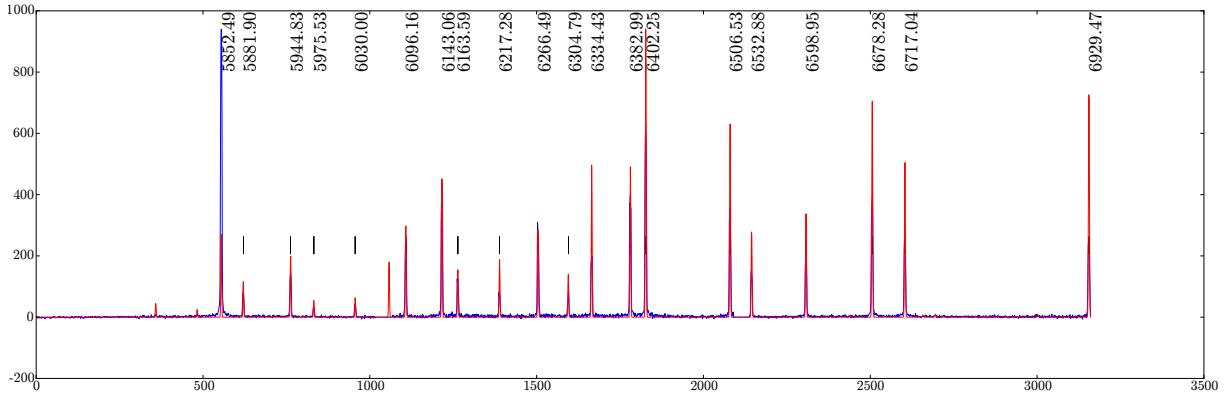


Figure 2.7: Example of an arc spectrum for NeAr taken with SALT’s RSS using the PG1800 grating at a grating angle of 34.625° , an articulation angle of 69.258° , and covering a wavelength range of $\sim 5600 - 6900 \text{ \AA}$. Plot adapted from SALT’s published Longslit Line Atlases, (2023).²

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/>

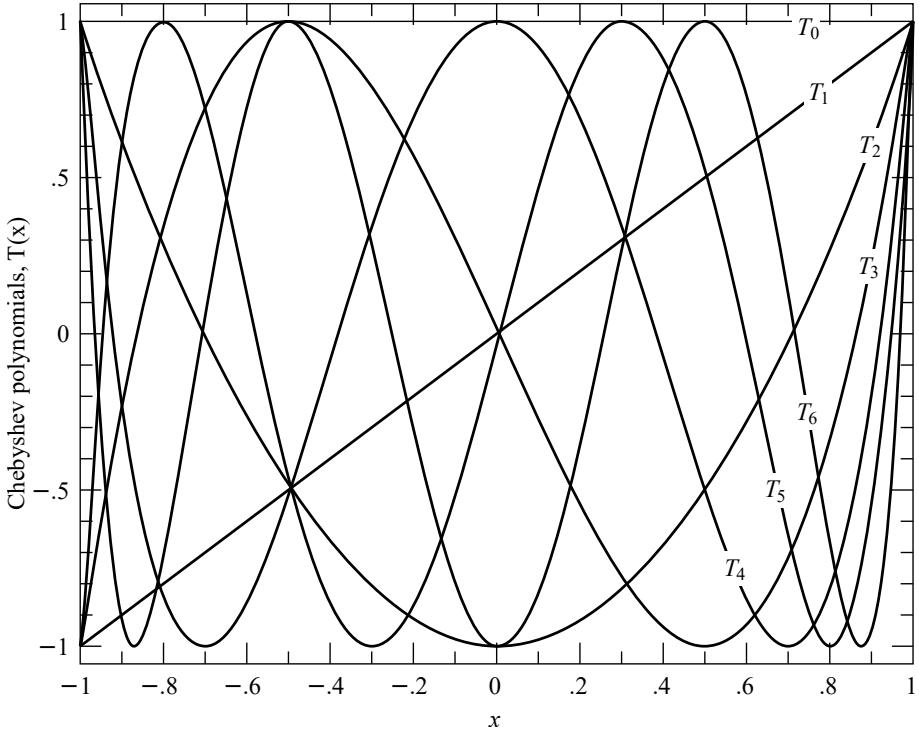


Figure 2.8: The first seven Chebyshev polynomials (T_0 through T_6) as defined by Equation 2.12 over the region $[-1, 1]$ for which they are orthogonal. Plot adapted from (Press et al., 2007) (2023)³

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’.

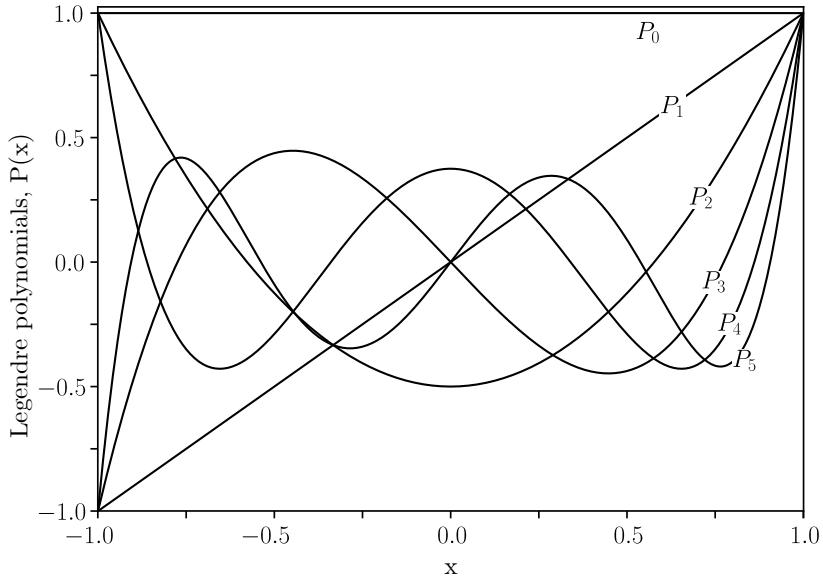


Figure 2.9: The first six Legendre polynomials (P_0 through P_5) as defined by Equation 2.20 over the region $[-1, 1]$ for which they are orthogonal. Plot adapted from Geek3, CC BY-SA 3.0, via Wikimedia Commons (2023).

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

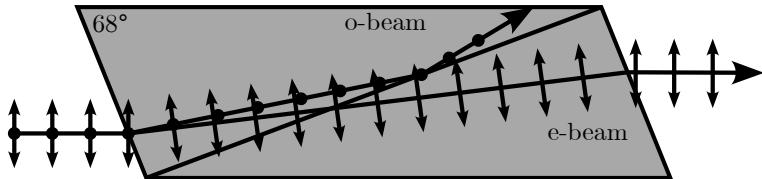


Figure 2.10: Diagram of a Nicol prism for incident non-polarized light. Diagram adapted from Fred the Oyster, CC BY-SA 4.0, via Wikimedia Commons (2023).

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:

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

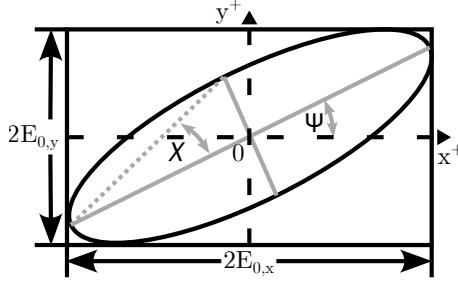


Figure 2.11: The polarization ellipse for an electric field vector propagating through free space. Diagram adapted from Inductiveload, PDM 1.0, via Wikimedia Commons (2023).

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

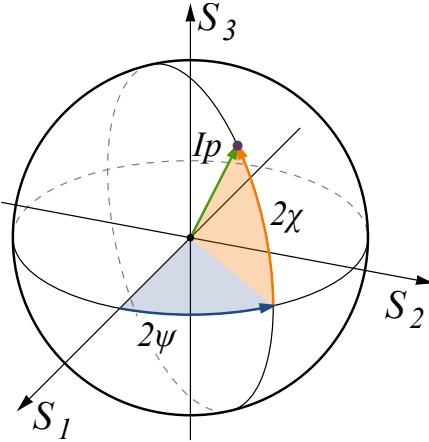


Figure 2.12: The Poincaré sphere describing the polarization properties of a wave-packet propagating through free space. Diagram adapted from Inductiveload, PDM 1.0, via Wikimedia Commons (2023).

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}

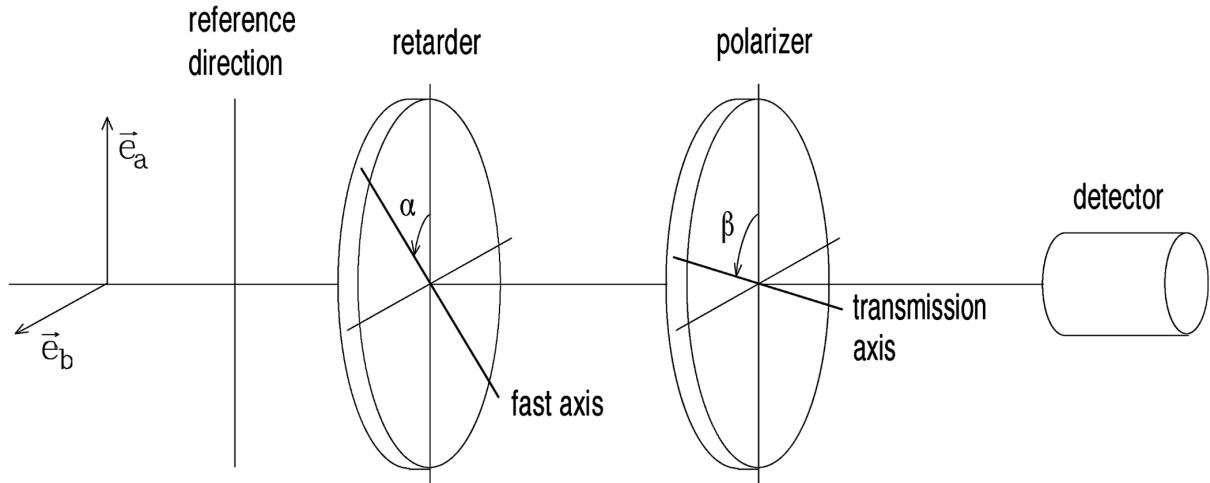


Figure 2.13: A diagram of an ideal polarimeter. Diagram adapted from Degl'Innocenti and Landolfi (2004).

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).

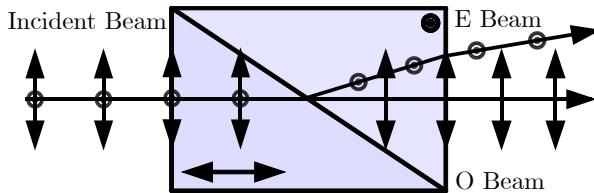


Figure 2.14: Diagram of a Rochon prism. Included in the diagram are the optical axes of the differing sections of the birefringent material as well as polarizing directions of the incident beam, denoted using the \leftrightarrow and \odot symbols, for the O - and E -beams, respectively. Figure adapted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

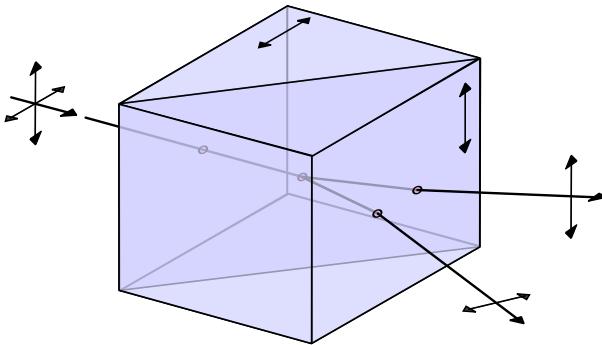


Figure 2.15: Diagram of a Wollaston prism. Included in the diagram are the optical axes of the differing sections of the birefringent material as well as polarizing directions of the incident beam, denoted using the \leftrightarrow and \ddagger symbols, for the O - and E -beams, respectively. Diagram 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.

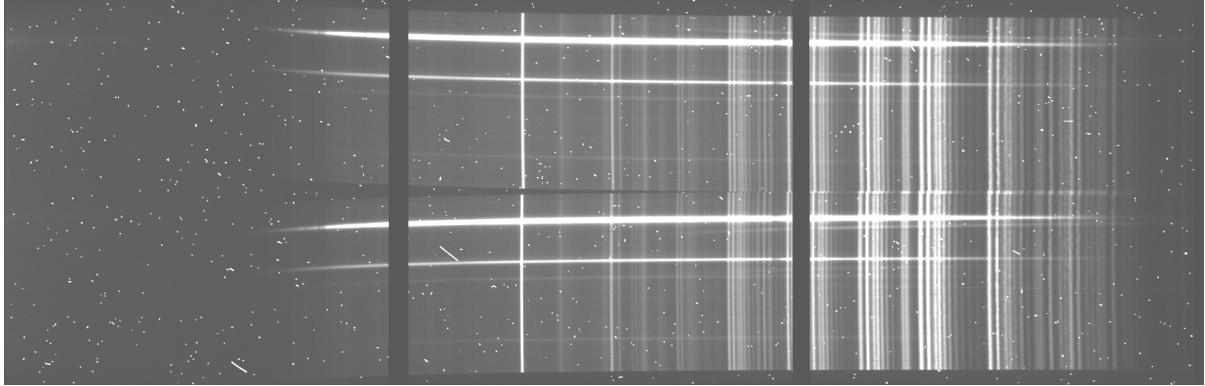


Figure 2.16: A spectropolarimetric target exposure as observed by the SALT RSS in spectropolarimetry mode.

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

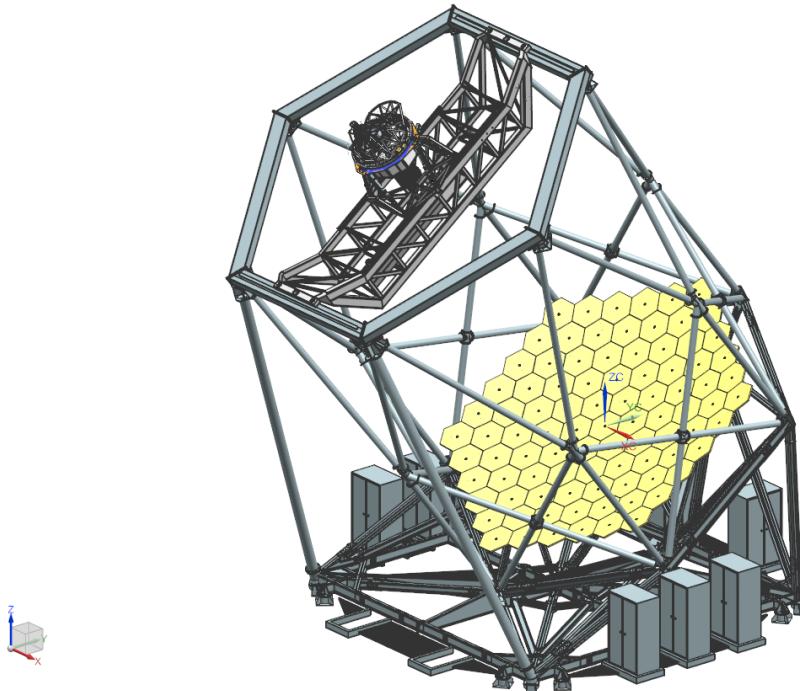


Figure 2.17: The tracker, supporting structure, and primary mirror of SALT. Figure adapted from the SALT call for proposals (2022).⁵

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

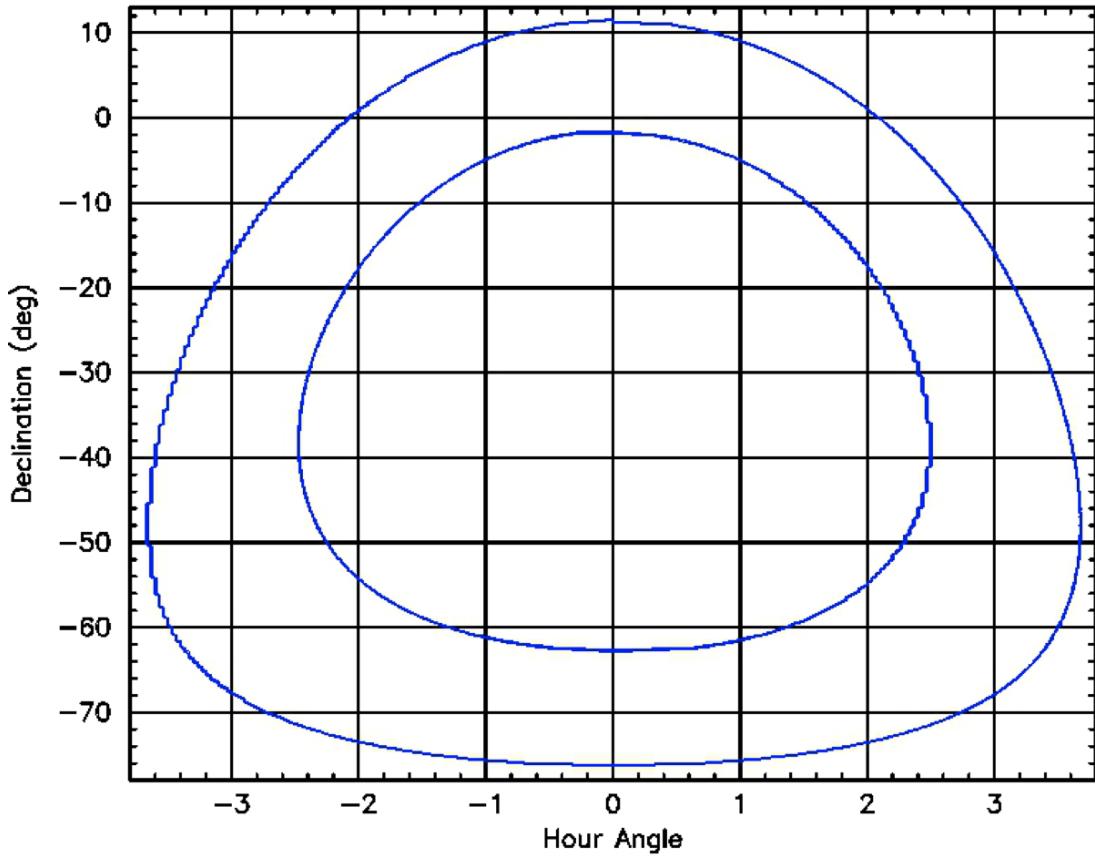


Figure 2.18: The visibility annulus of objects observable by SALT. Figure adapted from the SALT call for proposals (2013).⁶

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

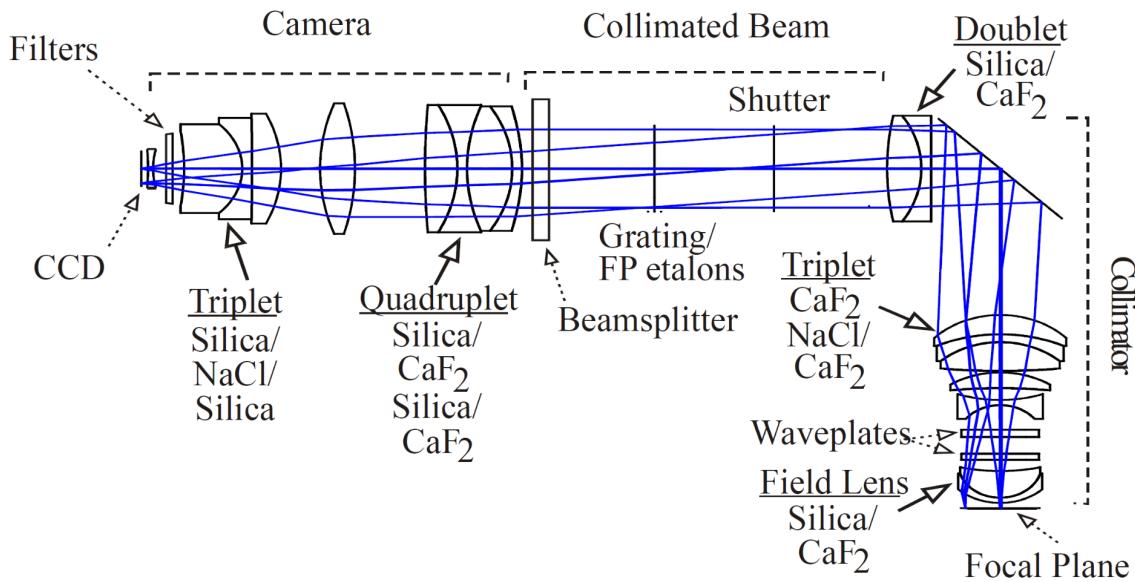


Figure 2.19: The optical path of the SALT RSS. Figure adapted from the SALT call for proposals (2023).⁷

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 POLSALT, IRAF, and STOPS

This chapter contains an overview of Polarimetric reductions for SALT (POLSALT) and the limitations faced during POLSALT wavelength calibrations ((§ 3.1)), a brief overview of the Image Reduction and Analysis Facility (IRAF) tasks relevant for spectropolarimetric wavelength calibrations (§ 3.2), and an overview of STOPS, the software developed to supplement the POLSALT 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 POLSALT - Polarimetric reductions for SALT

The POLSALT (Polarimetric reductions for SALT) pipeline 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), was the version adapted in this study. It includes a GUI, depicted in Figure 3.1, which allows for limited interactivity during key steps in the reduction process.²

The steps that make up the POLSALT 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 at each step are crucial for accurate results and are thus briefly discussed below. Further details for the reduction process may be found at the POLSALT GitHub wiki.³

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

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

²Installation 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.

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

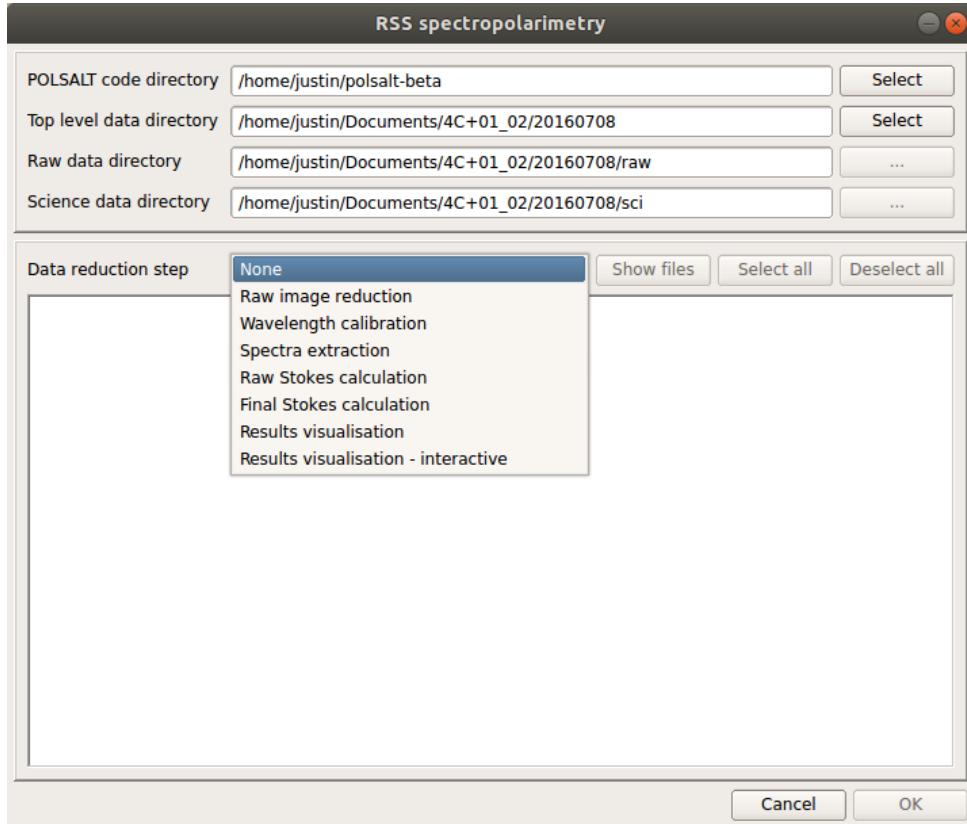


Figure 3.1: The layout of the `POLSALT` Graphical User Interface (GUI), including the contents of the reduction steps accessible via the dropdown menu. Note that there is no trailing forward slash after the ‘Top level data directory’. Figure created from a local instance of the `POLSALT` GUI.

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.

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 with Figure 3.2 depicting the interactive window used for spectral

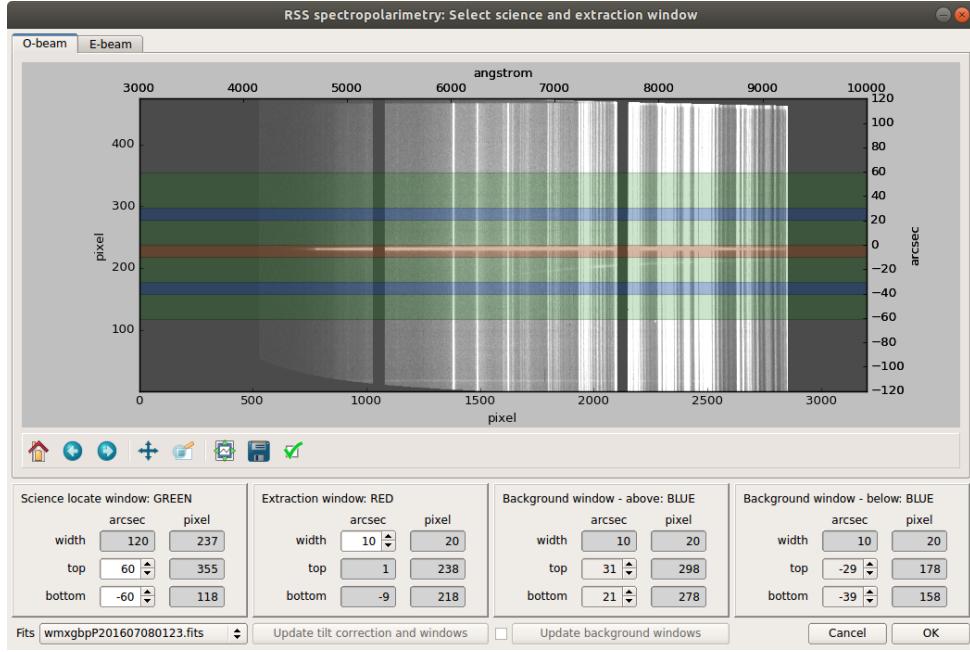


Figure 3.2: The layout of the interactive POLSALT spectra extraction GUI after selecting the ‘update tilt correction and windows’ button along the bottom border of the window. Figure created from a local instance of the POLSALT GUI.

extraction. The user, using the brightest trace in the image as a reference, defines regions which span the wavelength axis which define the background and trace regions for the sky subtraction and spectral extraction. Files with background and geometric 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

The 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 created files contain the raw Stokes information and use a very specific naming style, with most notably the index of the related waveplate pairs, from Table 2.2, being used included in the file names.

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 if a sufficient number of redundant exposures were taken, the raw Stokes signals are culled to eliminate outlier signals which may arise from, for example, temporary atmospheric conditions affecting the signal. The culling is

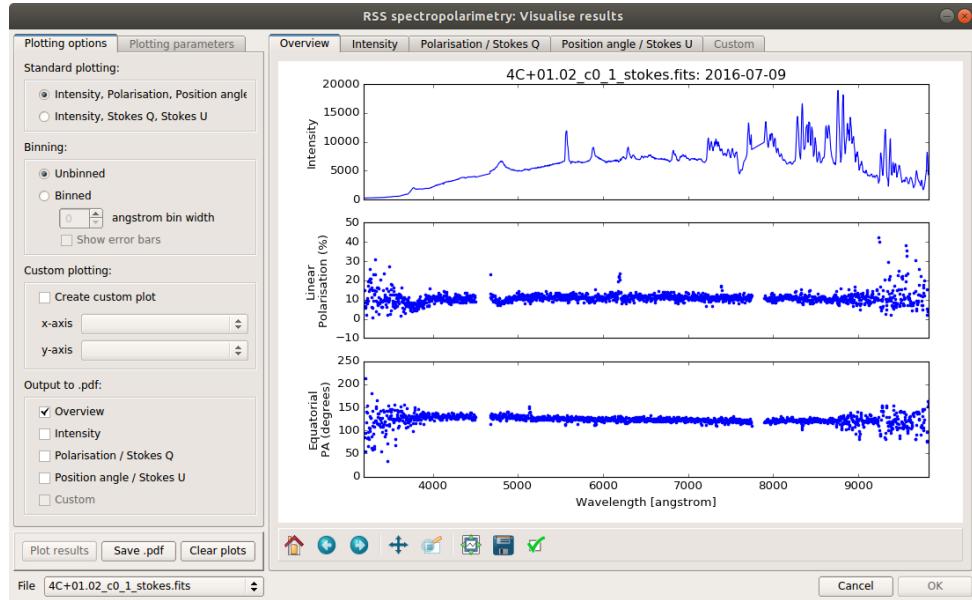


Figure 3.3: The layout of the interactive POLSALT visualization GUI after selecting the ‘Plot results’ button along the bottom border of the window. Figure created from a local instance of the POLSALT GUI.

performed by comparing observation cycles against one another, comparing the deviation of the signal means which estimate the baseline systematic polarization fluctuations (due to imperfections in repeatability), and performing a χ^2 analysis to eliminate any statistical 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.

Synthetic filtering is calculated via **specpolfilter.py** and computes the synthetically filtered polarization results. Any wavelength dependent throughput filter curve may be synthesized when defined by the user, but a few pre-defined filter curves are available, namely: the SALTICAM *U*, *B*, *V*, *R*, and *I* Johnson-Cousins filter curves.

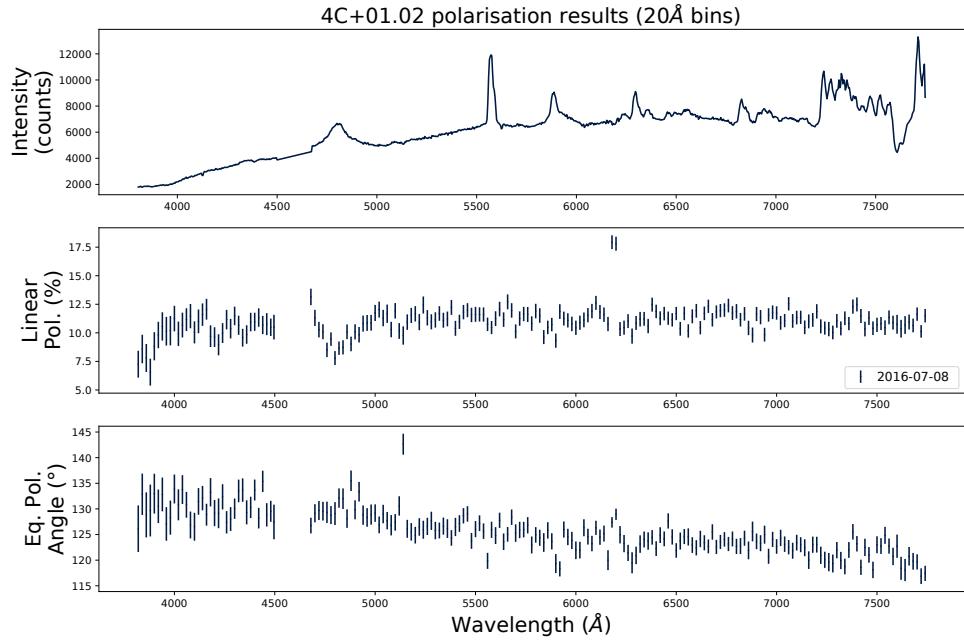


Figure 3.4: A typical plot resulting from the reduction process. Figure adapted from (Cooper et al., 2022).

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 program 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 led 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 higher order at large wavelengths (§ 2.1.7, Equation 2.5).

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

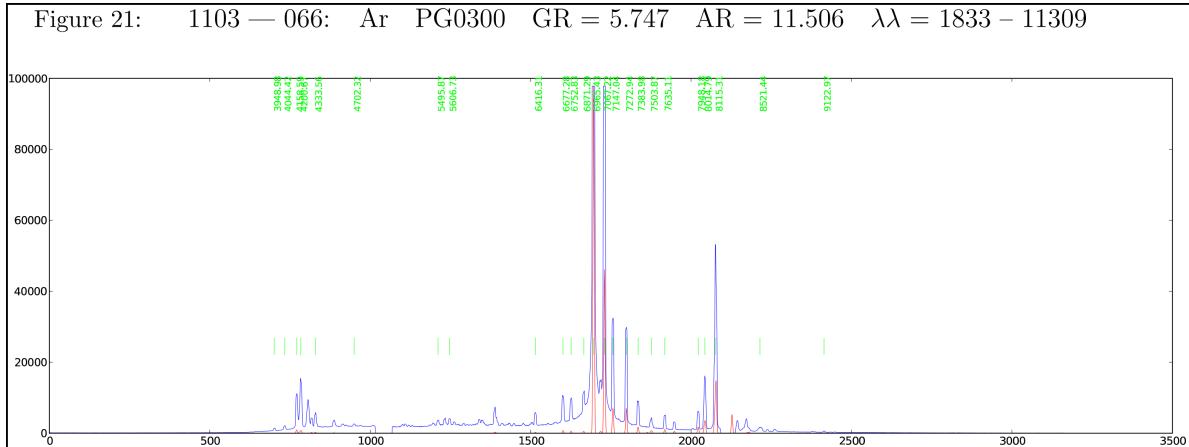


Figure 3.5: One of many Argon arc lamp spectra as provided by SALT for line identification. Plot adapted from SALT’s published Longslit Line Atlases (as of 2024), resized to fit within the document margins but otherwise unchanged.⁴

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 online⁵ 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,⁶ the `implot` task in the `plot` package which allows the rows or columns of an image to be interactively displayed,⁷ and the `eparam` task in the `language` package which allows the parameters of a task to be edited within the IRAF CLI.⁸

For wavelength calibrations of SALT spectropolarimetric data, the relevant tasks are

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

⁵<https://iraf.net/irafdocs/>

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

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

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

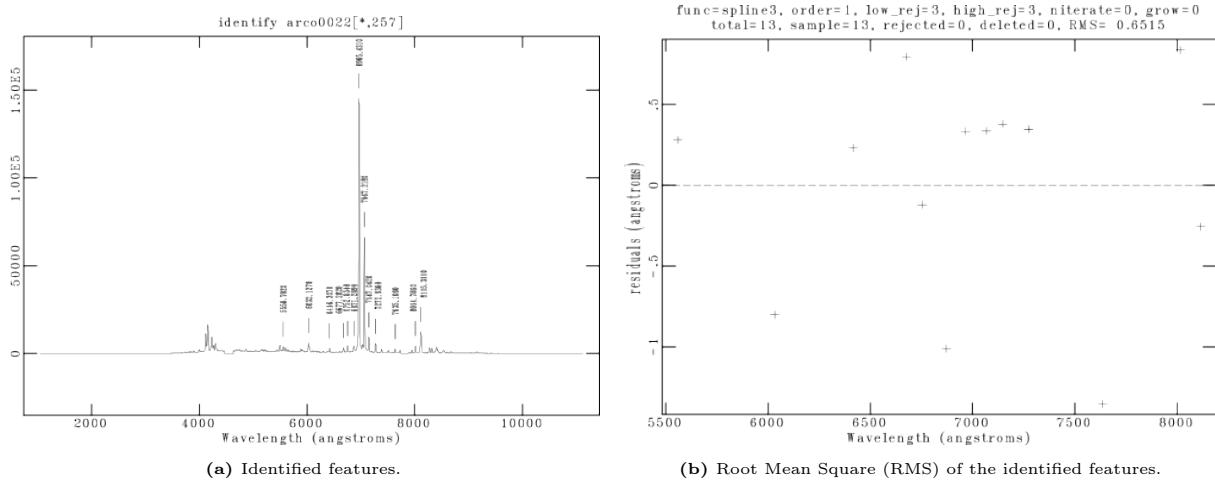


Figure 3.6: A plot and the RMS of the identified features found using the IRAF `identify` task. Figures created using the IRAF `identify` task.

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.⁹ The task creates the first approximation of the wavelength solution as well as a local database in which the solution is saved (see Listing 3.1). The initial 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 execution of `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.

⁹Help documentation for the `identify` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.onedspec.identify.html.

¹⁰See 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.¹⁰

```
# 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 (row) interval.¹¹ The task uses the one-dimensional wavelength solution stored in the database created by the initial `identify` call and refits the 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 if the task quit early. Regardless of whether the task quit successfully, the newly defined wavelength solutions are appended to the local database following the `identify` task database format, an example of which is given in Listing 3.1.

3.2.3 Fitcoords

The `fitcoords` task is used to find a two-dimensional surface function from the one-dimensional wavelength solutions found for specific rows in the previous steps.¹² 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 for each two-dimensional spectrum. It is saved using the `fitcoords` database format, an example of which is given in Listing 3.2, as the list of parameters and function coefficients required to recreate the closest two-dimensional model. The IRAF wavelength solution is used by the STOPS `join` method to create the wavelength extension required by POLSALT, further described in § 3.3.2.

3.2.4 Transform

The `transform` task is the optional final step in the IRAF wavelength calibration process.¹⁴ Simply put, `transform` converts the (pixel, pixel) units of an exposure to (wavelength, pixel) units which allows for an immediate check of whether the wavelength solution is consistent across the frame. Any general error in the wavelength solution may be spotted in the transformed images; ranging from minor errors, such as the arc lines or sky lines not being purely vertical across the frame, to more major errors, such as an incorrect wavelength solution skewing the exposure beyond recognition. For example, Figure 3.8a shows a good fit to the wavelength solution, as after transformation all the sky lines run exactly vertical. Figure 3.8b, on the other hand, shows a seemingly good fit, but closer

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

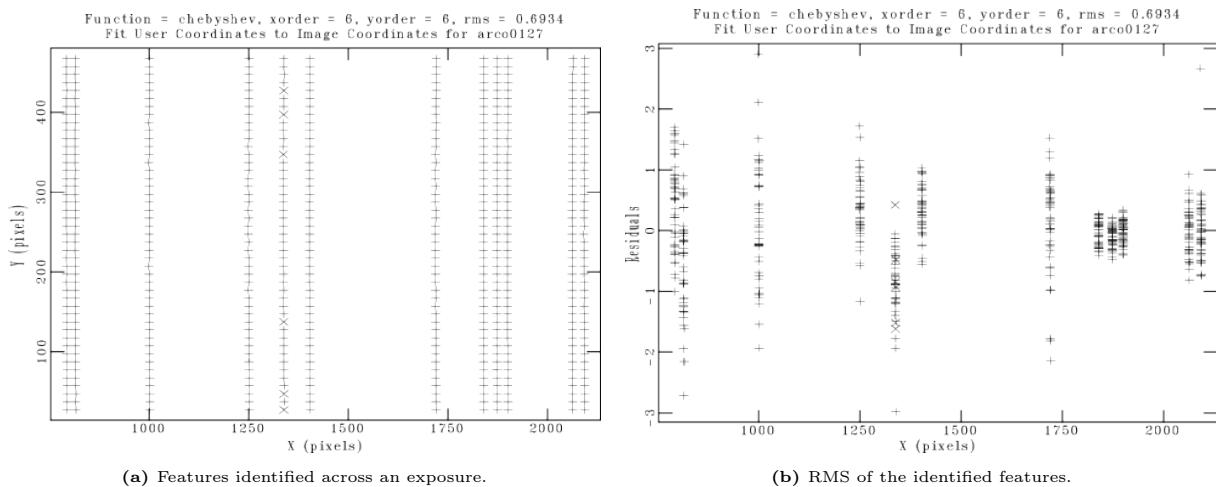
¹²Help documentation for the `fitcoords` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.twodspec.longslit.fitcoords.html.

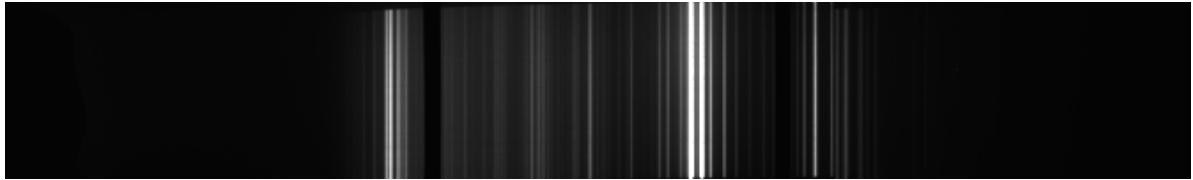
¹³See also <https://iraf.net/irafdocs/formats/fitcoords.php> for an explanation of the database contents.

¹⁴Help 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.¹³

```
# 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 poorly fit wavelength solution.

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

inspection reveals that the sky lines (especially towards the right of the frame) deviate from the vertical, indicating a poor fit to the wavelength solution.

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, 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 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 Flexible Image Transport System (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 """
99
```

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

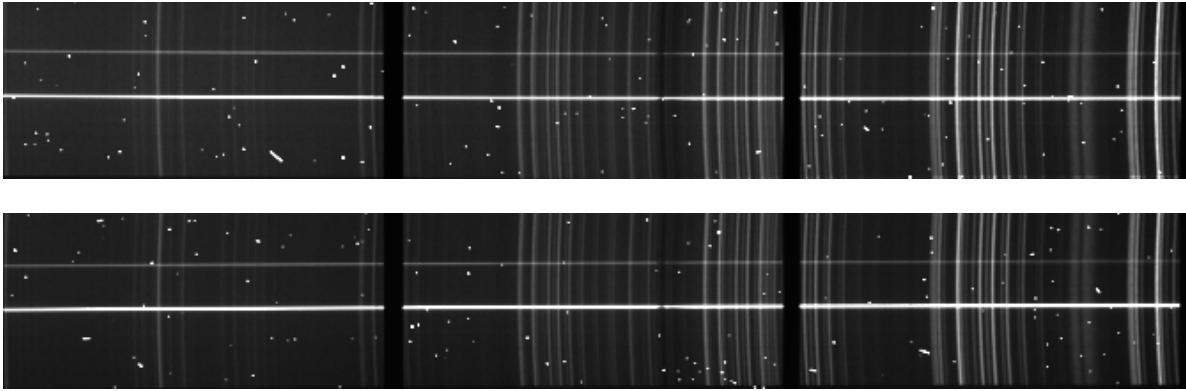


Figure 3.9: The split *O*- and *E*-beams as handed to IRAF. Figure created from the `STOPS split` method output.

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.

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.¹⁵ Otherwise, defaults, such as which row to split the beams along, were kept as close to the POLSALT pipeline as possible.

¹⁵Row 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 suggestions¹⁶ 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.

¹⁶Suggested 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

```

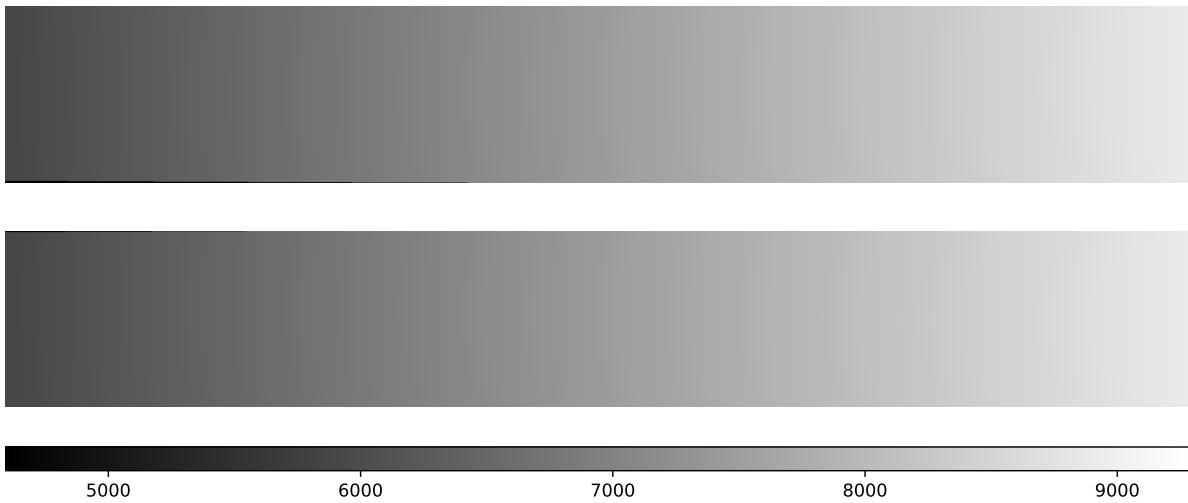


Figure 3.10: The wavelength extension of a FITS file ready to be handed back to the `POLSALT` pipeline. The color bar displays the wavelength in Å as displayed by the *O*- and *E*-beam sub-extensions. Note that regions which fall outside the exposed region are masked by setting the corresponding pixel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

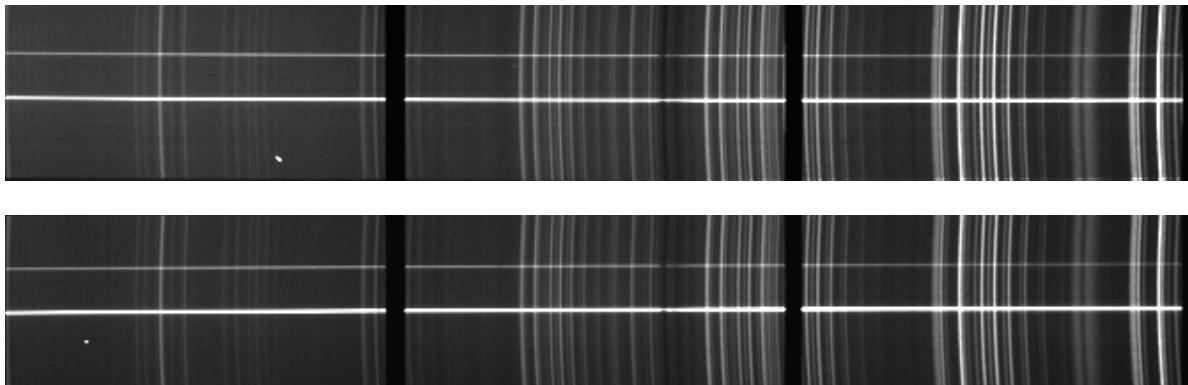


Figure 3.11: A representative science extension of a FITS file capable of being parsed by the `POLSALT` pipeline. The intensity of the *O*- and *E*-beam sub-extensions are displayed via the grayscale value at each pixel. Note the inclusion of regions of: solid black demarcating the chip gaps, horizontal 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,¹⁷ 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.¹⁸

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-

¹⁷The 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.

¹⁸The 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`

```

33 """
34     Class representing the Skylines object.
35
36     Parameters
37     -----
38     data_dir : Path
39         The directory containing the data files.
40     filenames : list[str]
41         The list of filenames to be processed.
42     beam : str, optional
43         The beam mode, by default "OE".
44     plot : bool, optional
45         Flag indicating whether to plot the continuum, by default False.
46     save_prefix : Path / None, optional
47         The prefix for saving the data, by default None.
48     **kwargs
49         Additional keyword arguments.
50
51     Attributes
52     -----
53     data_dir : Path
54         The directory containing the data files.
55     fits_list : list[str]
56         The list of fits file paths.
57     beam : str
58         The beam mode.
59     can_plot : bool
60         Flag indicating whether to plot the continuum.
61     save_prefix : Path / None
62         The prefix for saving the data.
63     wav_unit : str
64         The unit of wavelength.
65     rawWav : np.ndarray
66         The raw wavelength data.
67     rawSpec : np.ndarray
68         The raw spectral data.
69     rawBpm : np.ndarray
70         The raw bad pixel mask data.
71     corrWav : np.ndarray
72         The corrected wavelength data.
73     corrSpec : np.ndarray
74         The corrected spectral data.
75     spec : np.ndarray
76         The median spectrum.
77     normSpec : np.ndarray
78         The normalized spectrum.
79
80     Methods
81     -----
82     checkLoad(self, path1: str) -> np.ndarray:
83         Checks and loads the data from the given path.
84     transform(self, wav_sol: np.ndarray, spec: np.ndarray) -> np.ndarray:
85         Transforms the input wavelength and spectral data based on the given wavelength solution.
86     rmvCont(self) -> np.ndarray:
87         Removes the continuum from the spectrum.
88     process(self) -> None:
89         Placeholder method for processing the data.
90
91 """

```

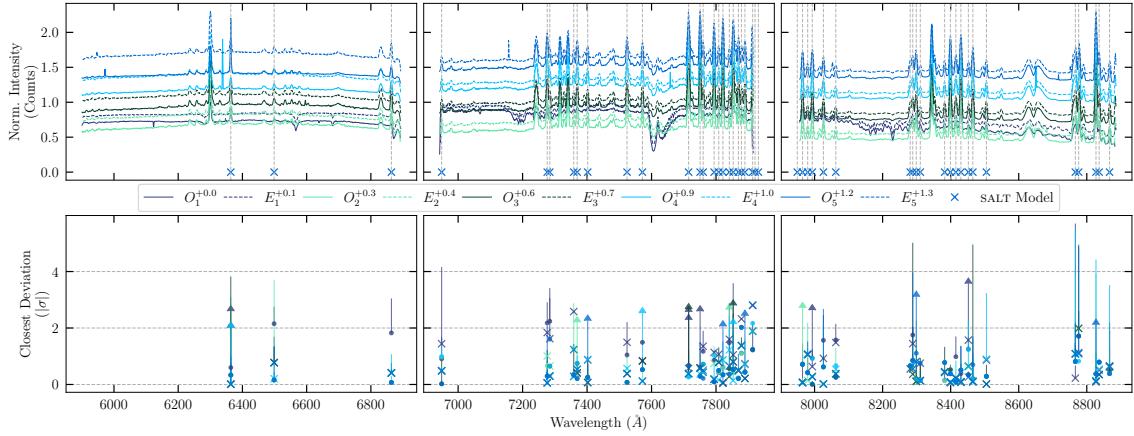


Figure 3.12: The resultant output plot of the `STOPS skyline` method, specifically for science images. Figure created via the `STOPS skyline` method.

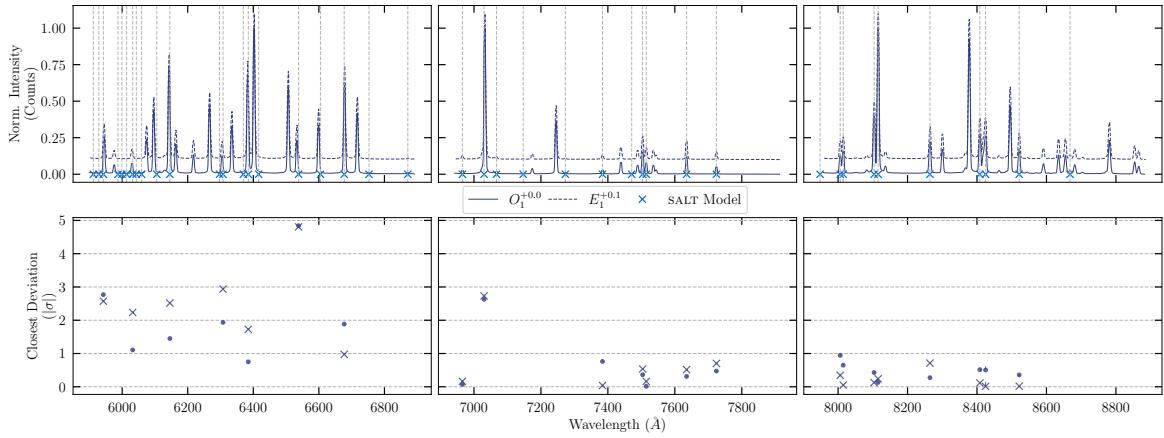


Figure 3.13: The resultant output plot of the `STOPS skyline` method, specifically for arc images. Figure created via the `STOPS skyline` method.

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.

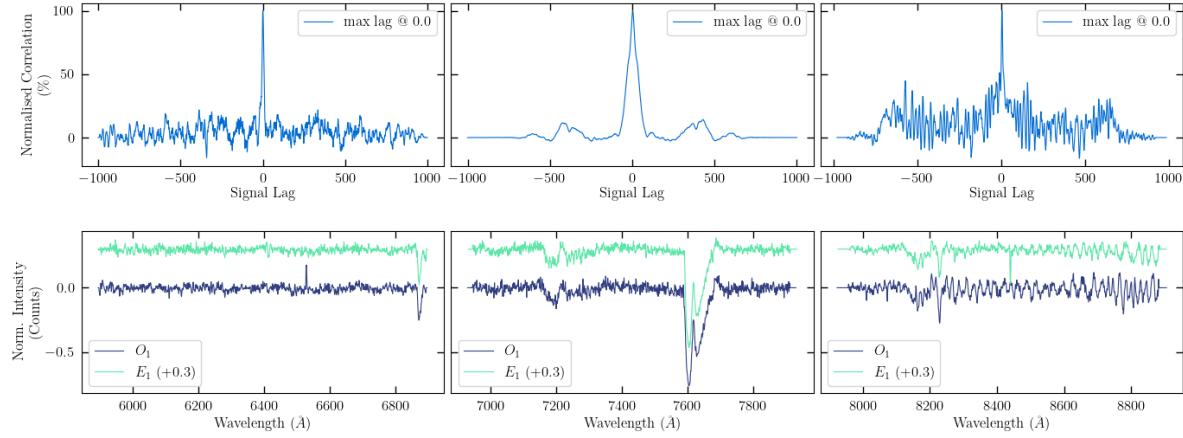


Figure 3.14: The resultant output plot of the `STOPS correlate` method. Figure created via the `STOPS correlate` method.

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.

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 3.14.

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

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 """

```

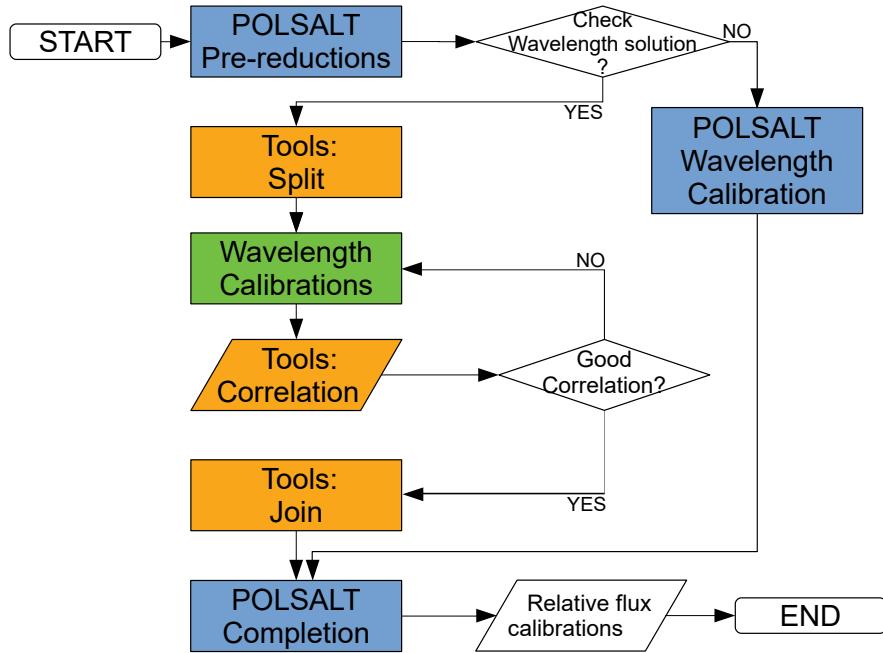


Figure 3.15: A general workflow for data reductions using a combination of POLSLT, IRAF, and the developed supplementary tools. Diagram adapted from Cooper et al. (2022).

that the software is running as intended.

3.4.1 Initial Setup

It is important to note that while POLSLT 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 POLSLT 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 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 POLSLT 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 POLSLT ‘beta’ scripts.

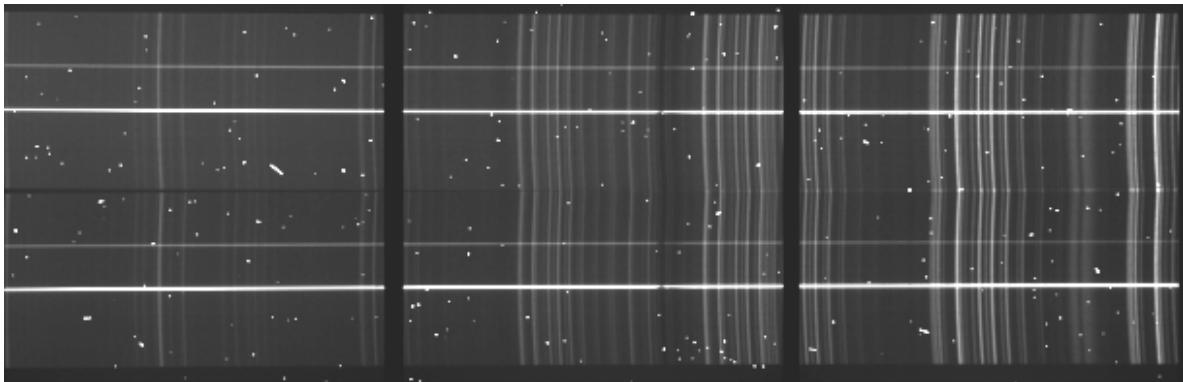


Figure 3.16: The science extension of a typical spectropolarimetric FITS file taken with the SALT RSS, after basic POLSALT CCD reductions have been completed. Figure created from the `STOPs split` output.

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.

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:¹⁹

```
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 `mkscript` 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.

¹⁹Please 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.

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 beamO* beamE* arcO* 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).²⁰

²⁰See the official POLSALT wiki or alternative online resources such as the SALT workshop slides.

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.

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.²¹

²¹Please 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, $\langle * \rangle$.

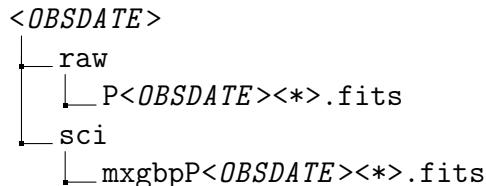


Figure I.1: The typical minimal file structure of data provided by SALT.

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 ("<0-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 ("@<0-beam FILES>",
>>> "t//@<0-beam FILES>", "<0-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.

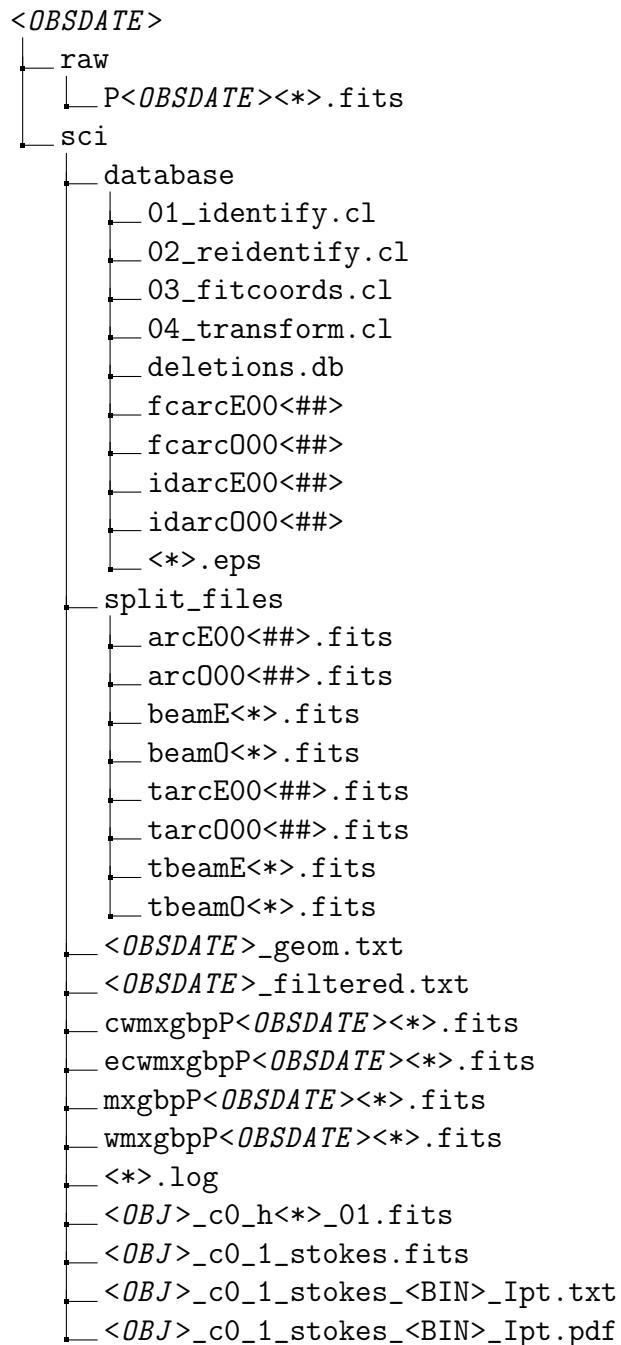


Figure I.2: The typical file structure after completing the reduction process.

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`

```

1  """Module for splitting ``polsalt`` FITS files."""
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 from copy import deepcopy
13 from pathlib import Path
14
15 import numpy as np
16 from astropy.io import fits as pyfits
17
18 from utils.SharedUtils import find_files, find_arc
19 from utils.Constants import SAVE_PREFIX, CROP_DEFAULT, SPLIT_ROW
20
21
22 # MARK: Split Class
23 class Split:
24
25     #-----split0-----
26
27     """
28     The `Split` class allows for the splitting of `polsalt` FITS files
29     based on the polarization beam. The FITS files must have basic
30     `polsalt` pre-reductions already applied (`mxgbp...` FITS files).
31
32     Parameters
33     -----
34     data_dir : str
35         The path to the data to be split
36     fits_list : list[str], optional
37         A list of pre-reduced `polsalt` FITS files to be split within `data_dir`.
38         (The default is None, `Split` will search for `mxgbp*.fits` files)
39     split_row : int, optional
40         The row along which to split the data of each extension in the
41         FITS file.
42         (The default is SPLIT_ROW (See Notes), the SALT RSS CCD's
43         middle row)
44     no_arc : bool, optional
45         Decides whether the arc frames should be recombined.
46         (The default is False, `polsalt` has no use for the arc after
47         wavelength calibrations)
48     save_prefix : dict[str, list[str]], optional
49         The prefix with which to save the O & E beams.
50         Setting `save_prefix` = ``None`` does not save the split O & E
51         beams.
52         (The default is SAVE_PREFIX (See Notes))
53
54     Attributes
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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     reverse: bool = True,
170 ) -> tuple[list[str], bool]:
171     """
172         Get the list of wavelength solution files.
173
174     Parameters
175     -----
176     wavlist : list[str] | None
177         A list of custom wavelength solutions files.
178         If ``None``, `Join` will search for wavelength solutions in
179         the `database` directory.
180     prefix : str, optional
181         The prefix of the wavelength solution files.
182         (Defaults to "fc")
183
184     Returns
185     -----
186     tuple[list[str], bool]
187         A tuple containing the list of wavelength solutions files
188         and
189         a boolean indicating whether custom solutions were provided.
190
191     """
192     # No custom solutions
193     if not wavlist:
194         # Handle finding solutions
195         ws = []
196         for fl in os.listdir(self.database):
197             if os.path.isfile(self.database / fl) and (prefix ==
198                 fl[0:len(prefix)]):
199                 ws.append(fl)
200
201         if len(ws) != 2:
202             # Handle incorrect number of solutions found
203             msg = (
204                 f"\"Incorrect amount of wavelength solutions \""
205                 f"\"{len(ws)} fc... files) found in the solution \""
206                 f"dir.: {self.database}\""
207             )
208             logging.error(msg)

```

```

    raise FileNotFoundError(msg)

208     sols = {i: j for i, j in zip(['0', 'E'], sorted(ws,
209         reverse=reverse))}
210     logging.debug(f"get_solutions - Found {sols} in
211         {self.database}")
212
213     return (sorted(ws, reverse=reverse), False)

214 # Custom solution
215 if len(wavlist) >= 2:
216     if len(wavlist) > 2:
217         logging.warning(f" Too many solutions, only
218             {wavlist[:2]} are considered")
219         wavlist = wavlist[:2]
220
221     for fl in wavlist:
222         if not os.path.isfile(os.path.join(self.data_dir, fl)):
223             msg = (
224                 f"{fl} not found in the "
225                 f"data directory {self.data_dir}"
226             )
227             logging.error(msg)
228             raise FileNotFoundError(msg)

229     sols = {i: j for i, j in zip(['0', 'E'], sorted(wavlist,
230         reverse=reverse))}
231     logging.debug(f"get_solutions - Found {sols} in
232         {self.database}")

233     return (sorted(wavlist, reverse=reverse), True)

234 # MARK: Parse 2D WAV Function
235 def parse_solution(
236     self,
237     fc_file: str,
238     xshape: int,
239     yshape: int
240 ) -> tuple[dict[str, int], np.ndarray]:
241     """
242         Parse the 2D wavelength solution function from `fc_file`.
243
244     Parameters
245     -----
246     fc_file : str
247         The filename of the wavelength solutions file.
248     xshape : int
249         The x-order of the 2D solution.
250     yshape : int
251         The y-order of the 2D solution.
252
253     Returns
254     -----
255     tuple[dict[str, int], np.ndarray]
256         A tuple containing a dictionary of the parameters of the
257             solution function
258             and the function coefficients.

```

```

258     """
259     fit_params = {}
260     coeff = []
261
262     if self.custom:
263         # Load coefficients
264         coeff = np.loadtxt(fc_file)
265
266         fit_params["xorder"] = coeff[0].astype(int)
267         fit_params["yorder"] = coeff[1].astype(int)
268         coeff = coeff[2:]
269
270         f_type = 3
271         if "cheb" in str(fc_file): f_type = 1
272         elif "leg" in str(fc_file): f_type = 2
273         fit_params["function"] = f_type
274
275         fit_params["xmin"], fit_params["xmax"] = 1, xshape
276         fit_params["ymin"], fit_params["ymax"] = 1, yshape
277
278     else:
279         # Parse IRAF fc database files
280         file_contents = []
281         with open(self.database / fc_file) as fcfile:
282             for i in fcfile:
283                 file_contents.append(re.sub(r"\n\t\s*", "", i))
284
285         if file_contents[9] != "1.": # xterms - Cross-term type
286             msg = (
287                 "Cross-term not recognised (always 1 for "
288                 "'FITCOORDS'), redo FITCOORDS or change manually."
289             )
290             raise Exception(msg)
291
292         fit_params["function"] = int(file_contents[6][-1])
293
294         fit_params["xorder"] = int(file_contents[7][-1])
295         fit_params["yorder"] = int(file_contents[8][-1])
296
297         fit_params["xmin"] = int(file_contents[10][-1])
298         fit_params["xmax"] = xshape
299         # int(file_contents[11][-1])# stretch fit over x
300         fit_params["ymin"] = int(file_contents[12][-1])
301         fit_params["ymax"] = yshape
302         # int(file_contents[13][-1])# stretch fit over y
303
304         coeff = np.array(file_contents[14:], dtype=float)
305
306         coeff = np.reshape(
307             coeff,
308             (fit_params["xorder"], fit_params["yorder"]))
309
310     return (fit_params, coeff)
311
312 # MARK: Join Files
313 def join_file(self, file: os.PathLike) -> None:
314     """
315

```

```

316 Join the `O`- and `E`-beams, attach the wavelength solutions,
317 perform cosmic ray cleaning, mask the extensions,
318 and checks cropping performed by `Split`.
319 Write the FITS file in a `polsalt` valid format.
320
321 Parameters
322 -----
323 file : os.PathLike
324     The path of the FITS file to be joined.
325
326 See Also
327 -----
328 IRAF - `fitcoords` task
329     https://iraf.net/irafdocs/formats/fitcoords.php,
330 numpy 2D grid functions
331     https://numpy.org/doc/stable/reference/generated/numpy
332 Chebyshev: + .polynomial.chebyshev.chebgrid2d.html
333 Legendre: + .polynomial.legendre.leggrid2d.html
334
335 """
336 # Create empty wavelength appended hdu list
337 whdu = pyfits.HDUList()
338 primary_ext = ""
339
340 # Handle prefix and names
341 pref = "arc" if file == self.arc else "beam"
342 o_file = self.save_prefix[pref][0] + file.name[-9:]
343 e_file = self.save_prefix[pref][1] + file.name[-9:]
344
345 # Open file
346 with pyfits.open(file) as hdu:
347     # Check if file has been cropped
348     cropsize = self.check_crop(hdu, o_file, e_file)
349
350     y_shape = int(hdu["SCI"].data.shape[0] / 2) - cropsize
351     x_shape = hdu["SCI"].data.shape[1]
352
353     # No differences in "PRIMARY" extention header
354     primary_ext = hdu["PRIMARY"]
355     whdu.append(primary_ext)
356
357     for ext in ["SCI", "VAR", "BPM"]:
358         whdu.append(pyfits.ImageHDU(name=ext))
359         whdu[ext].header = hdu[ext].header.copy()
360         whdu[ext].header["CTYPE3"] = "O,E"
361
362     # Create empty extentions with correct order and format
363     if ext == "BPM":
364         whdu[ext].data = np.zeros(
365             (2, y_shape, x_shape),
366             dtype="uint8"
367         )
368         whdu[ext].header["BITPIX"] = "-uint8"
369     else:
370         whdu[ext].data = np.zeros(
371             (2, y_shape, x_shape),
372             dtype=">f4"
373         )

```

```

374         whdu[ext].header["BITPIX"] = "-32"
375
376     # Fill in empty extention
377     if cropsize:
378         temp_split = split_sci(
379             hdu,
380             self.split_row,
381             ext=ext
382         )[ext].data
383         whdu[ext].data[0] = temp_split[0, cropsize:]
384         whdu[ext].data[1] = temp_split[1, 0:-cropsize]
385
386     else:
387         whdu[ext].data = split_sci(
388             hdu,
389             self.split_row,
390             ext=ext
391         )[ext].data
392     # End of hdu calls, close hdu
393
394     # MARK: Join (Wav. Ext.)
395     whdu.append(pyfits.ImageHDU(name="WAV"))
396     wav_header = whdu["SCI"].header.copy()
397     wav_header["EXTNAME"] = "WAV"
398     wav_header["CTYPE3"] = "O,E"
399     whdu["WAV"].header = wav_header
400
401     whdu["WAV"].data = np.zeros(
402         whdu["SCI"].data.shape,
403         dtype=">f4"
404     )
405
406     for num, fname in enumerate(self.fc_files):
407         params, coeffs = self.parse_solution(
408             fname,
409             x_shape,
410             y_shape
411         )
412
413         if params["function"] == 1: # Function type (1 = chebyshev)
414             # Set wavelength extention values to function
415             whdu["WAV"].data[num] = chebgrid2d(
416                 x=np.linspace(-1, 1, params["ymax"]),
417                 y=np.linspace(-1, 1, params["xmax"]),
418                 c=coeffs,
419             )
420
421         elif params["function"] == 2: # Function type (2 =
422             # legendre)
423             # Set wavelength extention values to function
424             whdu["WAV"].data[num] = leggrid2d(
425                 x=np.linspace(-1, 1, params["ymax"]),
426                 y=np.linspace(-1, 1, params["xmax"]),
427                 c=coeffs,
428             )
429
430         else:
431             msg = (

```

```

431             "Function type not recognised, please wavelength "
432             "calibrate using either chebychev or legendre."
433         )
434         raise Exception(msg)
435
436     # MARK: Cosmic Ray Cleaning
437     # See utils.Constants for `CR_PARAMS` discussion
438     whdu["SCI"].data[num] = lacosmic(
439         whdu["SCI"].data[num],
440         # contrast=CR_PARAMS['CR_CONTRAST'],
441         # threshold=CR_PARAMS['CR_THRESHOLD'],
442         # neighbor_threshold=CR_PARAMS['CR_NEIGH_THRESH'],
443         # effective_gain=CR_PARAMS['GAIN'],
444         # background=CR_PARAMS['BACKGROUND'],
445         readnoise=CR_PARAMS['READNOISE'],
446         gain=CR_PARAMS['GAIN'],
447         verbose=self.verbose,
448     )[0]
449
450     # MARK: WAV masking
451     # Left & Right Crop
452     whdu["WAV"].data[whdu["WAV"].data[:] < 3_000] = 0.0
453     whdu["WAV"].data[whdu["WAV"].data[:] >= 10_000] = 0.0
454
455     # Top & Bottom Crop (shift\tilt)
456     rpix_oc, cols, rbin, lam_c = read_wollaston(
457         whdu,
458         DATADIR + "wollaston.txt"
459     )
460
461     drow_oc = (rpix_oc - rpix_oc[:, int(cols / 2)][:, None]) / rbin
462
463     ## Cropping as suggested
464     for c, col in enumerate(drow_oc[0]):
465         if np.isnan(col):
466             continue
467
468         if int(col) < 0:
469             whdu["WAV"].data[0, int(col) :, c] = 0.0
470         elif int(col) > cropsize:
471             whdu["WAV"].data[0, 0 : int(col) - cropsize, c] = 0.0
472
473     for c, col in enumerate(drow_oc[1]):
474         if np.isnan(col):
475             continue
476
477         if int(col) > 0:
478             whdu["WAV"].data[1, 0 : int(col), c] = 0.0
479         elif (int(col) < 0) & (abs(int(col)) > cropsize):
480             whdu["WAV"].data[1, int(col) + cropsize :, c] = 0.0
481
482     # MARK: BPM masking
483     whdu["BPM"].data[0] = np.where(
484         whdu["WAV"].data[0] == 0,
485         1,
486         whdu["BPM"].data[0]
487     )
488     whdu["BPM"].data[1] = np.where(

```

```

489         whdu["WAV"].data[1] == 0,
490         1,
491         whdu["BPM"].data[1]
492     )
493
494     whdu.writeto(f"w{os.path.basename(file)}", overwrite="True")
495
496     return
497
498 # MARK: Check Crop
499 def check_crop(
500     self,
501     hdu: pyfits.HDUList,
502     o_file: str,
503     e_file: str
504 ) -> int:
505     """
506     Check if cropping is necessary when joining `O`- and `E`-beams.
507
508     Parameters
509     -----
510     hdu : astropy.io.fits.HDUList
511         The HDUList to check for cropping.
512     o_file : str
513         The name of the previously split `O`-beam FITS file.
514     e_file : str
515         The name of the previously split `E`-beam FITS file.
516
517     Returns
518     -----
519     int
520         The number of rows which were cropped by `Split`.
521
522     """
523     cropsize = 0
524     o_y = 0
525     e_y = 0
526
527     with pyfits.open(o_file) as o,
528         pyfits.open(e_file) as e:
529         o_y = o[0].data.shape[0]
530         e_y = e[0].data.shape[0]
531
532     if hdu["SCI"].data.shape[0] != (o_y + e_y):
533         # Get crop size, assuming crop same on both sides
534         cropsize = int((hdu["SCI"].data.shape[0] - o_y - e_y) / 2)
535
536     return cropsize
537
538 # MARK: Process all Listed Images
539 def process(self) -> None:
540     """Process all FITS images stored in the `fits_list`  

541     ↳ attribute"""
542     for target in self.fits_list:
543         logging.debug(f"Processing {target}")
544         self.join_file(target)
545

```

```
546
547
548 def main(argv) -> None:
549     """Main function."""
550     return
552
553
554 if __name__ == "__main__":
555     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         'OE' for same file, and 'O' 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     scipy
120         https://docs.scipy.org/doc/scipy/reference/generated/
121         correlation: scipy.signal.correlate.html
122
123     Notes
124     -----
125     Constants Imported (See utils.Constants):
126         SAVE_CORR
127
128     #-----corr1-----
129
130     # MARK: Correlate init
131     def __init__(
132         self,
133         data_dir: Path,
134         filenames: list[str],
135         beams: str = "OE",
136         split_ccd: bool = True,
137         cont_ord: int = 11,
138         plot: bool = False,
139         offset: int = 0,
140         save_prefix: Path | None = None,
141         **kwargs
142     ) -> None:
143         self.data_dir = data_dir
144         self.fits_list = find_files(
145             data_dir=self.data_dir,
146             filenames=filenames,
147             prefix="ecwmxgbp",
148             ext="fits",
149         )
150         self._beams = None
151         self.beams = beams
152         self.ccds = 1
153         if split_ccd:
154             # BPM == 2 near center of CCD if CCD count varies
155             with pyfits.open(self.fits_list[0]) as hdu:
156                 self.ccds = sum(hdu["BPM"].data.sum(axis=1)[0] == 2)
157
158         self.cont_ord = cont_ord
159         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
173     self.save_prefix = save_prefix
174     # Handle directory save name
175     if self.save_prefix and self.save_prefix.is_dir():
176         self.save_prefix /= SAVE_CORR
177         logging.warning((
178             f"Correlation save name resolves to a directory. "
179             f"Saving under {self.save_prefix}"
180         ))
181
182     self.wav_unit = "$\AA$"
183     self.wav_cdelt = 1
184
185     self.alt = self.FTCS if kwargs.get("FTCS") else None
186
187     logging.debug("__init__ - \n", self.__dict__)
188     return
189
190     # MARK: Beams property
191     @property
192     def beams(self) -> str:
193         return self._beams
194
195     @beams.setter
196     def beams(self, mode: str) -> None:
197         if mode not in ['O', 'E', 'OE']:
198             errMsg = f"Correlation mode '{mode}' not recognized."
199             logging.error(errMsg)
200             raise ValueError(errMsg)
201
202         self._beams = mode
203
204     return
205
206     # MARK: Load file
207     def load_file(
208         self,
209         filename: Path
210     ) -> tuple[np.ndarray, np.ndarray, np.ndarray]:
211         """
212             Load the data from a FITS file.
213
214             Parameters
215             -----
216             filename : Path
217                 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 != 'OE':
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 axs 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             ),

```

```

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             if self.beams != 'OE' and len(self.fits_list) == 1:
538                 # change mode to OE with warning
539                 logging.warning((
540                     f"`{self.beams}` correlation not possible for "
541                     "a single file. correlation `mode` changed to 'OE'."
542                 ))
543                 self.beams = 'OE'
544
545             # OE `mode` (same file, diff. ext.)
546             if self.beams == 'OE':
547                 for fl in self.fits_list:
548                     logging.info(f'"OE` correlation of {fl}.')
549                     (spec, wav, bpm), (corr, lags) = self.correlate(fl,
550                         ↪ alt=self.alt)
551                     self.plot(spec, wav, bpm, corr, lags)
552
553             # O/E `mode` (diff. files, same ext.)
554             for fl1, fl2 in iters.combinations(self.fits_list, 2):
555                 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
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, FIND_PEAK_PARAMS, ARC_FILE
22
23 # print([logging.getLogger(name) for name in
24 #        ↪ logging.root.manager.loggerDict])
25 mpl_logger = logging.getLogger('matplotlib')
26 mpl_logger.setLevel(logging.INFO)
27 pil_logger = logging.getLogger('PIL')
28 pil_logger.setLevel(logging.INFO)
29 # plt.rcParams['figure.figsize'] = (20, 4)
30
31 # MARK: Skylines Class
32 class Skylines:
33
34     """"
35         Class representing the Skylines object.
36
37         Parameters
38         -----
39         data_dir : Path
40             The directory containing the data files.
41         filenames : list[str]
42             The list of filenames to be processed.
43         beam : str, optional
44             The beam mode, by default "OE".
45         plot : bool, optional
46             Flag indicating whether to plot the continuum, by default False.
47         save_prefix : Path / None, optional
48             The prefix for saving the data, by default None.
49         **kwargs
50             Additional keyword arguments.
51
52         Attributes
53         -----
54         data_dir : Path

```

```

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

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

```

```

111         filenames=filenames ,
112         prefix="wmxgbp", # t[o/e]beam
113         ext="fits",
114         sep_arc=True ,
115     )
116     self._beams = None
117     self.beams = beams
118     self.ccds = 1
119     if split_ccd:
120         # See cross_correlate for initial implementation
121         self.ccds = 3
122
123     self.cont_ord = cont_ord
124     self.can_plot = plot
125     self.must_transform = transform
126
127     self.save_prefix = save_prefix
128     # Handle directory save name
129     if self.save_prefix and self.save_prefix.is_dir():
130         self.save_prefix /= SAVE_SKY
131         logging.warning((
132             f"Skylines save name resolves to a directory. "
133             f"Saving under {self.save_prefix}"
134         ))
135
136     self.max_difference = 5
137
138     self.wav_unit = "$\AA$"
139
140     logging.debug("__init__ - \n", self.__dict__)
141
142     return
143
144     # MARK: Beams property
145     @property
146     def beams(self) -> str:
147         return self._beams
148
149     @beams.setter
150     def beams(self, mode: str) -> None:
151         if mode not in ['O', 'E', 'OE']:
152             errMsg = f"Correlation mode '{mode}' not recognized."
153             logging.error(errMsg)
154             raise ValueErrorerrMsg
155
156         self._beams = mode
157
158     return
159
160     # MARK: Find Peaks
161     def find_peaks(
162         self,
163         spec: np.ndarray ,
164         axis: int | None = None ,
165         min_height: float = 0.5,
166         **kwargs ,
167     ) -> tuple[np.ndarray, np.ndarray]:
168         """

```

```

169     Finds the peaks in the given spectral data.
170
171     Parameters
172     -----
173     spec : np.ndarray
174         The spectral data.
175     bpm : np.ndarray
176         The bad pixel mask.
177     min_height : float, optional
178         The minimum height of the peaks, by default 0.5.
179     rel_height : float, optional
180         The relative height of the peaks, by default 0.05.
181
182     Returns
183     -----
184     peaks, properties : tuple[np.ndarray, dict]
185         The peaks and their properties.
186
187     """
188     peaks = []
189     props = []
190
191     for ext in range(len(self.beams)):
192         if axis is None:
193             row_mean = spec[ext]
194         else:
195             row_mean = np.mean(spec[ext], axis=axis)
196
197         peak, property = signal.find_peaks(
198             row_mean,
199             prominence=min_height * np.max(row_mean),
200             width=0,
201             **kwargs,
202         )
203         peaks.append(peak)
204         props.append(property)
205
206     if self.can_plot:
207         fig, axs = plt.subplots(2, 1)
208         for ext in range(len(self.beams)):
209             axs[ext].plot(row_mean, label=f"'E' if ext else 'O'")
210             axs[ext].plot(peak, row_mean[peak], "x", label=f"'E'"
211             ↪ if ext else 'O'} peaks")
212             axs[ext].legend()
213             plt.show()
214
215         logging.debug(f"find_peaks - peaks: {[len(i) for i in peaks]}")
216         logging.debug(f"find_peaks - props: {[key for key in
217             ↪ props[0].keys()]}")
218
219         return peaks, props
220
221     # MARK: Min. of Diff. Matrix
222     @staticmethod
223     def min_diff_matrix(A: np.ndarray, B: np.ndarray, max_diff: int =
224         100) -> np.ndarray:
225         """
226             Find the minimum difference between the elements of two arrays.

```

```

224
225     Parameters
226     -----
227     A : np.ndarray
228         The first 1d array.
229     B : np.ndarray
230         The second 1d array.
231     max_diff : int, optional
232         The maximum difference allowed, by default -1.
233
234     Returns
235     -----
236     A : np.ndarray (len(A))
237         The elements of the first array.
238     min_vals : np.ndarray (len(A))
239         The minimum difference between the elements of the two
240         ↪ arrays.
241     min_idxs : np.ndarray (len(A))
242         The indices of the minimum difference between the elements
243         ↪ of the two arrays.
244
245     """
246     # Compute the difference matrix using transpose
247     diff = np.abs(A - B[:, np.newaxis])
248
249     # Find the minimum value in each row (A) of `diff`
250     min_vals = np.min(diff, axis=0)
251     min_idxs = np.argmin(diff, axis=0)
252     # TODO: Recalculate min_val after selecting best min_val and
253     #       removing the corresponding row/column
254
255     max_mask = min_vals <= max_diff
256
257     return A[max_mask], min_vals[max_mask], min_idxs[max_mask]
258
259     # MARK: Load File Data
260     def load_file_data(
261         self,
262         filename: Path
263     ) -> tuple[np.ndarray, np.ndarray, np.ndarray]:
264         """
265             Loads the data from the given file.
266
267         Parameters
268         -----
269         filename : Path
270             The path to the file to be loaded.
271
272         Returns
273         -----
274         spec, wav, bpm : tuple[np.ndarray, np.ndarray, np.ndarray]
275             The wavelength, spectral, and bad pixel mask data.
276
277         """

```

```

278     # Load data from self.beams extension
279     with pyfits.open(filename) as hdul:
280         exts = [0, 1] if len(self.beams) == 2 else 0 + self.beams
281         ↪ == 'E'
282         spec2D = np.atleast_3d(hdul["SCI"].data[exts])
283         wav2D = np.atleast_3d(hdul["WAV"].data[exts])
284         bpm2D = np.atleast_3d(hdul["BPM"].data[exts].astype(bool))
285
286         logging.info(f"load_file_data - {filename.name} - shape:
287         ↪ {spec2D.shape}")
288
289     return spec2D, wav2D, bpm2D
290
291
292     # MARK: Load Sky or Arc Lines
293     def load_lines(
294         self,
295         filename: Path | None = None,
296         dtype: list[tuple] = [('wav', float), ('flux', float)],
297         skip_header: int = 3,
298         skip_footer: int = 1
299     ) -> np.ndarray:
300         """
301             Loads the sky or arc lines from the given file.
302
303             Parameters
304             -----
305             filename : Path / None, optional
306                 The path to the file to be loaded.
307                 Defaults to loading the skylines from `utils/sky.salt`.
308
309             Returns
310             -----
311             sky_lines : np.ndarray['wav', 'flux']
312                 The sky lines from the file.
313
314             """
315             usecols = None
316             if filename:
317                 filename = Path(__file__).parent.resolve() / filename
318                 usecols = (0, 1)
319             else:
320                 filename = Path(__file__).parent.resolve() /
321                 ↪ 'utils/sky.salt'
322
323             lines = np.genfromtxt(filename, dtype=dtype,
324             ↪ skip_header=skip_header, skip_footer=skip_footer,
325             ↪ usecols=usecols)
326
327             logging.debug(f"load_lines - {filename.name} - shape:
328             ↪ {lines.shape}")
329
330             return lines
331
332
333     # MARK: Mask Traces
334     def mask_traces(
335         self,
336         spec: np.ndarray,
337         bpm: np.ndarray,
338

```

```

330         max_traces: int = 1,
331         tr_pad: int = 5,
332         bg_margin: int = 10,
333         lr_margins: list[int] = [10, 10],
334         h_min: float = 0.5,
335         h_rel: float = 1 - 0.05,
336     ) -> np.ndarray:
337     """
338     Masks the traces in the bad pixel mask.
339
340     Parameters
341     -----
342     spec : np.ndarray
343         The spectral data.
344     bpm : np.ndarray
345         The bad pixel mask.
346
347     Returns
348     -----
349     bpm : np.ndarray
350         The updated bad pixel mask.
351
352     """
353     # Base mask
354     bpm[:, :bg_margin] = True
355     bpm[:, -bg_margin:] = True
356     bpm[:, :, :lr_margins[0]] = True
357     bpm[:, :, -lr_margins[1]:] = True
358
359     # Get the traces
360     traces, tr_props = self.find_peaks(spec, axis=1,
361                                         min_height=h_min, rel_height=h_rel)
362
363     for ext in range(len(self.beams)):
364         # Mask the traces
365         for i in range(len(traces[ext][:max_traces])):
366             lb = max(0, int(tr_props[ext]['left_ips'][i]) - tr_pad)
367             ub = min(spec.shape[-1],
368                     int(tr_props[ext]['right_ips'][i]) + tr_pad)
369             bpm[ext, lb : ub] = True
370             # TODO: Relocate targets after initial masking
371
372     logging.info(f"mask_traces - {min(max_traces, len(traces))} of
373                  {len(traces)} traces masked.")
374
375     return bpm
376
377     # MARK: Transform Spectra
378     def transform(
379         self,
380         spec: np.ndarray,
381         wav_sol: np.ndarray,
382         row_max: int | None = None,
383         resPlot: bool = False,
384     ) -> np.ndarray:
385     """
386     Transforms the input wavelength and spectral data based on the
387     given wavelength solution.

```

```

384
385     Parameters
386     -----
387     spec : np.ndarray
388         The spectral data.
389     wav_sol : np.ndarray
390         The wavelength solution.
391     resPlot : bool, optional
392         Flag indicating whether to plot the results, by default
393         ↪ False.
394
395     Returns
396     -----
397     spec, wav : np.ndarray
398         The transformed wavelength and spectral data.
399
400     """
401     # Create arrays to return
402     cs = np.zeros_like(spec)
403     cw = np.zeros_like(wav_sol.mean(axis=1))
404
405     for ext in range(len(self.beams)):
406
407         if row_max:
408             avg_max = row_max
409         else:
410             # Get middle row (to interpolate the rest of the rows
411             # to)
412             avg_max = np.mean(spec[ext], axis=1).argmax()
413
414             # Correct extensions based on wavelength
415             # Get wavelength values at row with most trace
416             cw[ext] = wav_sol[ext, avg_max]
417
418             # Spec ext
419             for row in range(cs.shape[1]):
420                 cs[ext, row] = np.interp(
421                     cw[ext],
422                     wav_sol[ext, row],
423                     spec[ext, row]
424                 )
425                 # f_2d = interpolate.interp2d(
426                 #     wav_sol[ext, row],
427                 #     np.arange(rows),
428                 #     spec[ext],
429                 # )
430                 # cs[ext] = f_2d(cw[ext], np.arange(rows))
431
432             # Plot results
433             if resPlot:
434                 fig, axs = plt.subplots(2, 1, figsize=[20, 4])
435                 for ext in range(len(self.beams)):
436                     axs[ext].imshow(
437                         cs[ext],
438                         vmax=cs[ext].mean() + 2*cs[ext].std(),
439                         vmin=cs[ext].mean() - 2*cs[ext].std()
440                     )

```

```

440         logging.debug(f"{'E' if ext else '0'} Average continuum
441             ↪ = {np.median(np.median(cs[ext], axis=0)):4.3f}")
442
443         axx = axs[ext].twinx()
444         axx.hlines(np.median(np.median(cs[ext], axis=0)), 0,
445             ↪ cs[ext].shape[-1], colors='black')
446         axx.plot(cs[ext].mean(axis=0), "k", label=f"mean {'E',
447             ↪ if ext else '0'}")
448         axx.plot(np.median(cs[ext], axis=0), "r",
449             ↪ label=f"median {'E' if ext else '0'}")
450         axx.legend()
451         plt.show()
452
453     logging.info(f"transform - {cs.shape} transformed.")
454
455     return cs, cw
456
457 # MARK: Plot
458 def plot(
459     self,
460     spectra,
461     wavelengths,
462     peaks,
463     properties,
464     arc: bool = False,
465 ) -> None:
466     plt.style.use(Path(__file__).parent.resolve() /
467             ↪ 'utils/STOPSS.mplstyle')
468
469     def norm(x):
470         return (x - np.min(x)) / (np.max(x) - np.min(x))
471
472     # Load known lines
473     if arc:
474         lines =
475             ↪ self.load_lines(filename=f'utils/RSS_arc_files/{ARC_FILE}')
476     else:
477         lines = self.load_lines()
478
479     lines = lines[
480         (lines['wav'] > wavelengths[1][0][0].min()) &
481         (lines['wav'] < wavelengths[1][0][0].max())
482     ]
483
484     # Create plot for results
485     fig, axs = plt.subplots(2, self.ccds, sharex='col',
486             ↪ sharey='row')
487
488     # Convert axs to a 2D array if ccd count is 1
489     if self.ccds == 1:
490         axs = np.swapaxes(np.atleast_2d(axs), 0, 1)
491
492     for fl in range(len(self.arc_list if arc else self.fits_list)):
493
494         # set color cycle
495         color=next(axs[0, 0]._get_lines.prop_cycler)['color']

```

```

491     for ext in range(len(self.beams)):
492
493         for ccd in range(self.ccds):
494
495             # spectrum (transformed)
496             ccdrange = spectra[1][fl][ext].shape[-1] //
497             ↪ self.ccds
498             axs[0, ccd].plot(
499                 wavelengths[1][fl][ext][ccdrange*ccd:ccdrange*(ccd+1)],
500                 norm(spectra[1][fl][ext][ccdrange*ccd:ccdrange*(ccd+1)])
501                 ↪ + 0.1 * ext + 0.3 * fl,
502                 color=color,
503                 linestyle='dashed' if ext else 'solid',
504                 label = f"${{{self.beams[ext]}}}_{{{fl +
505                 ↪ 1}}}]^{{+ {0.1*ext + 0.3*fl:.1f}}}" if ccd
506                 ↪ == 0 else None,
507             )
508
509             # deviation
510             sky_wavs, dev, peak_idx = self.min_diff_matrix(
511                 lines['wav'],
512                 wavelengths[1][fl][ext][peaks[1][fl][ext]],
513                 max_diff=self.max_difference,
514             )
515
516             # width/initial width
517             width = properties[1][fl][ext]['widths'][peak_idx]
518             width_i = np.zeros_like(width)
519
520             sky_i, i_dev, i_idx = self.min_diff_matrix(
521                 lines['wav'],
522                 wavelengths[0][fl][ext][peaks[0][fl][ext]],
523                 max_diff=self.max_difference,
524             )
525
526             width_i = np.array([
527                 properties[0][fl][ext]['widths'][np.where(wav
528                 ↪ == sky_i)[0][0]]
529                 if wav in sky_i else 1000
530                 for wav in sky_wavs
531             ])
532             width_ratio = (width / width_i) - 1
533             width_ratio[width_ratio < 0] = 0
534
535             ylolims = width_ratio > self.max_difference
536             width_ratio[width_ratio > self.max_difference] =
537                 ↪ self.max_difference // 2
538
539             ok = np.where(
540                 (sky_wavs >=
541                 ↪ wavelengths[1][fl][ext].data[ccdrange*ccd]) &
542                 (sky_wavs <=
543                 ↪ wavelengths[1][fl][ext].data[ccdrange*(ccd+1)])
544             )
545             axs[1, ccd].errorbar(
546                 sky_wavs[ok],
547                 dev.data[ok],
548                 yerr=(width_ratio[ok] * 0, width_ratio[ok]),
549             )
550

```

```

541         lolims=ylolims[ok],
542         fmt="." if ext else "x",
543         alpha=0.8,
544         color=color,
545         # markeredgedecolor='white',
546         # markeredgewidth=0.5,
547         # label=f"${self.beams[ext]}_{\{{\{fl + 1}\}}}$",
548     )
549
550     logging.debug(f"plot - RMS:
551                   → {np.sqrt(np.mean(dev**2)):.2f}")
552
553     for ccd in range(self.ccds):
554         # spectrum
555         ok = np.where(
556             (lines['wav'] >=
557             ↪ wavelengths[1][fl][0].data[ccdrange*ccd]) &
558             (lines['wav'] <=
559             ↪ wavelengths[1][fl][0].data[ccdrange*(ccd+1)])
560         )
561         axs[0, ccd].plot(
562             lines['wav'][ok],
563             lines['flux'][ok] * 0,
564             'x',
565             color='C4',
566             label="\textsc{salt} Model" if ccd == 0 else None,
567         )
568         for x in lines['wav'][ok]: axs[0, ccd].axvline(x,
569             ↪ ls='dashed', c='0.7')
570
571         axs[0, 0].set_ylabel("Norm. Intensity\n(Counts)")
572         axs[1, 0].set_ylabel("Closest Deviation\n($|\sigma|$)")
573         # for ax in axs[:, 0]:
574             # ax.legend(loc='upper left', ncols=(fl + 1) * (ext + 1) +
575             ↪ 1)
576         leg = fig.legend(loc='center', ncol=len(spectra[0]) *
577             ↪ len(spectra[0][0]) + 1, columnspacing=0.5)
578         leg.set_draggable(True)
579         for ax in axs[1, :]:
580             ax.grid(axis='y')
581
582         # fig.add_subplot(111, frameon=False)
583         # # hide tick and tick label of the big axis
584         # plt.tick_params(labelcolor='none', which='both', top=False,
585             ↪ bottom=False, left=False, right=False)
586         axs[-1, 0 if self.ccds == 1 else 1].set_xlabel(f"Wavelength
587             ↪ ({self.wav_unit})")
588
589         # plt.tight_layout()
590
591     plt.show()
592
593     # Save results
594     if self.save_prefix:
595         fig.savefig(fname=self.save_prefix)
596
597     return

```

```

591 # MARK: Process all listed images
592 def process(self, arc: bool=False) -> None:
593     files = self.fits_list
594     if arc:
595         files = self.arc_list
596
597     logging.info(f"Processing '{self.beams}' lines.")
598
599     spectra = [[], []]
600     wavs = [[], []]
601     peaks = [[], []]
602     peak_props = [[], []]
603
604     for fl in files:
605         # Load data
606         spec2d, wav2d, bpm2d = self.load_file_data(fl)
607
608         # Mask traces in BPM
609         bpm2d = self.mask_traces(spec2d, bpm2d, max_traces=0,
610         ↪ bg_margin=15, h_min=0.05)
611         m_spec2d = np.ma.masked_array(spec2d, mask=bpm2d) # spec2d
612         m_wav2d = np.ma.masked_array(wav2d, mask=bpm2d) # wav2d
613
614         # Initial spectra
615         spec_i = np.mean(m_spec2d, axis=-2)
616         wav_i = np.mean(m_wav2d, axis=-2)
617
618         # Transform data
619         t_spec2d, t_wav = self.transform(m_spec2d, m_wav2d,
620         ↪ resPlot=self.can_plot)
621
622         # Final spectra
623         spec_f = np.mean(t_spec2d, axis=-2)
624         wav_f = t_wav
625
626         # Find peaks
627         peaks_i, props_i = self.find_peaks(spec_i,
628         ↪ **FIND_PEAK_PARAMS)
629         peaks_f, props_f = self.find_peaks(spec_f,
630         ↪ **FIND_PEAK_PARAMS)
631
632         spectra[0].append([*spec_i])
633         spectra[1].append([*spec_f])
634         wavs[0].append([*wav_i])
635         wavs[1].append([*wav_f])
636         peaks[0].append([*peaks_i])
637         peaks[1].append([*peaks_f])
638         peak_props[0].append([*props_i])
639         peak_props[1].append([*props_f])
640
641         # Plot results
642         self.plot(spectra, wavs, peaks, peak_props, arc=arc)
643
644     if arc:
645         return
646     elif self.arc_list:
647         self.process(arc=True)

```

```
645         return
646
647
648 # MARK: Main function
649 def main(argv) -> None:
650     return
651
652 if __name__ == "__main__":
653     main(sys.argv[1:])
```


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List of Acronyms

ADC	Analog-to-Digital Converter
Ar	Argon
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
IRAF	Image Reduction and Analysis Facility
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
POLSLT	Polarimetric reductions for SALT
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
STOPs	Supplementary Tools for POLSLT Spectro-polarimetry
UV	Ultraviolet
VPH	Volume Phase Holographic

Glossary

Johnson-Cousins photometric system

U The ultraviolet filter, typically centered around 3640 Å.

B The blue filter, typically centered around 4420 Å.

V The visual filter, designed to approximate human visual sensitivity and typically centered around 5400 Å.

R The red filter, typically centered around 6580 Å.

I The infrared filter, typically centered around 8060 Å.