

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: STOPS, POLSALT, IRAF, SALT, RSS, Development: Python, Pipeline, Calibration: wavelength, Polarization: optical, galaxies: AGN, Blazars, Spectropolarimetry, Astrophysics, Astronomy,

TODO:

- Add Keywords → look up the astronomy journal keywords
- Look up keywords for pipeline development and data reduction.

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- **TODO: Add acknowledgements!**

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List of Acronyms and Symbols

A-DC	Analog-to-Digital Converter
ADC	Atmospheric Dispersion Compensator
Ar	Argon
CCD	Charged-Coupled Device
CLI	Command Line Interface
CMOS	Complementary Metal-Oxide-Semiconductor
CuAr	Copper-Argon
FITS	Flexible Image Transport System
FWHM	Full Width at Half Maximum
GUI	Graphical User Interface
HDU	Header and Data Unit
HEASA	High Energy Astrophysics South Africa
HET	Hobby-Eberly Telescope
HgAr	Mercury-Argon
HRS	High Resolution Spectrograph
IRAF	<i>Image Reduction and Analysis Facility</i>
L+45°	Linear +45° Polarized
L−45°	Linear −45° Polarized
LCP	Left Circularly Polarized
LHP	Linear Horizontally Polarized
LVP	Linear Vertically Polarized
Ne	Neon-Argon
NIR	Near Infra-Red
NIRWALS	Near Infra-Red Washburn Labs Spectrograph
POLSLAT	<i>Polarimetric reductions for SALT</i>
RCP	Right Circularly Polarized
RMS	Root Mean Square
RSS	Robert Stobie Spectrograph
S/N	Signal-to-Noise Ratio
SAAO	South African Astronomical Observatory
SAC	Spherical Aberration Corrector
SALT	Southern African Large Telescope
SALTICAM	SALT Imaging Camera
STOPs	<i>Supplementary Tools for POLSALT Spectropolarimetry</i>
ThAr	Thorium-Argon
UV	Ultraviolet

VPH Volume Phase Holographic
Xe Xenon

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 (A-DC) 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

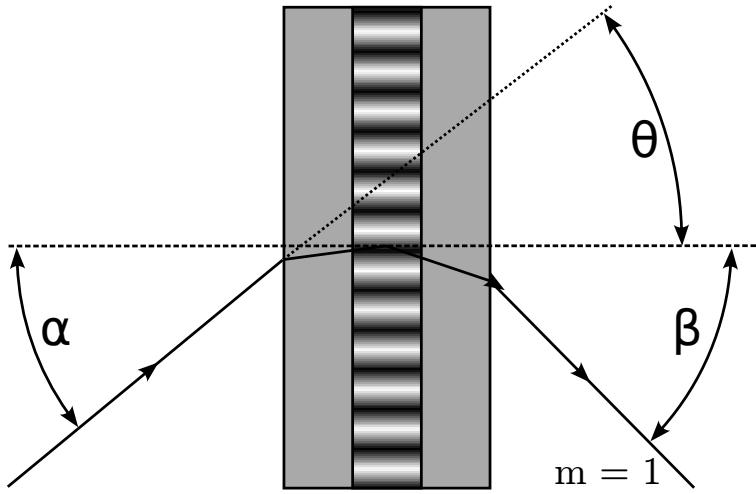


Figure 2.5: Diagram of a VPH grating for an incident monochromatic beam of light. Diagram adapted from Birney et al. (2006).

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.

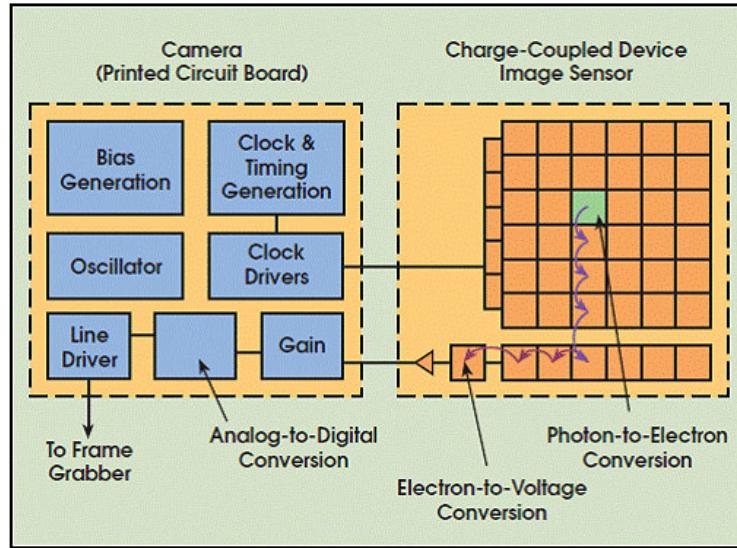


Figure 2.6: Diagram of the inner logic of a CCD. Figure adapted from Litwiller (2001).

Additive noise, such as bias and dark currents, is inherent to CCD images, and as such 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 of a telescope's 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.

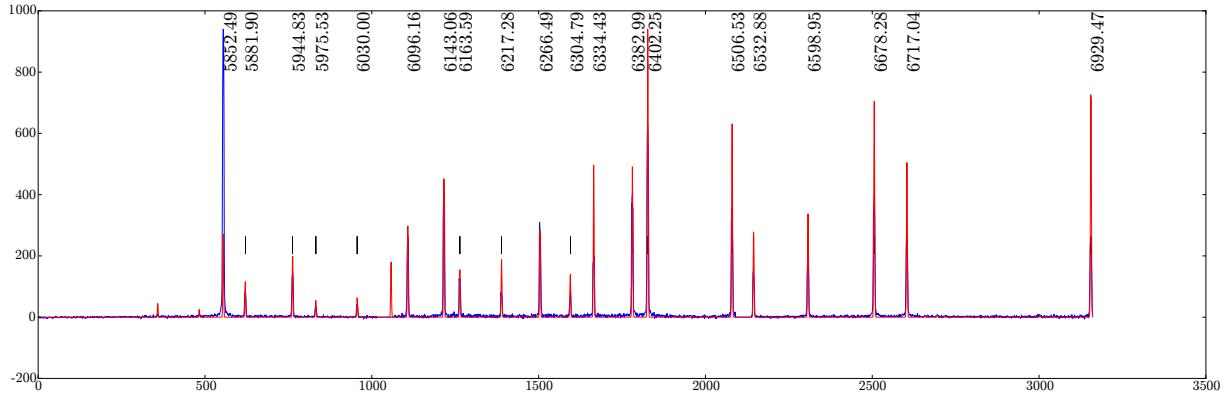


Figure 2.7: Example of an arc spectrum for NeAr taken with SALT’s RSS using the PG1800 grating at a grating angle of 34.625° , an articulation angle of 69.258° , and covering a wavelength range of $\sim 5600 - 6900 \text{ \AA}$. Plot adapted from SALT’s published Longslit Line Atlases, (2023).²

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/N at the cost of careful timing of the images.

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.

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

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 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.

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

Chebyshev Polynomials The Chebyshev polynomials are defined explicitly as:

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

or recursively as:

$$\begin{aligned} T_0(x) &= 1 , \\ T_1(x) &= x , \text{ and} \\ T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x) , \text{ for } n \geq 1 , \end{aligned} \quad (2.12)$$

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). A Chebyshev approximation 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 orders (Arfken and Weber, 1999).

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).

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

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

or recursively as:

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \text{ and} \\ (n+1)P_{n+1}(x) &= (2n+1)xP_n(x) - nP_{n-1}(x), \text{ for } n \geq 1, \end{aligned} \quad (2.18)$$

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). A Legendre approximation 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 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:

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

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.

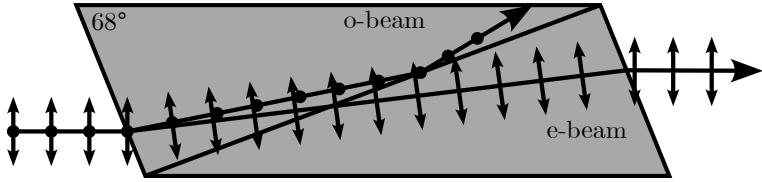


Figure 2.10: Diagram of a Nicol prism for incident non-polarized light. Diagram adapted from Fred the Oyster, CC BY-SA 4.0, via Wikimedia Commons (2023).

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:

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

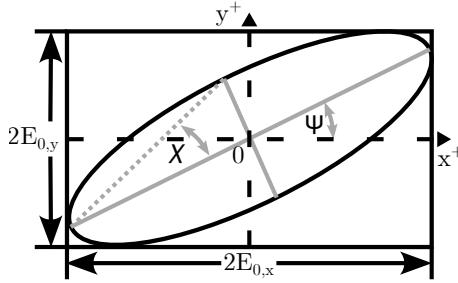


Figure 2.11: The polarization ellipse for an electric field vector propagating through free space. Diagram adapted from Inductiveload, PDM 1.0, via Wikimedia Commons (2023).

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:

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

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)



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).

(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 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.



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

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} 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



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 ChrisHodgesUK, CC BY-SA 3.0, via Wikimedia Commons (2023).

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).

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



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 \updownarrow symbols, for the O - and E -beams, respectively. Diagram adapted from fgalore, CC BY-SA 3.0, via Wikimedia Commons (2023).

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. 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



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

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 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.



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

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 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).

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

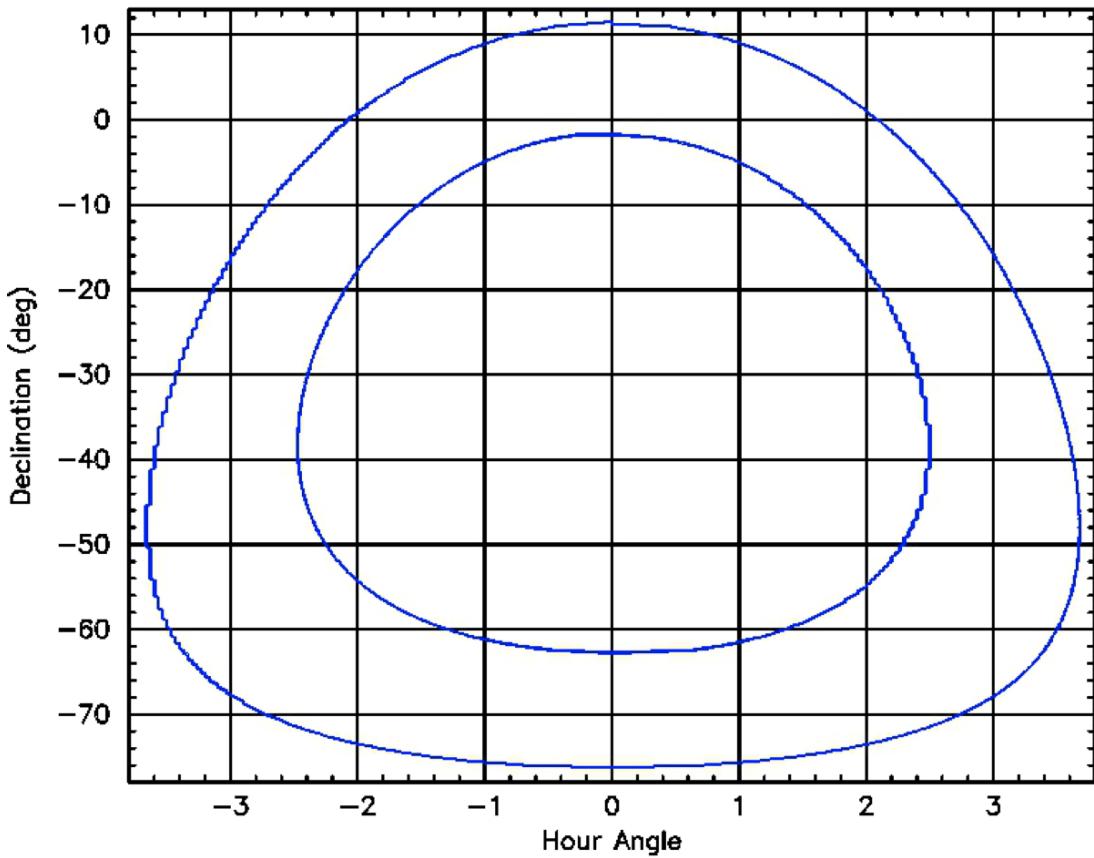


Figure 2.18: The visibility annulus of objects observable by SALT. Figure adapted from the SALT call for proposals (2013).⁶

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 of $\sim 7 \text{ m}$ 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 (SAC) (O'Donoghue, 2000), and an Atmospheric Dispersion Compensator (ADC) (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 \AA . 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. The tracker also houses the calibration system which contains the Ar, CuAr, HgAr, Ne, ThAr, and Xe wavelength calibration lamps (Buckley et al., 2008).

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



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

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.

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.

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

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).

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 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 sourced 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 *Supplementary Tools for POLSALT Spectropolarimetry* (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 A, 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 raw image 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

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.sao.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.

3.1.1 Raw Image Reductions

Raw image reductions are run via `imred.py` and apply the necessary basic reductions to the raw data before any calibrations are applied. These reductions include overscan subtractions, gain corrections, crosstalk corrections, and mosaicking as well as attaching the bad pixel maps and pixel variance information. Files with raw image reductions performed have “`mxgbp`” prepended to their names. As of February 2022, raw image 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 ‘`WAV`’ wavelength extension to each science FITS file, which are prefixed with a “`w`”, and the *O*- and *E*-beams of the extensions are split into their own sub-extensions.



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

3.1.3 Spectral Extraction

Background subtraction and spectral extraction is run via `specpoleextract_dev.py` which corrects for the beam-splitter distortion and tilt, performs sky subtraction, and extracts a one dimensional wavelength dependent spectrum for each beam sub-extension. This step is interactive with Figure 3.2 showing the interactive window used for spectral 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; most notably the indexes of the related waveplate pairs, from Table 2.2, are included in the file names.



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

3.1.5 Final Stokes Calculations

The Final Stokes calculations are performed via `specpolfinalstokes.py` and, using the waveplate pattern along with the raw Stokes signals, calibrates for the polarimetric zero-point and waveplate efficiency, and calculates the final Stokes parameters. Before the final Stokes calculations are performed, and 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 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 is done using `specpolview.py`, which 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 allowing the user control over various options, such as the wavelength range, binning, etc., with the GUI shown in Figure 3.3.

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.



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

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 SALTICAMs *U*, *B*, *V*, *R*, and *I* Johnson-Cousins filter curves.

3.1.8 POLSALT Limitations and the Need for Supplementary Tools

The creation of supplementary tools for POLSALT spectropolarimetric reductions stemmed from the limitations of the wavelength calibration process and a need to compare wavelength solutions across the perpendicular *O* and *E* polarization beams. The process of calibrating wavelength solutions using the POLSALT pipeline is time-consuming for the average user, and often results in unexpected 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 anything 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 Ar 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,



Figure 3.5: One of many Ar 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

since minor deviations of identified spectral features resulted 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 longer 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.

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*

The IRAF (*Image Reduction and Analysis Facility*) software is a collection of software designed specifically for the reduction and analysis of astronomical images and spectra (Tody, 1986, 1993). The software consists of many tasks which perform specific operations and which are grouped into relevant packages. Only a brief overview of the tasks will be provided here. Help documentation for any of the IRAF tasks may be found online 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.⁵

Useful IRAF tasks that deserve a brief mention are: the `mkscript` task in the `system` package which allows a user to create and save a task along with the defined parameters

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

⁵Online help for IRAF is available at <https://iraf.net/irafdocs/>

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 the wavelength calibration of SALT spectropolarimetric data, the relevant tasks are the `identify` and `reidentify` tasks located in the `noao.onedspec` package, and the `fitcoords` and the (optional) `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 (see Figure 3.6) 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 any features which negatively impact the wavelength solution. A balance must be found between the number of identified features, the parameters of the fit, and the deviation of the fit from the known features.

3.2.2 Reidentify

The `reidentify` task is used to run the `identify` task autonomously and repeatedly across the entirety of the arc frame at defined (row) intervals.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`.

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.

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.

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

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
```

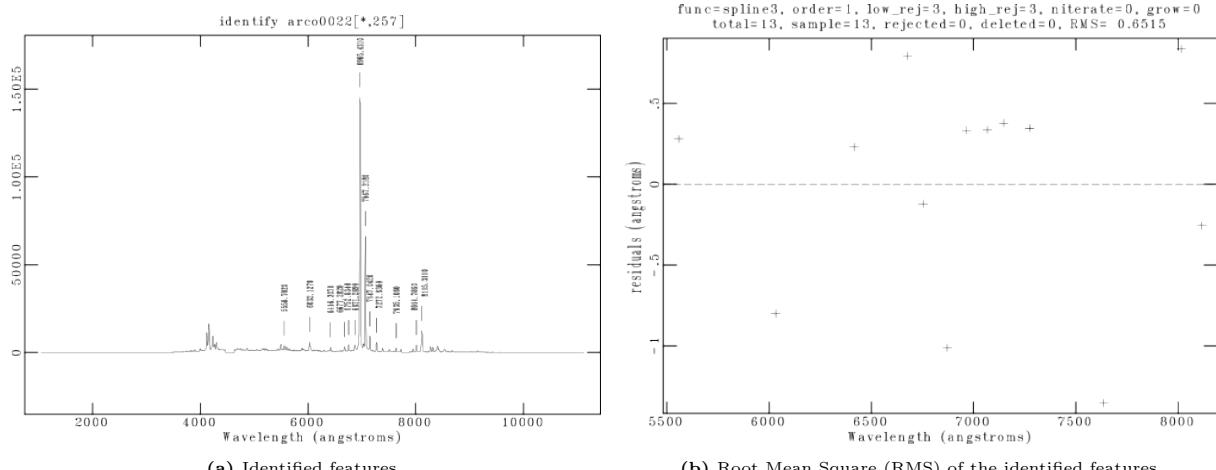


Figure 3.6: A plot and the RMS of the identified features found using the IRAF identify task. Figures created using the IRAF identify task.

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
```

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 (see Figure 3.7).

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 ‘WAV’ extension required by POLSALT, further described in § 3.3.2.

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.



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.

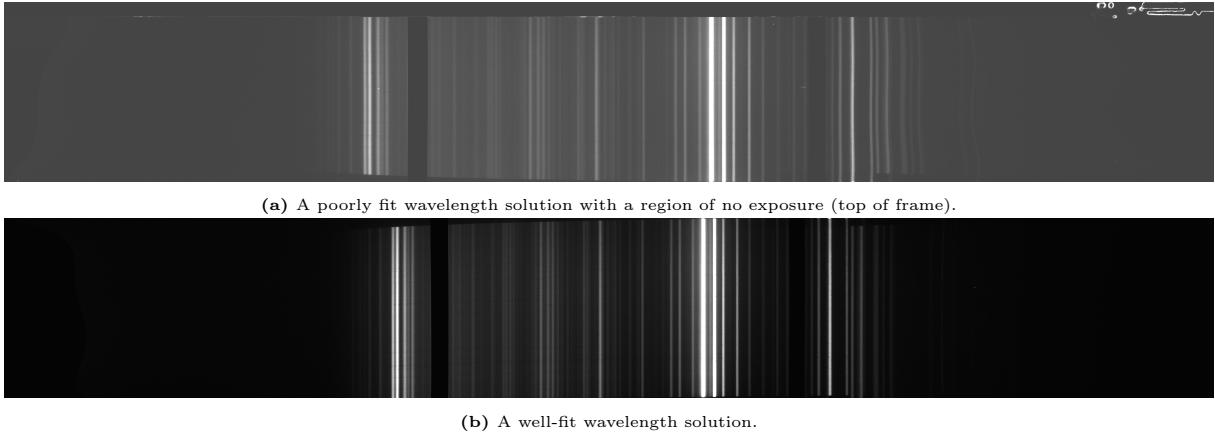


Figure 3.8: Examples of a poor fit (a) and well-fit (b) wavelength solution applied to the *O*- and *E*-beams of an arc image. The contrast of the figures were scaled to best capture any deviation of the arc lines. Figures created by the IRAF `transform` task.

3.2.4 Transform

The `transform` task is the optional final step in the IRAF wavelength calibration process.¹⁴ Simply put, `transform` converts the (x_p, y_p) pixel units of an exposure to (λ, y_p) wavelength 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 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.

¹⁴Help documentation for the `transform` task may be found at https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.twodspec.longsit.transform.html.

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 (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 on the usage of STOPS in a CLI can be viewed by running:

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

which retrieves and prints the help documentation to the CLI from Listing B.1 (in Appendix B), such as how to enable logging or increase the verbosity, or change default parameters of the various methods. Finally, help documentation for the specific STOPS methods may be found within this section (Listing 3.3 to 3.6) or in Appendix B.

3.3.1 Splitting

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

While IRAF is capable of dealing with multiple traces in an extension or lists of input files, it 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**).

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

```

24 """
25 The `Split` class allows for the splitting of `polsalt` FITS files
26 based on the polarization beam. The FITS files must have basic
27 `polsalt` pre-reductions already applied (`mzgbp...` FITS files).
28
29 Parameters
30 -----
31 data_dir : str / Path
32     The path to the data to be split
33 fits_list : list[str], optional
34     A list of pre-reduced `polsalt` FITS files to be split within `data_dir`.
35     (The default is None, `Split` will search for `mzgbp*.fits` files)
36 split_row : int, optional
37     The row along which to split the data of each extension in the FITS file.
38     (The default is SPLIT_ROW (See Notes), the SALT RSS CCD's middle row)
39 no_arc : bool, optional
40     Decides whether the arc frames should be recombined.
41     (The default is False, `polsalt` has no use for the arc after wavelength calibrations)
42 save_prefix : dict[str, list[str]], optional
43     The prefix with which to save the O & E beams.
44     Setting `save_prefix` = ``None`` does not save the split O & E beams.
45     (The default is SAVE_PREFIX (See Notes))
46
47 Attributes
48 -----
49 arc : str
50     Name of arc FITS file within `data_dir`.
51     `arc` = `""` if `no_arc` or not detected in `data_dir`.
52 o_files, e_files : list[str]
53     A list of the `O`- and `E`-beam FITS file names.
54     The first entry is the arc file if `arc` defined.
55 data_dir
56 fits_list
57 split_row
58 save_prefix
59
60 Methods
61 -----
62 split_file(file: os.PathLike)
63     -> tuple[astropy.io.fits.HDUList]
64     Handles creation and saving the separated FITS files
65 split_ext(hdulist: astropy.io.fits.HDUList, ext: str = 'SCI')
66     -> astropy.io.fits.HDUList
67     Splits the data in the `ext` extension along the `split_row`
68 crop_file(hdulist: astropy.io.fits.HDUList, crop: int = CROP_DEFAULT (See Notes))
69     -> tuple[numpy.ndarray]
70     Crops the data along the edge of the frame, that is,
71     `O`-beam cropped as [crop:], and
72     `E`-beam cropped as [:crop].
73 update_beam_lists(o_name: str, e_name: str)
74     -> None
75     Updates `o_files` and `e_files`.
76 save_beam_lists(file_suffix: str = 'frames')
77     -> None
78     Creates (Overwrites if exists) and writes the `o_files` and `e_files` to files named
79     `o_{file_suffix}` and `e_{file_suffix}`, respectively.
80 process()
81     -> None
82     Calls `split_file` and `save_beam_lists` on each file in `fits_list` for automation.
83
84 Other Parameters
85 -----
86 **kwargs : dict
87     keyword arguments. Allows for passing unpacked dictionary to the class constructor.
88
89 Notes
90 -----
91 Constants Imported (See utils.Constants):
92     SAVE_PREFIX
93     CROP_DEFAULT
94     SPLIT_ROW
95
96
97 """

```

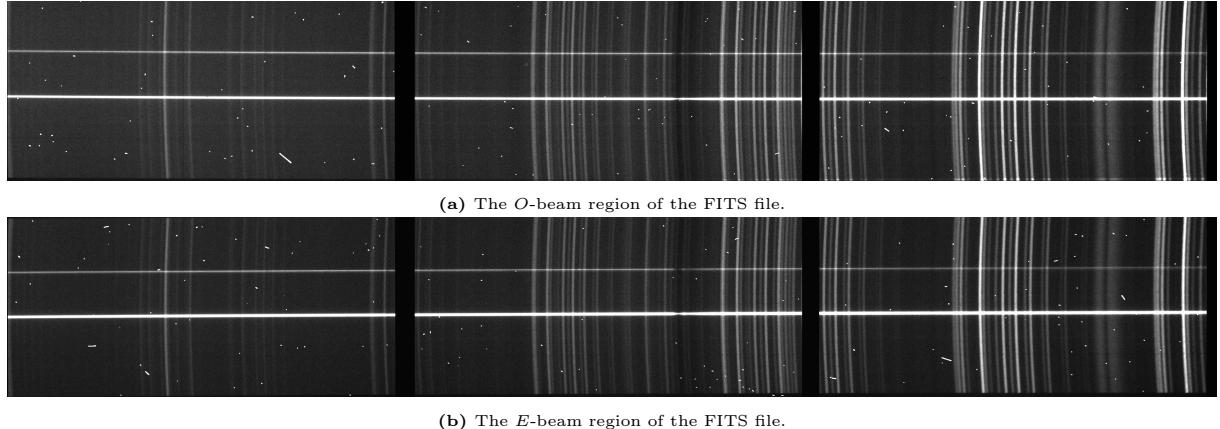


Figure 3.9: The split *O*- (a) and *E*-beams (b) as handed to **IRAF**. Figure created from the **STOPS** **split** method output.

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 and Data Unit (HDU) structures for each FITS file (i.e. for both the *O*- and *E*-beam), and appends all header and science data necessary for wavelength calibration to the relevant HDU structure. Otherwise, defaults, such as which row to split the image along to separate the beams, were kept as close to the POLSALT pipeline as possible.

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 by only including the header and ‘SCI’ science extension. To aid the scripting of the **IRAF** wavelength calibration process, the **split** method also performs row cropping to exclude CCD regions which are not exposed to light, and creates files listing the split *O*- and *E*-beam FITS files which may be passed to the **IRAF** task inputs. Row cropping was decided on as **IRAF** does not handle rows with no exposure well, specifically when it comes to the autonomous **reidentify** task. The full **STOPS** **split** class docstring is given in Listing 3.3.

3.3.2 Joining

After the **IRAF** **fitcoords** task has been successfully run for both the *O*- and *E*-beams, the **STOPS** **join** method is used to extract and parse the wavelength solution from the **IRAF** database, and to create the wavelength calibrated FITS files required by the POLSALT pipeline. More specifically, the **join** method performs the following steps:

First, **join** parses the wavelength database file, described in § 3.2.3, for either a ‘Chebyshev’ or ‘Legendre’ solution, and calculates the wavelength at each (x_p, y_p) pixel position. This new image containing the corresponding wavelength values, seen in Figure 3.10, is appended to the wavelength calibrated FITS file as the ‘WAV’ extension.

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 / Path
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 `mxbgp*.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, x_shape: int, y_shape: 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 Chebyshev 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 """

```

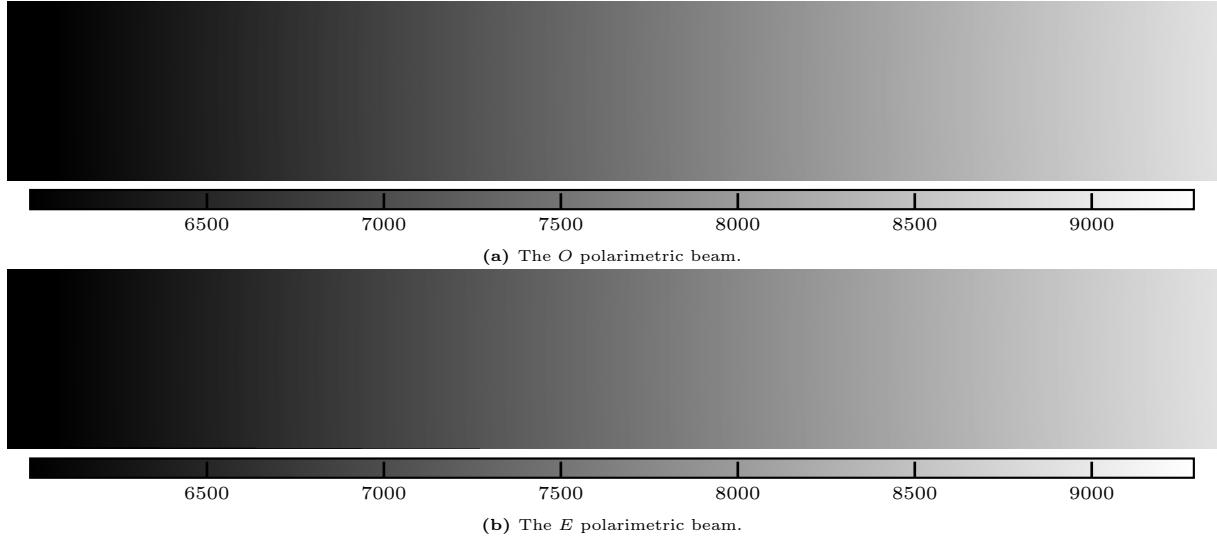


Figure 3.10: A representative ‘WAV’ extension of a FITS file, for the *O*- (a) and *E*-beam (b), ready to be processed by the POLSALT pipeline. The color bars show the wavelength in Å. Note that regions which fall outside the exposed region are masked by setting the corresponding pixel values of the wavelength and ‘BPM’ extensions to 0. Figure created from the `STOPS join` method output.

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

Next, `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 ‘WAV’ 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. The full STOPS `join` class docstring is given in Listing 3.4.

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

```

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

```



Figure 3.11: A representative ‘SCI’ extension of a FITS file, for the *O*- (a) and *E*-beam (b), ready to be processed by the POLSALT pipeline. The observed intensity is displayed via the grayscale value at each pixel. Figure created from the `STOPSjoin` method output.

3.3.3 Sky Line Checks

The `skyline` method has been implemented to compare the position of the sky lines on the ‘SCI’ extension, or arc lines in the arc exposure, to the known positions of the sky lines, or arc lines, as measured by SALT, respectively.¹⁶ This provides an additional check of the accuracy of the wavelength solution across the frame. This method accepts both the IRAF `transform` FITS file or the ‘wmxgbp’ FITS files created by the `join` method as the input.

The `skyline` method loads the wavelength calibrated files, masks the traces present in the frames, transforms the frames from (x_p, y_p) pixel to $(\text{\AA}, y_p)$ wavelength units if the frame was not transformed by `transform`,¹⁷ and compares the peak wavelength position of the sky lines to the reference sky lines as measured by SALT. Finally, a figure is created containing a plot of the background spectra (offset by the respective legend entries superscript) with the known sky lines marked with a vertical line, and a plot of the closest identified peaks of said spectra.

Minor variations in the comparison of the sky lines are expected, such as those seen in Figure 3.12, but any uniform trends, such as those in Figure 3.13 (bottom left), indicate an underlying poor fit across the horizontal axis of the wavelength solution. The full STOPS `skyline` class docstring is given in Listing 3.5.

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 by the difference between the *O*- and *E*-beams, a direct comparison is not appropriate.

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

¹⁶Both sky and arc lines are available at <https://astronomers.salt.ac.za/data/salt-longslit-line-atlas/>.

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.

Listing 3.6: The ‘docstring’ for `cross_correlate.py`

```

31 """
32 Cross correlate allows for comparing the extensions of multiple
33 FITS files, or comparing the O and E beams of a single FITS file.
34
35 Parameters
36 -----
37 data_dir : str / Path
38     The path to the data to be cross correlated
39 filenames : list[str]
40     The ecwmagbp*.fits files to be cross correlated.
41     If only one filename is defined, correlation is done against the two polarization beams.
42 split_ccd : bool, optional
43     Decides whether the CCD regions should each be individually cross correlated.
44     (The default is True, which splits the spectrum up into its separate CCD regions)
45 cont_ord : int, optional
46     The degree of a chebyshev to fit to the continuum.
47     (The default is 11)
48 plot : bool, optional
49     Decides whether the continuum fitting should be plotted
50     (The default is False, so no continua plots are displayed)
51 save_prefix : str, optional
52     The name or directory to save the figure produced to.
53     "" saves a default name to the current working. A default name is also used when save_prefix is a directory.
54     (The default is None, I.E. The figure is not saved, only displayed)
55
56 Attributes
57 -----
58 data_dir
59 fits_list
60 beams : str
61     The mode of correlation.
62     'OE' for same file, and 'O' or 'E' for different files but same extension.
63 ccds : int
64     The number of CCD's in the data. Used to split the CCD's if split_ccd is True.
65 cont_ord : int
66     The degree of the chebyshev to fit to the continuum.
67 can_plot : bool
68     Decides whether the continuum fitting should be plotted
69 offset : int
70     The amount the spectrum is shifted, mainly to test the effect of the cross correlation
71     (The default is 0, I.E. no offset introduced)
72 save_prefix
73 wav_unit : str
74     The units of the wavelength axis.
75     (The default is Angstroms)
76 wav_cdel : int
77     The wavelength increment.
78     (The default is 1)
79 alt : Callable
80     An alternate method of cross correlating the data.
81     (The default is None)
82
83 Methods
84 -----
85 load_file(filename: Path) -> tuple[np.ndarray, np.ndarray, np.ndarray]
86     Loads the data from a FITS file.
87 get_bounds(bpm: np.ndarray) -> np.ndarray
88     Finds the bounds for the CCD regions.
89 remove_cont(spec: list, wav: list, bpm: list, plot_cont: bool) -> None
90     Removes the continuum from the data.
91 correlate(filename1: Path, filename2: Path / None = None) -> None
92     Cross correlates the data.
93 ftcs(filename1: Path, filename2: Path / None = None) -> None
94     Cross correlates the data using the Fourier Transform.
95 plot(spec, wav, bpm, corrdb, lagsdb) -> None
96     Plots the data.
97 process() -> None
98     Processes the data.
99
100 Other Parameters
101 -----
102 offset : int, optional
103     The amount the spectrum is shifted, mainly to test the effect of the cross correlation
104     (The default is 0, I.E. no offset introduced)
105 **kwargs : dict
106     keyword arguments. Allows for passing unpacked dictionary to the class constructor.
107 ftcs : bool, optional
108     Decides whether the Fourier Transform should be used for cross correlation.
109
110 See Also
111 -----
112 scipy
113     https://docs.scipy.org/doc/scipy/reference/generated/scipy.signal.correlate.html
114
115 Notes
116 -----
117 Constants Imported (See utils.Constants):
118     SAVE_CORR
119
120
121 """

```



Figure 3.12: An example of a well calibrated wavelength solution, specifically shown for science images. Figure created via the `STOPS skyline` method.

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. The full `STOPS split` class docstring is given in Listing 3.6.

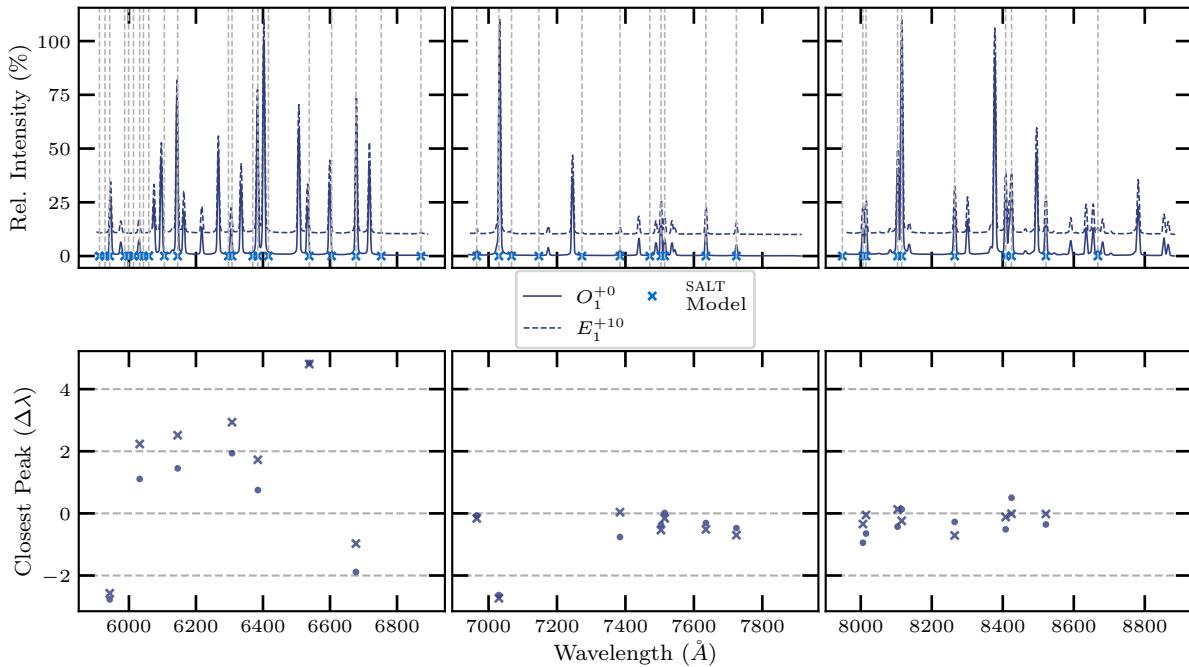


Figure 3.13: An example of a wavelength solution with a poor fit at shorter wavelengths (bottom left), specifically shown for an arc image. Arc lines are Figure created via the `STOPS` `skyline` method.

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 A. 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 general order, seen in Figure 3.15, and commands necessary to complete each step of the reduction process are discussed, assuming that the software is running as intended.

3.4.1 Initial Setup

It is important to note that while POLSALT was developed in Python 2 (2.7), the STOPS supplementary tools were developed in, and require, Python 3 (3.11+), as well as the 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 has been deprecated, nor would it have been reasonable to update POLSALT to Python 3.

It is therefore recommended that the different versions of Python are managed using separate virtual environments. While the `anaconda` package manager was used in this 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 A.1 or the Listings 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.



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

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

3.4.2 POLSALT Pre-Reductions

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

The POLSALT GUI may be launched by opening a CLI and running the commands given in Listing A.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.



Figure 3.15: A general workflow for data reductions using a combination of POLSALT, IRAF, and STOPS. Diagram adapted from Cooper et al. (2022).

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 A.2 to A.8, but it should be noted that the art of wavelength calibration consists of modifying the parameters to achieve a well-fit calibration function.

Preparing the Data for IRAF

Splitting the data is presented in Listing A.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 the `identify`, `reidentify`, `fitcoords`, and optionally `transform` tasks.

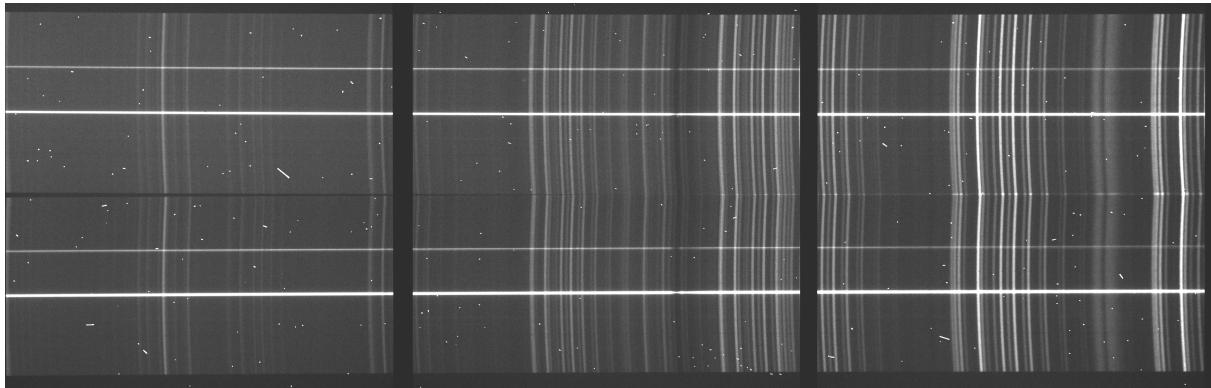


Figure 3.16: The ‘SCI’ extension of a typical spectropolarimetric FITS file taken with the SALT RSS, after basic POLSALT CCD reductions have been completed. Figure created from the `STOPS split` output.

In general, these tasks are run directly in the IRAF terminal using:¹⁸

```
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 A, namely Listing A.4 to A.7, describes how the tasks may be scripted and saved 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.

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

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 A.8.

Similar to the `split` procedure, the `join` procedure has the same defaults defined. The onus of keeping track of any previously changed default parameters falls to the user, but logging is implemented in STOPS (see the discussion on help documentation in § 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 A.9. 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 A.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 A.10, but they may also be removed using:

```
$ rm beam*.fits arc*.fits frame* <any user created files>
```

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.

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 specpolwavmap import specpolwavmap
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=""
# specpolwavmap(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)

```

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 A (p. 72 onwards).¹⁹

POLSALT Beta through a CLI

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

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

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

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

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

The POLSALT analysis scripts may be run using:

```
$ python script.py
```

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

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

Chapter 4

Testing and Application

This chapter contains an overview of the testing performed for the development of STOPS (§ 4.1) and the checking of the replaced wavelength solutions (§ 4.2), as well as the application of STOPS on observations (§ 4.3.1) and its application in publications (§ 4.3.2).

4.1 Testing STOPS

The main challenge faced when developing STOPS was ensuring that the software was compatible with both the POLSALT and IRAF file structures. As development is an iterative process, STOPS was continually checked to ensure compatibility such that the varying STOPS method inputs were correctly parsed, and that their outputs were parsable by the relevant IRAF tasks or POLSALT methods.

To this end, observations which were verified to have been accurately reduced were duplicated for testing purposes, allowing for continual checks of the STOPS pipeline to be made during the development process. As the STOPS `split` and `join` methods are designed to convert between the POLSALT and IRAF file structures, greater emphasis was made to ensure that the output of both methods provided accurate and consistent results.

4.1.1 Testing the split Method

The STOPS `split` method requires any POLSALT pre-reduced ('mxgbp'- prefixed) FITS files as input and outputs IRAF compatible ('(arc|beam)(O|E)'- prefixed) FITS file structures. As no 'split' FITS files are created during pure POLSALT reductions, the STOPS `split` method was tested by comparing the pre-reduced POLSALT files to the `split` method's output files, ensuring the correct structure and data integrity of the files handed off to IRAF.

Table 4.1 shows the FITS file information for the files before and after splitting. The split FITS files contain the split 'SCI' extension data and the 'Primary' header from the pre-reduced files, with any Header or Data differences mentioned below.

The header is left mostly untouched, and is only updated to represent the new data

Filename	No.	Name	Type	Cards	Dimensions	Format
POLSLT	0	‘Primary’	PrimaryHDU	161	()	
	1	‘SCI’	ImageHDU	19	(3199, 1028)	float32
	2	‘VAR’	ImageHDU	8	(3199, 1028)	float32
	3	‘BPM’	ImageHDU	8	(3199, 1028)	uint8
STOPSLT split ‘O’	0	‘Primary’	PrimaryHDU	162	(3199, 474)	float32
	0	‘Primary’	PrimaryHDU	162	(3199, 474)	float32

Table 4.1: A comparison of the contents of a POLSLT pre-reduced FITS file to the STOPSLT split O- and E-beam FITS files. Table created using the `Astropy fitsinfo` CLI tool.



(a) The difference in the ‘SCI’ extensions, for the ‘O’ polarization beam.



(b) The difference in the ‘SCI’ extensions, for the ‘E’ polarization beam.

Figure 4.1: The difference between the POLSLT pre-reduced (‘mxgbp’- prefixed) FITS files and the STOPSLT ‘split’ (‘arc|beam)(O|E’- prefixed) files. Figures created using both the `POLSLT Raw image reduction` and `STOPSLT split` method outputs.

type and shape: the ‘BITPIX’ value is updated, from 8 to –32, and the ‘NAXIS’ value is updated, from 0 to 2; the ‘NAXIS1’ and ‘NAXIS2’ keywords are added, and their values are set to the new split ‘SCI’ data shape; and the ‘EXTEND’ keyword is removed.¹ This accounts for the discrepancy in the ‘Cards’ between the POLSLT and STOPSLT file header entries in Table 4.1.

Figure 4.1 shows that the POLSLT ‘SCI’ data is unmodified when copying the data to the STOPSLT FITS file, but only includes half of the data, for the relevant O- or E-polarization beam, Figure 4.1a and Figure 4.1b, respectively, with a cropping which defaults to 40 pixels (see § 3.3.1), introduced to the top- and bottom-most rows of the POLSLT data. This accounts for the discrepancy in the ‘Dimensions’ between the POLSLT and STOPSLT files in Table 4.1.

This output file structure was chosen for IRAF compatibility, and was tested over multiple grating and articulation angles, as well as with various data sets to ensure that the `split` method was robust and reliable.

4.1.2 Testing the join Method

The `join` method requires both an IRAF database with wavelength solutions (or a custom wavelength solution) for both polarimetric beams and the POLSLT pre-reduced files

¹The ‘EXTEND’ keyword indicates that the FITS file contains multiple extensions while the ‘NAXIS1’ and ‘NAXIS2’ keywords indicate the shape and size of the data stored in the relevant extension.

Filename	No.	Name	Type	Cards	Dimensions	Format
POLSLT	0	'Primary'	PrimaryHDU	161	()	
	1	'SCI'	ImageHDU	21	(3199, 514, 2)	float32
	2	'VAR'	ImageHDU	10	(3199, 514, 2)	float32
	3	'BPM'	ImageHDU	10	(3199, 514, 2)	uint8
	4	'WAV'	ImageHDU	21	(3199, 514, 2)	float32
STOPs join	0	'Primary'	PrimaryHDU	161	()	
	1	'SCI'	ImageHDU	21	(3199, 474, 2)	float32
	2	'VAR'	ImageHDU	10	(3199, 474, 2)	float32
	3	'BPM'	ImageHDU	10	(3199, 474, 2)	uint8
	4	'WAV'	ImageHDU	21	(3199, 474, 2)	float32

Table 4.2: A comparison of the POLSLT wavelength calibrated FITS file to the (IRAF wavelength calibrated) STOPs join FITS file. Table created using the Astropy `fitsinfo` CLI tool.

as input and outputs POLSLT spectra extraction compatible ('wmxgbp'- prefixed) FITS file structures. Ensuring that the output format was correct was paramount as the POLSLT spectra extraction method is unable to process the files otherwise, thus halting the reduction process. Thankfully, the `join` method output could be compared to the POLSLT wavelength calibration method output files, ensuring that any changes introduced by the STOPs pipeline were well characterized.

Table 4.2 shows the FITS file information for both the POLSLT and STOPs wavelength calibrated files. Other than the 'Dimensions' of each 'ImageHDU' extension,² the FITS files are identical in structure.

Although the 'Cards' count is the same, minor differences across the headers are present. The 'HISTORY' keyword, which contains the POLSLT 'CRCLEAN' parameters and which default to 'upper= 4.0, lower= 1.5, sigmaveto= 2.0', is left as 'None' in the STOPs file.³ Although STOPs performs cosmic ray cleaning (see § 3.3.2), the parameters are not stored in the header as POLSLT and STOPs implement different methods for cosmic ray cleaning. Other minor differences such as the date-times stored in the 'SALT-TLM' and 'SMOSAIC' keywords may also differ as they contain the date-times relating to the completion of the POLSLT pre-reductions. This accounts for the differences in the 'Cards' between the POLSLT and STOPs file header entries in Table 4.2.

Figure 4.2 shows the differences in the data between the POLSLT and STOPs wavelength calibrated files. It can be seen that the 'VAR' extensions (Figure 4.2b) are identical. The 'SCI' extensions (Figure 4.2a) differ only in that the cosmic ray cleaning has been applied to the STOPs data, whereas the POLSLT data applies a mask to the cosmic rays using the 'BPM' extension (Figure 4.2c). The 'BPM' and 'WAV' extensions (Figure 4.2d) are also masked to account for the valid wavelength calibrated region. The 'WAV' extensions contain the differing wavelength solutions and as such naturally differ. This accounts for the differences in the data between the POLSLT and STOPs files.

²The 'Dimensions' differ due to the before mentioned cropping of the top- and bottom-most rows of the data.

³The POLSLT pipeline performs cosmic ray cleaning using a 10σ spike to cull cosmic rays. See the POLSLT source code for more information.

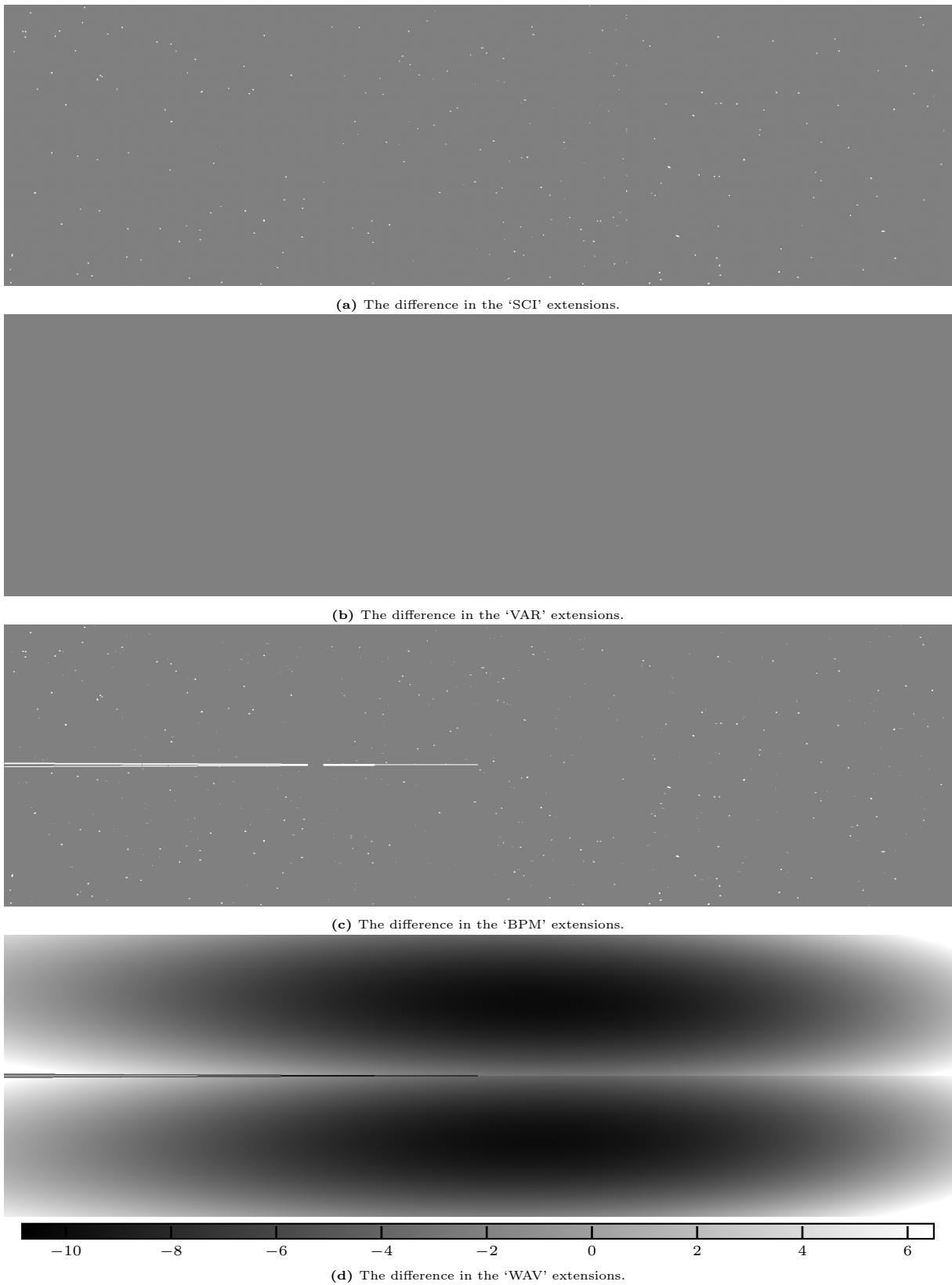


Figure 4.2: The difference of the FITS file extensions between the `POLSALT` and `STOPS` ('wmxgbp'- prefixed) wavelength calibrated files. Figures created using both the `POLSALT` and `STOPS` versions of the `POLSALT spectral extraction` input.

Finally, the STOPS `join` method was tested to ensure compatibility and correctness of the output data in comparison to POLSALT. This involved testing the `join` method with various data sets to ensure that the output files were accurate and consistent.

4.2 Wavelength Solution Checks

The secondary challenge encountered when developing STOPS was ensuring that the wavelength solutions parsed by STOPS were unaffected by the pipeline and that they were similar to those created by POLSALT. This was achieved through the `correlate` and `skylines` methods, which were designed to validate the wavelength solutions produced by IRAF, but were later modified to parse both the IRAF and POLSALT wavelength solutions, allowing for further inspection of the two-dimensional wavelength solution.

Before the POLSALT wavelength calibrations were replaced with the IRAF wavelength calibrations, the accuracy of the new wavelength solutions needed to be validated. This was done both through the IRAF tasks, ensuring an accurate wavelength solution, and through the STOPS `correlate` and `skylines` methods, allowing the integration of the wavelength solutions to be validated.

TODO: Add RMS results (Table / Figures / Both?) from wavelength solution checks (IRAF RMS, POLSALT RMS) to quantify differences.

TODO: Plot IRAF vs POLSALT RMS for sources?

4.2.1 Cross Correlation Checks

The `correlate` method returns plots validating the wavelength solutions and so only has to accept the POLSALT `spectra extraction` ('ecwmxgbp'- prefixed) method output files as input.

The STOPS `correlate` method was tested by cross correlating generated *O*- and *E*-beam spectra with known offsets, with the aim of reacquiring said offsets, as shown in Figure 4.3. The spectra were generated with a feature in each CCD region, randomly offset in both the wavelength and intensity axes, Figure 4.3a.

Through cross correlation, Figure 4.3b, the introduced offsets, or ‘max lag’, were reacquired. For spectral regions with few features or features not much more significant than the continuum noise (such as the left most CCD region of Figure 4.3b), correlation may fail to determine the correct offset. It is clear that the returned ‘max lag’ is incorrect when the ‘max lag’ peak is not significantly larger than any noise of the continuum in the correlation plot.

4.2.2 Sky Line Checks

The `skylines` method returns plots validating the wavelength solutions and so only has to accept either the IRAF `transform` task or STOPS `join` method output files as input.

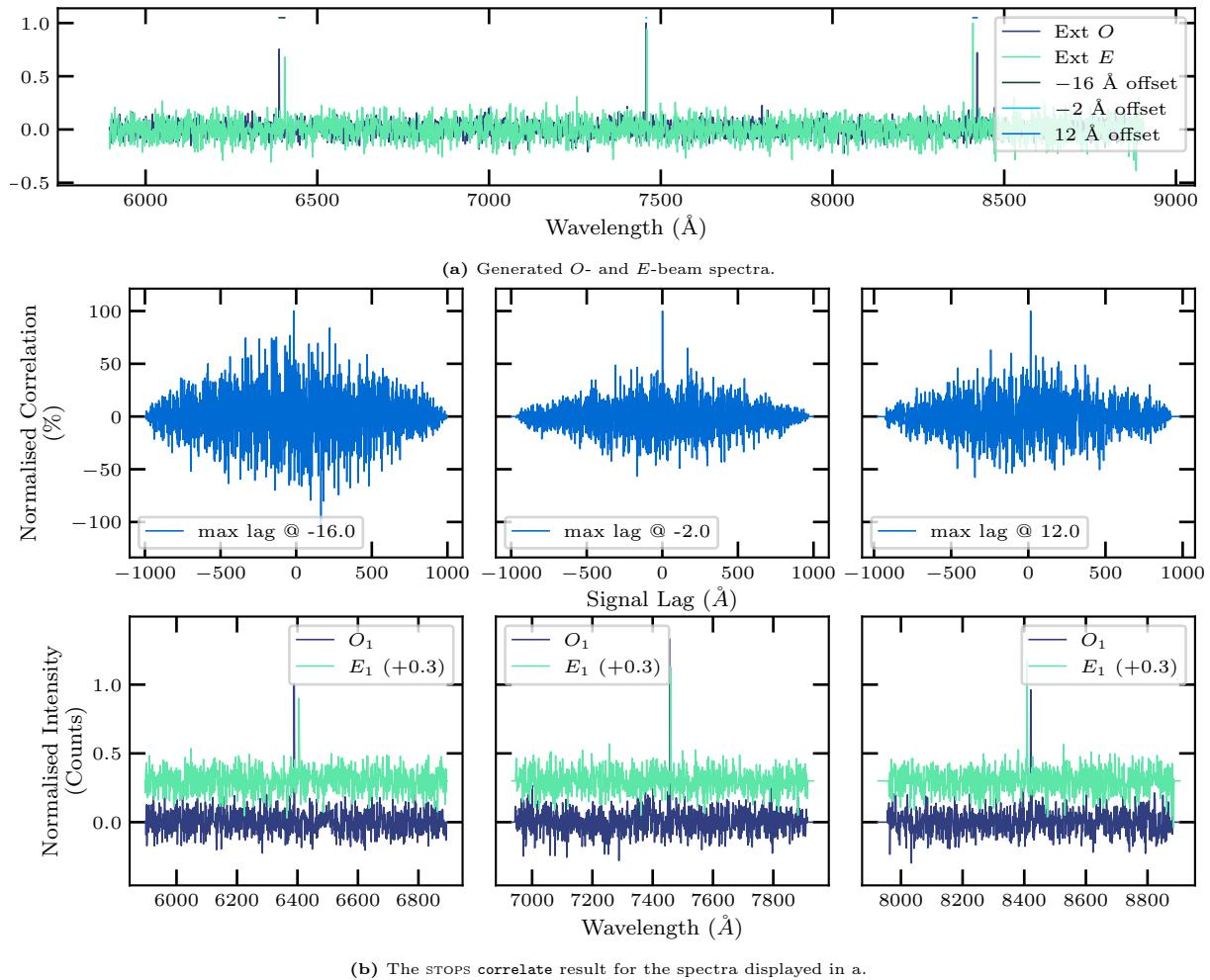


Figure 4.3: Reacquisition of the offsets introduced to the O - and E -beam spectra (a) by cross-correlation (b).

TODO: Compare skylines from STOPS to ‘poor’ POLSALT spectral extraction (I.E. spectral extraction with no trace in the ‘target’ window and the ‘background’ window on region with no skylines).

TODO: Test ‘skylines’ using known spectral sky lines / telluric lines.

TODO: Insert figure illustrating skyline identification accuracy.

4.3 Application of STOPS

TODO: 1-2 paragraph intro mentioning both standards used for testing and (flaring blazar) science targets used. Mention results discussed for optical region, and briefly why (SALT).

4.3.1 Spectropolarimetric Standards

Testing included the use of spectropolarimetric standards, comprising four highly polarized and two non-polarized objects. **TODO: VERIFY CORRECT**

TODO: Insert table listing the spectropolarimetric standards used, with their properties.

Source

TODO: For each standard:

TODO: Mention basic background information and a general discussion for source (A little more detail than included in paper).

TODO: General reduction steps performed (not necessary to constantly repeat self). Highlight any differences in reduction steps compared to science targets.

TODO: Insert figure(s) showing comparison plots of spectrum/polarization parameters from POLSALT and STOPS(or leave out POLSALT and just show comparison to (*FORS1/2*) published results). Also short discussion (what the results can tell us and why it is useful). Focus on polarization results.

TODO: Add a ‘see reference’ to final paragraph and, if one of my papers, mention attached in appendix.

4.3.2 Spectropolarimetric Science Targets

Tested using 3C 279, 4C+01.02, and preliminary testing data provided by David. **TODO: VERIFY CORRECT**

TODO: Insert table listing the spectropolarimetric targets used, with their properties. (?)

Development of Tools for the SALT/RSS Spectropolarimetry Reductions:
Application to the Blazar 3C 279
(HEASA 2021)

TODO: Mention in appendix.

TODO: Mention basic background information and a general discussion for source (summary of paper + necessary extra).

TODO: Brief/unique reduction steps performed.

TODO: Insert figure(s) showing comparison plots of spectrum/polarization parameters from POLSALT and STOPS(or leave out POLSALT and just show published results). Also short discussion (what the results can tell us and why it is useful). Focus on polarization results.

SALT Spectropolarimetric Pipeline Comparisons

(HEASA 2022)

TODO: Mention in appendix.

TODO: Mention basic background information and a general discussion for source (summary of paper + necessary extra).

TODO: Brief/unique reduction steps performed.

TODO: Insert figure(s) showing comparison plots of spectrum/polarization parameters from POLSALT and STOPS(or leave out POLSALT and just show published results). Also short discussion (what the results can tell us and why it is useful). Focus on polarization results.

Chapter 5

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.

5.1 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 A

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, $\langle * \rangle$.

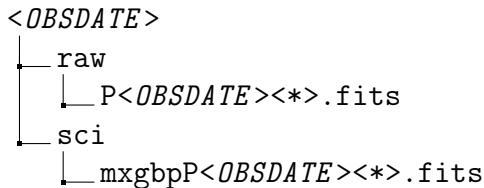


Figure A.1: The typical minimal file structure of data provided by SALT.

Ensure the data is formatted in a file structure similar to that in Figure A.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 A.2. The POLSALT GUI is launched from the default CLI running the commands in Listing A.1.

Listing A.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 A.2.

Listing A.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 A.3.

Listing A.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 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 A.4.

Listing A.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 $<O\text{-beam } ARC>$ with $<E\text{-beam } ARC>$.

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

Listing A.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="")
```

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

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.

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

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

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

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

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

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

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

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

The `transform` task will run autonomously.⁶ Repeat the `transform` procedure, replacing the $\langle O\text{-beam } FILES \rangle$ and $\langle O\text{-beam } ARC \rangle$ with $\langle E\text{-beam } FILES \rangle$ and $\langle E\text{-beam } ARC \rangle$ at both parameter locations. 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.

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

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

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.

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

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

Listing A.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, *<FILE(S)>*, using the commands in Listing A.9.

Listing A.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 A.10, moving all the files relevant to the wavelength calibrations into either the ‘database’ or ‘split_files’ directories.

Listing A.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 A.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’.

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

Listing A.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 A.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 A.2.

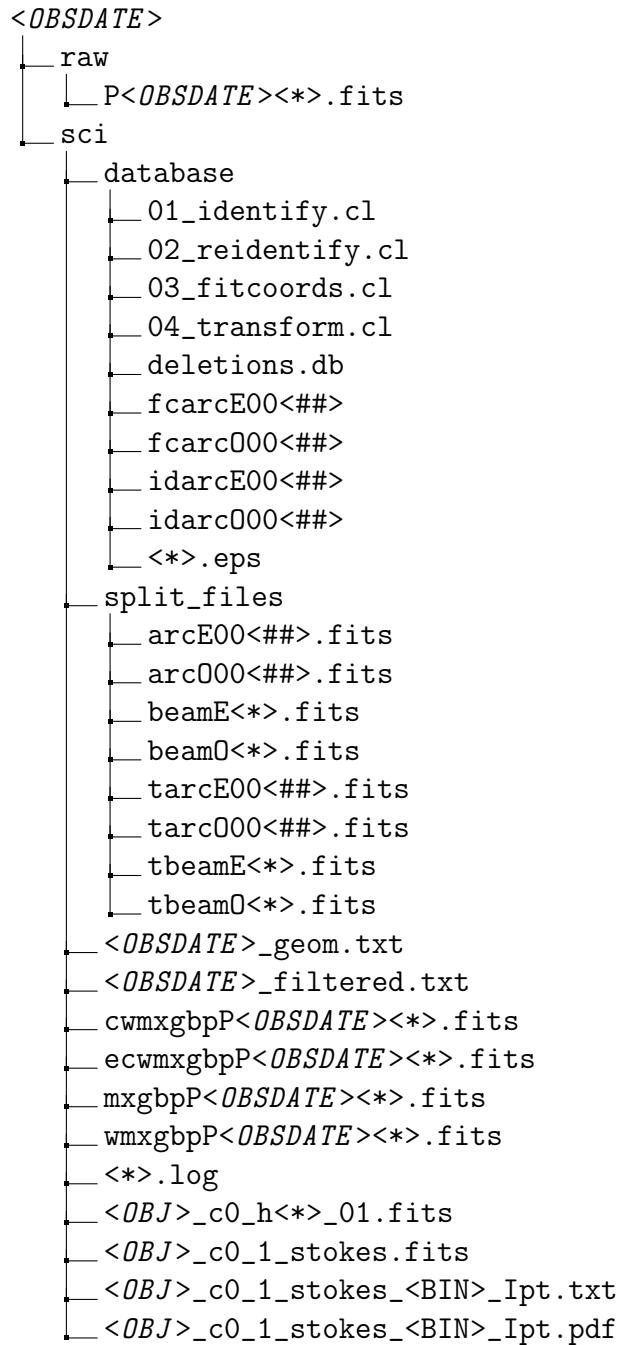


Figure A.2: The typical file structure after completing the reduction process.

Appendix B

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 B.1: The source code for `__main__.py`

```
1 #!/usr/bin/env python3
2 # -*- coding: utf-8 -*-
3
4 """Argument parser for STOPS."""
5
6 # MARK: Imports
7 import sys
8 import argparse
9 import logging
10 from pathlib import Path
11
12 from STOPS import __version__
13 from STOPS import Split, Join, CrossCorrelate, Skylines
14 from STOPS.utils import ParserUtils as Parser
15 from STOPS.utils.Constants import SPLIT_ROW, PREFIX, PARSE, SAVE_CORR, SAVE_SKY
16
17 # MARK: Constants
18 PROG = "STOPS"
19 DESCRIPTION = """
20 Supplementary TOols for Polsalt Spectropolarimetry (STOPS) is a
21 collection of supplementary tools created for SALT's POLSALT pipeline,
22 allowing for wavelength calibrations with IRAF. The tools provide
23 support for splitting and joining polsalt formatted data as well as
24 cross correlating complementary polarimetric beams.
25
26 DOI: 10.22323/1.401.0056
27 """
28
29
30 # MARK: Universal Parser
31 parser = argparse.ArgumentParser(
32     prog=PROG,
33     description=DESCRIPTION,
34     formatter_class=argparse.RawDescriptionHelpFormatter,
35 )
36 parser.add_argument(
37     "-V",
38     "--version",
39     action="version",
40     version=f"%(prog)s as of {__version__}",
41 )
```

```

42 parser.add_argument(
43     "-v",
44     "--verbose",
45     action="count",
46     default=PARSE['VERBOSE'],
47     help=(
48         "Counter flag which enables and increases verbosity. "
49         "Use -v or -vv for greater verbosity levels."
50     ),
51 )
52 parser.add_argument(
53     "-l",
54     "--log",
55     action="store",
56     type=Parser.parse_logfile,
57     help=(
58         "Filename of the logging file. "
59         "File is created if it does not exist. Defaults to None."
60     ),
61 )
62 parser.add_argument(
63     "data_dir",
64     action="store",
65     nargs="?",
66     default=PARSE['DATA_DIR'],
67     type=Parser.parse_path,
68     help=(
69         "Path of the directory which contains the working data. "
70         f"Defaults to the cwd -> '{PARSE['DATA_DIR']}' (I.E. '..')."
71     ),
72 )
73
74
75 # MARK: Split\Join Parent
76 split_join_args = argparse.ArgumentParser(add_help=False)
77 split_join_args.add_argument(
78     "-n",
79     "--no_arc",
80     action="store_true",
81     help="Flag to exclude arc files from processing.",
82 )
83 split_join_args.add_argument(
84     "-s",
85     "--split_row",
86     default=SPLIT_ROW,
87     type=int,
88     help=(
89         "Row along which the O and E beams are split. "
90         f"Defaults to polsalt's default -> {SPLIT_ROW}."
91     ),
92 )
93 split_join_args.add_argument(
94     "-p",
95     "--save_prefix",
96     nargs=2,
97     default=PREFIX,
98     help=(
99         "Prefix appended to the filenames, "
100        "with which the O and E beams are saved. "
101        f"Defaults to {PREFIX}."
102     ),
103 )
104
105
106 # MARK: Correlate\Skylines Parent
107 corr_sky_args = argparse.ArgumentParser(add_help=False)
108 corr_sky_args.add_argument(
109     "filenames",
110     action="store",
111     nargs="+",
112     type=Parser.parse_file,
113     help=(
114         "File name(s) of FITS file(s) to be processed."

```

```

115     "A minimum of one filename is required."
116 ),
117 )
118 corr_sky_args.add_argument(
119     "-b",
120     "--beams",
121     choices=["O", "E", "OE"],
122     type=str.upper,
123     default=PARSE['BEAMS'],
124     help=(
125         "Beams to process."
126         f"Defaults to {PARSE['BEAMS']}, but "
127         "may be given 'O', 'E', or 'OE' to "
128         "determine which beams are processed."
129     ),
130 )
131 corr_sky_args.add_argument(
132     "-ccd",
133     "--split_ccd",
134     action="store_false",
135     help=(
136         "Flag to NOT split CCD's."
137         "Recommended to leave off unless the chip gaps "
138         "have been removed from the data."
139     ),
140 )
141 corr_sky_args.add_argument(
142     "-c",
143     "--continuum_order",
144     type=int,
145     default=PARSE['CONT_ORD'],
146     dest="cont_ord",
147     help=(
148         "Order of continuum to remove from spectra."
149         "Higher orders recommended to remove most variation, "
150         "leaving only significant features."
151     ),
152 )
153 corr_sky_args.add_argument(
154     "-p",
155     "--plot",
156     action="store_true",
157     help="Flag for additional plot outputs.",
158 )
159
160
161 # MARK: Create subparser modes
162 subparsers = parser.add_subparsers(
163     dest="mode",
164     help="Operational mode of supplementary tools",
165 )
166
167
168 # MARK: Split Subparser
169 split_parser = subparsers.add_parser(
170     "split",
171     aliases=["s"],
172     help="Split mode",
173     parents=[split_join_args],
174 )
175 # 'children' split args here
176 # Change defaults here
177 split_parser.set_defaults(
178     mode="split",
179     func=Split,
180 )
181
182
183 # MARK: Join Subparser
184 join_parser = subparsers.add_parser(
185     "join",
186     aliases=["j"],
187     help="Join mode",

```

```

188     parents=[split_join_args],
189 )
190 # 'children' join args here
191 join_parser.add_argument(
192     "-c",
193     "--coefficients",
194     dest="solutions_list",
195     nargs='*',
196     type=Parser.parse_file,
197     help=(
198         "Custom coefficients to use instead of the `IRAF` fitcoords "
199         "database. Use as either '-c <o_solution> <e_solution>' or "
200         "a regex descriptor '-c <*solution*extention>'."
201     ),
202 )
203 # Change defaults here
204 join_parser.set_defaults(
205     mode="join",
206     func=Join,
207 )
208
209
210 # MARK: Correlate Subparser
211 corr_parser = subparsers.add_parser(
212     "correlate",
213     aliases=["x"],
214     help="Cross correlation mode",
215     parents=[corr_sky_args],
216 )
217 # 'children' correlate args here
218 corr_parser.add_argument(
219     "-o",
220     "--offset",
221     type=int,
222     default=PARSE['OFFSET'],
223     help=(
224         "Introduces an offset when correcting for "
225         "known offset in spectra or for testing purposes. "
226         f"Defaults to {PARSE['OFFSET']}. "
227         "(For testing, not used during regular operation.)"
228     ),
229 )
230 corr_parser.add_argument(
231     "-s",
232     "--save_prefix",
233     action="store",
234     nargs="?",
235     type=lambda path: Path(path).expanduser().resolve(),
236     const=SAVE_CORR,
237     help=(
238         "Prefix used when saving plot. "
239         "Excluding flag does not save output plot, "
240         f"flag usage of option uses default prefix, "
241         "and a provided prefix overwrites default prefix."
242     ),
243 )
244 # Change defaults here
245 corr_parser.set_defaults(
246     mode="correlate",
247     func=CrossCorrelate,
248 )
249
250
251 # MARK: Skyline Subparser
252 sky_parser = subparsers.add_parser(
253     "skylines",
254     aliases=["sky"],
255     help="Sky line check mode",
256     parents=[corr_sky_args],
257 )
258 # 'children' skyline args here
259 sky_parser.add_argument(
260     "-t",

```

```

261     "--transform",
262     action="store_false",
263     help=(
264         "Flag to force transform images. "
265         "Recommended to use only when input image(s) "
266         "are prefixed 't' but are not yet transformed."
267     ),
268 )
269 sky_parser.add_argument(
270     "-s",
271     "--save_prefix",
272     action="store",
273     nargs="?",
274     type=lambda path: Path(path).expanduser().resolve(),
275     const=SAVE_SKY,
276     help=(
277         "Prefix used when saving plot. "
278         "Excluding flag does not save output plot, "
279         f"flag usage of option uses default prefix, "
280         "and a provided prefix overwrites default prefix."
281     ),
282 )
283 # Change defaults here
284 sky_parser.set_defaults(
285     mode="skyline",
286     func=Skylines,
287 )
288
289
290 # MARK: Keyword Clean Up
291 args = parser.parse_args()
292
293 if len(sys.argv) == 1:
294     parser.print_help(sys.stderr)
295     sys.exit(2)
296
297 args.verbose = Parser.parse_loglevel(args.verbose)
298
299 if 'log' in args and args.log not in [None]:
300     args.log = args.data_dir / args.log
301
302 if "filenames" in args:
303     args.filenames = Parser.flatten(args.filenames)
304
305 if "solutions_list" in args and isinstance(args.solutions_list, list):
306     args.solutions_list = Parser.flatten(args.solutions_list)
307
308 # MARK: Begin logging
309 logging.basicConfig(
310     filename=args.log,
311     format="%(asctime)s - %(module)s - %(levelname)s - %(message)s",
312     datefmt="%Y-%m-%d %H:%M:%S",
313     level=args.verbose,
314 )
315
316 # MARK: Call Relevant Class(Args)
317 logging.debug(f"Argparse namespace: {args}")
318 logging.info(f"Mode:{args.mode}")
319 args.func(**vars(args)).process()
320
321
322 # Confirm all processes completed and exit without error
323 logging.info("All done! Come again!\n")

```

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

```

1 #!/usr/bin/env python3
2 # -*- coding: utf-8 -*-
3
4 """Module for splitting ``polsalt`` FITS files."""
5
6 # MARK: Imports
7 import os
8 import sys
9 import logging
10 from copy import deepcopy
11 from pathlib import Path
12
13 import numpy as np
14 from astropy.io import fits as pyfits
15
16 from STOPS.utils.SharedUtils import find_files, find_arc
17 from STOPS.utils.Constants import SAVE_PREFIX, CROP_DEFAULT, SPLIT_ROW
18
19
20 # MARK: Split Class
21 class Split:
22
23     #-----split0-----
24
25     """
26     The `Split` class allows for the splitting of `polsalt` FITS files
27     based on the polarization beam. The FITS files must have basic
28     `polsalt` pre-reductions already applied (`mxbgp...` FITS files).
29
30     Parameters
31     -----
32     data_dir : str / Path
33         The path to the data to be split
34     fits_list : list[str], optional
35         A list of pre-reduced `polsalt` FITS files to be split within `data_dir`.
36         (The default is None, `Split` will search for `mxbgp*.fits` files)
37     split_row : int, optional
38         The row along which to split the data of each extension in the FITS file.
39         (The default is SPLIT_ROW (See Notes), the SALT RSS CCD's middle row)
40     no_arc : bool, optional
41         Decides whether the arc frames should be recombined.
42         (The default is False, `polsalt` has no use for the arc after wavelength
43         ↪ 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]

```

```

71     Crops the data along the edge of the frame, that is,
72     `O`-beam cropped as [crop:], and
73     `E`-beam cropped as [: - crop].
74     update_beam_lists(o_name: str, e_name: str)
75         -> None
76         Updates `o_files` and `e_files`.
77     save_beam_lists(file_suffix: str = 'frames')
78         -> None
79         Creates (Overwrites if exists) and writes the `o_files` and `e_files` to files
80         ↳ 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
85         ↳ automation.
86
87     Other Parameters
88     -----
89
90     Notes
91     -----
92     Constants Imported (See utils.Constants):
93         SAVE_PREFIX
94         CROP_DEFAULT
95         SPLIT_ROW
96
97     """
98
99     #-----split1-----
100
101    # MARK: Split init
102    def __init__(
103        self,
104        data_dir: Path,
105        fits_list: list[str] = None,
106        split_row: int = SPLIT_ROW,
107        no_arc: bool = False,
108        save_prefix: Path | None = None,
109        **kwargs,
110    ) -> None:
111        self.data_dir = data_dir
112        self.fits_list = find_files(
113            data_dir=data_dir,
114            filenames=fits_list,
115            prefix="mxgbp",
116            ext="fits"
117        )
118        self.split_row = split_row
119        self.save_prefix = SAVE_PREFIX
120        if isinstance(save_prefix, dict):
121            self.save_prefix = save_prefix
122
123        self.arc = "" if no_arc else find_arc(self.fits_list)
124        self.o_files = []
125        self.e_files = []
126
127        logging.debug("__init__ - \n", self.__dict__)
128        return
129
130    # MARK: Split Files
131    def split_file(
132        self,
133        file: os.PathLike
134    ) -> tuple[pyfits.HDUList, pyfits.HDUList]:
135        """
136            Split the single FITS file into separated `O`- and `E`- FITS files.
137
138        Parameters
139        -----
140        file : os.PathLike

```

```

141     The name of the FITS file to be split.
142
143     Returns
144     -----
145     tuple[astropy.io.fits.HDUList, astropy.io.fits.HDUList]
146         Tuple containing the split O and E beam HDULists.
147
148     """
149     # Create empty HDUList
150     o_beam = pyfits.HDUList()
151     e_beam = pyfits.HDUList()
152
153     # Open file and split O & E beams
154     with pyfits.open(file) as hdul:
155         o_beam.append(hdul["PRIMARY"].copy())
156         e_beam.append(hdul["PRIMARY"].copy())
157
158     # Split specific extention
159     raw_split = self.split_ext(hdul, "SCI")
160
161     # o_beam[0].data = raw_split['SCI'].data[1]
162     # e_beam[0].data = raw_split['SCI'].data[0]
163     o_beam[0].data, e_beam[0].data = self.crop_file(raw_split)
164
165     # Handle prefix and names
166     pref = "arc" if file == self.arc else "beam"
167     o_name = self.save_prefix[pref][0] + file.name[-9:]
168     e_name = self.save_prefix[pref][1] + file.name[-9:]
169
170     # Add split data to O & E beam lists
171     self.update_beam_lists(o_name, e_name, pref == "arc")
172
173     # Handle don't save case
174     if self.save_prefix is None:
175         return o_beam, e_beam
176
177     # Handle save case
178     o_beam.writeto(o_name, overwrite=True)
179     e_beam.writeto(e_name, overwrite=True)
180
181     return o_beam, e_beam
182
183     # MARK: Split extensions
184     def split_ext(
185         self,
186         hdulist: pyfits.HDUList,
187         ext: str = "SCI"
188     ) -> pyfits.HDUList:
189         """
190             Split the data of the specified extension of `hdulist` into
191             its 'O'- and 'E'- beams.
192
193             Parameters
194             -----
195             hdulist : astropy.io.fits.HDUList
196                 The FITS HDUList to be split.
197             ext : str, optional
198                 The name of the extension to be split.
199                 (Defaults to 'SCI')
200
201             Returns
202             -----
203             astropy.io.fits.HDUList
204                 The HDUList with the split applied.
205
206             """
207             hdu = deepcopy(hdulist)
208             rows, cols = hdu[ext].data.shape
209
210             # if odd number of rows, strip off the last one
211             rows = int(rows / 2) * 2
212
213             # how far split is from center of detector

```

```

214     offset = int(self.split_row - rows / 2)
215
216     # split arc into o/e images
217     ind_rc = np.indices((rows, cols))[0]
218     padbins = (ind_rc < offset) | (ind_rc > rows + offset)
219
220     # Roll split_row to be centre row
221     image_rc = np.roll(hdu[ext].data[:rows, :], -offset, axis=0)
222     image_rc[padbins] = 0.0
223
224     # Split columns equally
225     hdu[ext].data = image_rc.reshape((2, int(rows / 2), cols))
226
227     return hdu
228
229 # MARK: Crop files
230 @staticmethod
231 def crop_file(
232     hdulist: pyfits.HDUList,
233     crop: int = CROP_DEFAULT
234 ) -> tuple[np.ndarray, np.ndarray]:
235     """
236         Crop the data with respect to the `O`/`E` beam.
237
238     Parameters
239     -----
240     hdulist : astropy.io.fits.HDUList
241         The HDUList containing the data to be cropped.
242     crop : int, optional
243         The number of rows to be cropped from the bottom and top
244         of the `O` and `E` beam, respectively.
245         (Defaults to 40)
246
247     Returns
248     -----
249     tuple[numpy.ndarray, np.ndarray]
250         Tuple containing the cropped O and E beam data arrays.
251
252     """
253     o_data = hdulist["SCI"].data[1, 0:-crop]
254     e_data = hdulist["SCI"].data[0, crop:]
255
256     return o_data, e_data
257
258 # MARK: Update beam lists
259 def update_beam_lists(
260     self,
261     o_name,
262     e_name,
263     arc: bool = True
264 ) -> None:
265     """
266         Update the `o_files` and `e_files` attributes.
267
268     Parameters
269     -----
270     o_name : str
271         The filename of the O beam.
272     e_name : str
273         The filename of the E beam.
274     arc : bool, optional
275         Indicates whether the first entry should be the arc frame.
276         (Defaults to True)
277
278     Returns
279     -----
280     None
281
282     """
283     if arc:
284         self.o_files.insert(0, o_name)
285         self.e_files.insert(0, e_name)
286     else:

```

```
287         self.o_files.append(o_name)
288         self.e_files.append(e_name)
289
290     return
291
292 # MARK: Save beam lists
293 def save_beam_lists(self, file_suffix: str = 'frames') -> None:
294     with open(f'o_{file_suffix}', 'w+') as f_o, \
295             open(f'e_{file_suffix}', 'w+') as f_e:
296         for i, j in zip(self.o_files, self.e_files):
297             f_o.write(i + '\n')
298             f_e.write(j + '\n')
299
300     return
301
302 # MARK: Process all Listed Images
303 def process(self) -> None:
304     """
305     Process all FITS images stored in the `fits_list` attribute
306
307     Returns
308     -----
309     None
310
311     """
312     for target in self.fits_list:
313         logging.debug(f"Processing {target}")
314         self.split_file(target)
315
316     self.save_beam_lists()
317
318     return
319
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 B.3: The source code for `join.py`

```

1 #!/usr/bin/env python3
2 # -*- coding: utf-8 -*-
3
4 """
5 Module for joining the split FITS files with an external wavelength solution.
6 """
7
8 # MARK: Imports
9 import os
10 import sys
11 import logging
12 import re
13 from pathlib import Path
14
15 import numpy as np
16 from numpy.polynomial.chebyshev import chebgrid2d as chebgrid2d
17 from numpy.polynomial.legendre import leggrid2d as leggrid2d
18 from astropy.io import fits as pyfits
19
20 # from lacosmic import lacosmic # Replaced: ccdproc is ~6x faster
21 from ccdproc import cosmicray_lacosmic as lacosmic
22
23 from STOPS.utils.specpolpy3 import read_wollaston, split_sci
24 from STOPS.utils.SharedUtils import find_files, find_arc
25 from STOPS.utils.Constants import DATADIR, SAVE_PREFIX, SPLIT_ROW, CR_PARAMS
26
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 and the
35     appending of an external wavelength solution in the `polsalt` FITS file format.
36
37     Parameters
38     -----
39     data_dir : str / Path
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 `mxbp*.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
49         ↪ 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
79     Methods
80     -----
81     get_solutions(wavlist: list / None, prefix: str = "fc") -> (fc_files, custom):
82         tuple[list[str], bool]
83             Parse `solutions_list` and return valid solution files and if they are
84             non-`IRAF` solutions.
85     parse_solution(fc_file: str, x_shape: int, y_shape: int) -> tuple[dict[str, int],
86         np.ndarray]
87         Loads the wavelength solution file and parses keywords necessary for creating
88         the wavelength extension.
89     join_file(file: os.PathLike) -> None
90         Joins the files,
91         attaches the wavelength solutions,
92         performs cosmic ray cleaning,
93         masks the extension,
94         and checks cropping performed in `Split`.
95         Writes the FITS file in a `polsalt` valid format.
96     check_crop(hdu: pyfits.HDUList, o_file: str, e_file: str) -> int
97         Opens the split `O`- and `E`-beam FITS files and returns the amount of cropping
98         that was performed.
99     process() -> None
100        Calls `join_file` on each file in `fits_list` for automation.
101
102
103     Other Parameters
104     -----
105     no_arc : bool, optional
106         Deprecated. Decides whether the arc frames should be processed.
107         (The default is False, `polsalt` has no use for the arc after wavelength
108         calibrations)
109     **kwargs : dict
110         keyword arguments. Allows for passing unpacked dictionary to the class
111         constructor.
112
113     Notes
114     -----
115     Constants Imported (See utils.Constants):
116         DATADIR, SAVE_PREFIX, SPLIT_ROW, CR_PARAMS
117
118     Custom wavelength solutions must be formatted containing:
119         `x`, `y`, *coefficients...
120     where a solution are of order (`x` by `y`) and must contain  $x \times y$  coefficients,
121     all separated by newlines. The name of the custom wavelength solution file
122     must contain either "cheb" or "leg" for Chebyshev or Legendre
123     wavelength solutions, respectively.
124
125     Cosmic ray rejection is performed using lacosmic [1]_ implemented in ccdproc via
126     astroscreappy [2]_.
127
128     References
129     -----
130     .. [1] van Dokkum 2001, PASP, 113, 789, 1420 (article :
131         <https://adsabs.harvard.edu/abs/2001PASP..113.1420V>
132     .. [2] https://zenodo.org/records/1482019
133
134     """
135
136     #-----join1-----
137
138     # MARK: Join init
139     def __init__(self,
140                  data_dir: Path,
141                  database: str = "database",
142                  fits_list: list[str] = None,
143

```

```

135     solutions_list: list[Path] = None,
136     split_row: int = SPLIT_ROW,
137     no_arc: bool = True,
138     save_prefix: Path | None = None,
139     verbose: int = 30,
140     **kwargs,
141 ) -> None:
142     self.data_dir = data_dir
143     self.database = Path(data_dir) / database
144     self.fits_list = find_files(
145         data_dir=self.data_dir,
146         filenames=fits_list,
147         prefix="mxgbp",
148         ext="fits",
149     )
150     self.fc_files, self.custom = self.get_solutions(solutions_list)
151     self.split_row = split_row
152     self.save_prefix = SAVE_PREFIX
153     if isinstance(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
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
179         in the `database` directory.
180     prefix : str, optional
181         The prefix of the wavelength solution files.
182         (Defaults to "fc")
183     reverse : bool, optional
184         Whether to reverse the wavelength solution files.
185         Necessary when `wavlist` ordered ['O', 'E']
186         (Defaults to True)
187
188     Returns
189     -----
190     tuple[list[str], bool]
191         A tuple containing the list of wavelength solutions files and
192         a boolean indicating whether custom solutions were provided.
193
194     """
195     # No custom solutions
196     if not wavlist:
197         # Handle finding solutions
198         ws = []
199         for fl in os.listdir(self.database):
200             if os.path.isfile(self.database / fl) and (prefix == fl[0:len(prefix)]):
201                 ws.append(fl)
202
203         if len(ws) != 2:
204             # Handle incorrect number of solutions found
205             msg = (
206                 f"Incorrect amount of wavelength solutions "
207                 f"({len(ws)} fc... files) found in the solution "

```

```

208             f"dir.: {self.database}"
209         )
210         logging.error(msg)
211         raise FileNotFoundError(msg)
212
213     sols = {
214         i: j for i, j in zip(['0', 'E'], sorted(ws, reverse=reverse))
215     }
216     logging.debug(f"get_solutions - Found {sols} in {self.database}")
217
218     return sorted(ws, reverse=reverse), False
219
220     # Custom solution
221     if len(wavlist) >= 2:
222         if len(wavlist) > 2:
223             logging.warning(f" Too many solutions, only {wavlist[:2]} are
224             ↪ considered")
225             wavlist = wavlist[:2]
226
227         for fl in wavlist:
228             if not os.path.isfile(os.path.join(self.data_dir, fl)):
229                 msg = (
230                     f"{fl} not found in the "
231                     f"data directory {self.data_dir}"
232                 )
233                 logging.error(msg)
234                 raise FileNotFoundError(msg)
235
236         sols = {
237             i: j for i, j in zip(['0', 'E'], sorted(wavlist, reverse=reverse))
238         }
239         logging.debug(f"get_solutions - Found {sols} in {self.database}")
240
241     return sorted(wavlist, reverse=reverse), True
242
243     # MARK: Parse 2D WAV Function
244     def parse_solution(
245         self,
246         fc_file: str,
247         x_shape: int,
248         y_shape: int
249     ) -> tuple[dict[str, int], np.ndarray]:
250         """
251             Parse the 2D wavelength solution function from `fc_file`.
252
253             Parameters
254             -----
255             fc_file : str
256                 The filename of the wavelength solutions file.
257             x_shape : int
258                 The x-order of the 2D solution.
259             y_shape : int
260                 The y-order of the 2D solution.
261
262             Returns
263             -----
264             tuple[dict[str, int], np.ndarray]
265                 A tuple containing a dictionary of
266                 the parameters of the solution function
267                 and the function coefficients.
268
269             fit_params = {}
270
271             if self.custom:
272                 # Load coefficients
273                 coeff = np.loadtxt(fc_file)
274
275                 fit_params["xorder"] = int(coeff[0].astype(int))
276                 fit_params["yorder"] = int(coeff[1].astype(int))
277                 coeff = coeff[2:]
278
279             f_type = 3

```

```

280         if "cheb" in str(fc_file):
281             f_type = 1
282         elif "leg" in str(fc_file):
283             f_type = 2
284         fit_params["function"] = f_type
285
286         fit_params["xmin"], fit_params["xmax"] = 1, x_shape
287         fit_params["ymin"], fit_params["ymax"] = 1, y_shape
288
289     else:
290         # Parse IRAF fc database files
291         file_contents = []
292         with open(self.database / fc_file) as fcfile:
293             for i in fcfile:
294                 file_contents.append(re.sub(r"\n\t\s*", "", i))
295
296         if file_contents[9] != "1.": # xterms - Cross-term type
297             msg = (
298                 "Cross-term not recognised (always 1 for "
299                 "'FITCOORDS'), redo FITCOORDS or change manually."
300             )
301             raise Exception(msg)
302
303         fit_params["function"] = int(file_contents[6][-1])
304
305         fit_params["xorder"] = round(float(file_contents[7][-1]), None)
306         fit_params["yorder"] = round(float(file_contents[8][-1]), None)
307
308         fit_params["xmin"] = int(file_contents[10][-1])
309         fit_params["xmax"] = x_shape
310         # int(file_contents[11][-1])# stretch fit over x
311         fit_params["ymin"] = int(file_contents[12][-1])
312         fit_params["ymax"] = y_shape
313         # int(file_contents[13][-1])# stretch fit over y
314
315         coeff = np.array(file_contents[14:], dtype=float)
316
317         coeff = np.reshape(
318             coeff,
319             (fit_params["xorder"], fit_params["yorder"]))
320
321     return fit_params, coeff
322
323
324 # MARK: Join Files
325 def join_file(self, file: os.PathLike) -> None:
326     """
327     Join the `O`- and `E`-beams, attach the wavelength solutions,
328     perform cosmic ray cleaning, mask the extensions,
329     and checks cropping performed by `Split`.
330     Write the FITS file in a `polsalt` valid format.
331
332     Parameters
333     -----
334     file : os.PathLike
335         The path of the FITS file to be joined.
336
337     See Also
338     -----
339     IRAF - `fitcoords` task
340         https://iraf.net/irafdocs/formats/fitcoords.php,
341     numpy 2D grid functions
342         https://numpy.org/doc/stable/reference/generated/numpy.polynomial.chebyshev.chebgrid2d.html,
343         https://numpy.org/doc/stable/reference/generated/numpy.polynomial.legendre.leggrid2d.html
344
345     """
346
347     # Create empty wavelength appended hdu list
348     whdu = pyfits.HDUList()
349
350     # Handle prefix and names
351     pref = "arc" if file == self.arc else "beam"
352     o_file = self.save_prefix[pref][0] + file.name[-9:]

```

```

353     e_file = self.save_prefix[pref][1] + file.name[-9:]
354
355     # Open file
356     with pyfits.open(file) as hdu:
357         # Check if file has been cropped
358         cropsize = self.check_crop(hdu, o_file, e_file)
359
360         y_shape = int(hdu["SCI"].data.shape[0] / 2) - cropsize
361         x_shape = hdu["SCI"].data.shape[1]
362
363         # No differences in "PRIMARY" extention header
364         primary_ext = hdu["PRIMARY"]
365         primary_ext.header["HISTORY"] = f"CRCLEAN: {CR_PARAMS}"
366         whdu.append(primary_ext)
367
368         for ext in ["SCI", "VAR", "BPM"]:
369             whdu.append(pyfits.ImageHDU(name=ext))
370             whdu[ext].header = hdu[ext].header.copy()
371             whdu[ext].header["CTYPE3"] = "O,E"
372
373             # Create empty extentions with correct order and format
374             if ext == "BPM":
375                 whdu[ext].data = np.zeros(
376                     (2, y_shape, x_shape),
377                     dtype="uint8"
378                 )
379                 whdu[ext].header["BITPIX"] = "-uint8"
380             else:
381                 whdu[ext].data = np.zeros(
382                     (2, y_shape, x_shape),
383                     dtype=">f4"
384                 )
385                 whdu[ext].header["BITPIX"] = "-32"
386
387             # Fill in empty extentions
388             if cropsize:
389                 temp_split = split_sci(
390                     hdu,
391                     self.split_row,
392                     ext=ext
393                 )[ext].data
394                 whdu[ext].data[0] = temp_split[0, cropsize:]
395                 whdu[ext].data[1] = temp_split[1, 0:-cropsize]
396
397             else:
398                 whdu[ext].data = split_sci(
399                     hdu,
400                     self.split_row,
401                     ext=ext
402                 )[ext].data
403             # End of hdu calls, close hdu
404
405             # MARK: Join (Wav. Ext.)
406             whdu.append(pyfits.ImageHDU(name="WAV"))
407             wav_header = whdu["SCI"].header.copy()
408             wav_header["EXTNAME"] = "WAV"
409             wav_header["CTYPE3"] = "O,E"
410             whdu["WAV"].header = wav_header
411
412             whdu["WAV"].data = np.zeros(
413                 whdu["SCI"].data.shape,
414                 dtype=">f4"
415             )
416
417             for num, fname in enumerate(self.fc_files):
418                 params, coeffs = self.parse_solution(
419                     fname,
420                     x_shape,
421                     y_shape
422                 )
423
424                 if params["function"] == 1: # Function type (1 = chebyshev)
425                     # Set wavelength extention values to function

```

```

426         whdu["WAV"].data[num] = chebgrid2d(
427             x=np.linspace(-1, 1, params["ymax"]),
428             y=np.linspace(-1, 1, params["xmax"]),
429             c=coeffs,
430         )
431
432     elif params["function"] == 2: # Function type (2 = legendre)
433         # Set wavelength extention values to function
434         whdu["WAV"].data[num] = leggrid2d(
435             x=np.linspace(-1, 1, params["ymax"]),
436             y=np.linspace(-1, 1, params["xmax"]),
437             c=coeffs,
438         )
439
440     else:
441         msg = (
442             "Function type not recognised, please wavelength "
443             "calibrate using either Chebyshev or Legendre."
444         )
445         raise Exception(msg)
446
447     # MARK: Cosmic Ray Cleaning
448     # See utils.Constants for `CR_PARAMS` discussion
449     whdu["SCI"].data[num] = lacosmic(
450         whdu["SCI"].data[num],
451         # contrast=CR_PARAMS['CR_CONTRAST'],
452         # threshold=CR_PARAMS['CR_THRESHOLD'],
453         # neighbor_threshold=CR_PARAMS['CR_NEIGH_THRESH'],
454         # effective_gain=CR_PARAMS['GAIN'],
455         # background=CR_PARAMS['BACKGROUND'],
456         readnoise=CR_PARAMS['READNOISE'],
457         gain=CR_PARAMS['GAIN'],
458         verbose=self.verbose,
459     )[0]
460
461     # MARK: WAV masking
462     # Left & Right Crop
463     whdu["WAV"].data[whdu["WAV"].data[:] < 3_000] = 0.0
464     whdu["WAV"].data[whdu["WAV"].data[:] >= 10_000] = 0.0
465
466     # Top & Bottom Crop (shift\tilt)
467     rpix_oc, cols, rbin, lam_c = read_wollaston(
468         whdu,
469         DATADIR + "wollaston.txt"
470     )
471
472     drow_oc = (rpix_oc - rpix_oc[:, int(cols / 2)][:, None]) / rbin
473
474     # Cropping as suggested
475     for c, col in enumerate(drow_oc[0]):
476         if np.isnan(col):
477             continue
478
479         if int(col) < 0:
480             whdu["WAV"].data[0, int(col):, c] = 0.0
481         elif int(col) > cropsize:
482             whdu["WAV"].data[0, 0: int(col) - cropsize, c] = 0.0
483
484     for c, col in enumerate(drow_oc[1]):
485         if np.isnan(col):
486             continue
487
488         if int(col) > 0:
489             whdu["WAV"].data[1, 0: int(col), c] = 0.0
490         elif (int(col) < 0) & (abs(int(col)) > cropsize):
491             whdu["WAV"].data[1, int(col) + cropsize:, c] = 0.0
492
493     # MARK: BPM masking
494     whdu["BPM"].data[0] = np.where(
495         whdu["WAV"].data[0] == 0,
496         1,
497         whdu["BPM"].data[0]
498     )

```

```

499     whdu["BPM"].data[1] = np.where(
500         whdu["WAV"].data[1] == 0,
501         1,
502         whdu["BPM"].data[1]
503     )
504
505     whdu.writeto(f"w{os.path.basename(file)}", overwrite="True")
506
507     return
508
509 # MARK: Check Crop
510 @staticmethod
511 def check_crop(
512     hdu: pyfits.HDUList,
513     o_file: str,
514     e_file: str
515 ) -> int:
516     """
517     Check if cropping is necessary when joining `O`- and `E`-beams.
518
519     Parameters
520     -----
521     hdu : astropy.io.fits.HDUList
522         The HDUList to check for cropping.
523     o_file : str
524         The name of the previously split `O`-beam FITS file.
525     e_file : str
526         The name of the previously split `E`-beam FITS file.
527
528     Returns
529     -----
530     int
531         The number of rows which were cropped by `Split`.
532
533     """
534     cropsize = 0
535
536     with pyfits.open(o_file) as o, \
537         pyfits.open(e_file) as e:
538         o_y = o[0].data.shape[0]
539         e_y = e[0].data.shape[0]
540
541     if hdu["SCI"].data.shape[0] != (o_y + e_y):
542         # Get crop size, assuming crop same on both sides
543         cropsize = int((hdu["SCI"].data.shape[0] - o_y - e_y) / 2)
544
545     return cropsize
546
547 # MARK: Process all Listed Images
548 def process(self) -> None:
549     """
550     Process all FITS images stored in the `fits_list` attribute
551     """
552     for target in self.fits_list:
553         logging.debug(f"Processing {target}")
554         self.join_file(target)
555
556
557 def main(argv) -> None:
558     """
559     Main function.
560     """
561
562
563 if __name__ == "__main__":
564     main(sys.argv[1:])

```

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

```

1 #!/usr/bin/env python3
2 # -*- coding: utf-8 -*-
3
4 """Module for cross correlating polarization beams."""
5
6 # MARK: Imports
7 import sys
8 import logging
9 import itertools as iters
10 from pathlib import Path
11 from typing import Callable
12
13 import numpy as np
14 from numpy.polynomial import chebyshev
15 import matplotlib.pyplot as plt
16 import matplotlib.axes
17 from astropy.io import fits as pyfits
18 from scipy import signal
19
20 from STOPS.utils.SharedUtils import find_files, continuum
21 from STOPS.utils.Constants import SAVE_CORR, OFFSET
22
23 mpl_logger = logging.getLogger('matplotlib')
24 mpl_logger.setLevel(logging.INFO)
25
26
27 # MARK: Correlate class
28 class CrossCorrelate:
29
30     #-----corr0-----
31
32     """
33     Cross correlate allows for comparing the extensions of multiple
34     FITS files, or comparing the O and E beams of a single FITS file.
35
36     Parameters
37     -----
38     data_dir : str / Path
39         The path to the data to be cross correlated
40     filenames : list[str]
41         The ecwma*gbp*.fits files to be cross correlated.
42         If only one filename is defined, correlation is done against the two
43         ↪ polarization beams.
44     split_ccd : bool, optional
45         Decides whether the CCD regions should each be individually cross correlated.
46         (The default is True, which splits the spectrum up into its separate CCD regions)
47     cont_ord : int, optional
48         The degree of a chebyshev to fit to the continuum.
49         (The default is 11)
50     plot : bool, optional
51         Decides whether the continuum fitting should be plotted
52         (The default is False, so no continua plots are displayed)
53     save_prefix : str, optional
54         The name or directory to save the figure produced to.
55         "." saves a default name to the current working. A default name is also used
56         ↪ 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 extension.
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 the continuum fitting should be plotted

```

```

70     offset : int
71         The amount the spectrum is shifted, mainly to test the effect of the cross
72         ↵ correlation
73         (The default is 0, I.E. no offset introduced)
74     save_prefix
75     wav_unit : str
76         The units of the wavelength axis.
77         (The default is Angstroms)
78     wav_cdel : int
79         The wavelength increment.
80         (The default is 1)
81     alt : Callable
82         An alternate method of cross correlating the data.
83         (The default is None)
84
85     Methods
86     -----
87     load_file(filename: Path) -> tuple[np.ndarray, np.ndarray, np.ndarray]
88         Loads the data from a FITS file.
89     get_bounds(bpm: np.ndarray) -> np.ndarray
90         Finds the bounds for the CCD regions.
91     remove_cont(spec: list, wav: list, bpm: list, plot_cont: bool) -> None
92         Removes the continuum from the data.
93     correlate(filename1: Path, filename2: Path | None = None) -> None
94         Cross correlates the data.
95     ftcs(filename1: Path, filename2: Path | None = None) -> None
96         Cross correlates the data using the Fourier Transform.
97     plot(spec, wav, bpm, corrd, lagsdb) -> None
98         Plots the data.
99     process() -> None
100        Processes the data.
101
102    Other Parameters
103    -----
104    offset : int, optional
105        The amount the spectrum is shifted, mainly to test the effect of the cross
106        ↵ 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
110        ↵ constructor.
111        ftcs : bool, optional
112            Decides whether the Fourier Transform should be used for cross correlation.
113
114    See Also
115    -----
116    scipy
117        https://docs.scipy.org/doc/scipy/reference/generated/
118        correlation: scipy.signal.correlate.html
119
120    Notes
121    -----
122    Constants Imported (See utils.Constants):
123        SAVE_CORR
124
125    # -----corr1-----
126
127    # MARK: Correlate init
128    def __init__(
129        self,
130        data_dir: Path,
131        filenames: list[str],
132        beams: str = "OE",
133        split_ccd: bool = True,
134        cont_ord: int = 11,
135        plot: bool = False,
136        offset: int = 0,
137        save_prefix: Path | None = None,
138        **kwargs,
139    ) -> None:

```

```

140     self.data_dir = data_dir
141     self.fits_list = find_files(
142         data_dir=self.data_dir,
143         filenames=filenames,
144         prefix="ecwmxgbp",
145         ext="fits",
146     )
147     self._beams = None
148     self.beams = beams
149     self.ccds = 1
150     if split_ccd:
151         # BPM == 2 near center of CCD if CCD count varies
152         with pyfits.open(self.fits_list[0]) as hdu:
153             self.ccds = sum(hdu["BPM"].data.sum(axis=1)[0] == 2)
154
155     self.cont_ord = cont_ord
156     self.can_plot = plot
157     self.offset = offset
158     if offset != 0:
159         logging.warning("'offset' is only for testing.")
160
161     err_msg = "Offset removed after finalizing testing."
162     logging.error(err_msg)
163     raise ValueError(err_msg)
164     # Add an offset to the spectra to test cross correlation
165     # self.spec1 = np.insert(
166     #     self.spec1, [0] * offset, self.spec1[:, :offset], axis=-1
167     # )[:, :self.spec1.shape[-1]]
168
169     self.save_prefix = save_prefix
170     # Handle directory save name
171     if self.save_prefix and self.save_prefix.is_dir():
172         self.save_prefix /= SAVE_CORR
173         logging.warning((
174             f"Correlation save name resolves to a directory. "
175             f"Saving under {self.save_prefix}"
176         ))
177
178     self.wav_unit = "$\AA$"
179     self.wav_cdelt = 1
180
181     self.alt = self.ftcs if kwargs.get("ftcs") else None
182
183     logging.debug("__init__ - \n", self.__dict__)
184     return
185
186     # MARK: Beams property
187     @property
188     def beams(self) -> str:
189         return self._beams
190
191     @beams.setter
192     def beams(self, mode: str) -> None:
193         if mode not in ['O', 'E', 'OE']:
194             err_msg = f"Correlation mode '{mode}' not recognized."
195             logging.error(err_msg)
196             raise ValueError(err_msg)
197
198         self._beams = mode
199
200     return
201
202     # MARK: Load file
203     def load_file(
204         self,
205         filename: Path
206     ) -> tuple[np.ndarray, np.ndarray, np.ndarray]:
207         """
208             Load the data from a FITS file.
209
210             Parameters
211             -----
212             filename : Path

```

```

213     The name of the FITS file to load.
214
215     Returns
216     -----
217     tuple[np.ndarray, np.ndarray, np.ndarray]
218         The spectrum, wavelength, and bad pixel mask.
219
220     """
221
222     # Open HDU
223     with pyfits.open(filename) as hdul:
224         spec = hdul["SCI"].data.sum(axis=1)
225         wav = (
226             np.arange(spec.shape[-1])
227             * hdul["SCI"].header["CDELT1"]
228             + hdul["SCI"].header["CRVAL1"]
229         )
230         wav = np.array((wav, wav))
231         bpm = hdul["BPM"].data.sum(axis=1)
232
233         self.wav_cdel = float(hdul["SCI"].header["CDELT1"])
234
235         if hdul["SCI"].header["CTYPE1"] != 'Angstroms':
236             self.wav_unit = hdul["SCI"].header["CTYPE1"]
237
238     return spec, wav, bpm
239
240 # MARK: Get bounds
241 def get_bounds(self, bpm: np.ndarray) -> np.ndarray:
242     """
243         Find the bounds for a file based on the CCD count.
244
245         Parameters
246         -----
247         bpm : np.ndarray
248             The bad pixel mask.
249
250         Returns
251         -----
252         np.ndarray
253             The bounds for the CCD regions.
254
255     """
256     # bounds.shape -> (0/E, CCD's, low./up. bound)
257     if self.ccds == 1:
258         return np.array(
259             [(0, bpm[0].shape[-1]), (0, bpm[1].shape[-1])])
260         .astype(int)
261
262     bounds = np.zeros((2, self.ccds, 2))
263
264     # Get lower and upper bound for each ccd, save to bounds
265     # Lower -> min is zero, Upper -> max is bpm length
266     for ext, ccd in iter.product(range(2), range(self.ccds)):
267         mid = np.where(bpm[ext] == 2)[0][ccd]
268         ccds = self.ccds * 2
269         bounds[ext, ccd] = (
270             max(mid - bpm.shape[-1] // ccds, 0),
271             min(mid + bpm.shape[-1] // ccds, bpm.shape[-1])
272         )
273
274     return bounds.astype(int)
275
276 # MARK: Remove Continua
277 def remove_cont(
278     self,
279     spec: np.ndarray,
280     wav: np.ndarray,
281     bpm: np.ndarray,
282     plot_cont: bool
283 ) -> np.ndarray:
284     """
285         Remove the continuum from the data.

```

```

286
287     Parameters
288     -----
289     spec : np.ndarray
290         The spectrum to remove the continuum from.
291     wav : np.ndarray
292         The wavelength of the spectrum.
293     bpm : np.ndarray
294         The bad pixel mask.
295     plot_cont : bool
296         Decides whether the continuum fitting should be plotted
297
298     Returns
299     -----
300     spec : np.ndarray
301
302     """
303     # Mask out the bad pixels for fitting continua
304     okwav = np.where(bpm != 1)
305
306     # Define continua
307     ctm = continuum(
308         wav[okwav],
309         spec[okwav],
310         deg=self.cont_ord,
311         plot=plot_cont,
312     )
313
314     # Normalise spectra
315     spec /= chebyshev.chebval(wav, ctm)
316     spec -= 1
317
318     return spec
319
320     # MARK: Correlate
321     def correlate(
322         self,
323         filename1: Path,
324         filename2: Path | None = None,
325         alt: Callable = None
326     ) -> tuple[np.ndarray, np.ndarray, np.ndarray, list[list], list[list]]:
327         """
328             Cross correlates the data.
329
330         Parameters
331         -----
332         filename1 : Path
333             The name of the first FITS file to cross correlate.
334         filename2 : Path, optional
335             The name of the second FITS file to cross correlate.
336             (Defaults to None)
337         alt : Callable, optional
338             An alternate method of cross correlating the data.
339             (Defaults to None)
340
341         Returns
342         -----
343         spec, wav, bpm, lagsdb, corrdb: tuple[np.ndarray, np.ndarray, np.ndarray,
344             ↵ list[list], list[list]]
345
346         """
347         # mode: 'OE' -> 'O1' & 'E1', 'O' -> 'O1' & 'O2', 'E' -> 'E1' & 'E2'
348         # Load data
349         spec, wav, bpm = self.load_file(filename1)
350         if filename2 and self.beams != 'OE':
351             def unpack(exts, *args):
352                 return [arr[exts] for arr in args]
353
354             if self.beams == 'O':
355                 spec[-1], wav[-1], bpm[-1] = unpack(
356                     0, *self.load_file(filename2)
357                 )

```

```

358     else:
359         spec[0], wav[0], bpm[0] = spec[-1], wav[-1], bpm[-1]
360         spec[-1], wav[-1], bpm[-1] = unpack(
361             -1, *self.load_file(filename2)
362         )
363
364     bounds = self.get_bounds(bpm)
365
366     logging.debug(
367         f"correlate - data shape:\n{tspec/wav/bpm: {spec.shape}}"
368     )
369
370     corrdb = [[] for _ in range(self.ccdb)]
371     lagsdb = [[] for _ in range(self.ccdb)]
372     for ccd in range(self.ccdb):
373         sig = []
374         for ext in range(2):
375             lb, ub = bounds[ext, ccd]
376
377             if self.cont_ord > 0:
378                 spec[ext, lb:ub] = self.remove_cont(
379                     spec[ext, lb:ub],
380                     wav[ext, lb:ub],
381                     bpm[ext, lb:ub],
382                     self.can_plot
383                 )
384
385             # Invert BPM (and account for 2); zero bad pixels
386             sig.append((
387                 spec[ext, lb:ub]
388                 * abs(bpm[ext, lb:ub] * -1 + 1)
389             ))
390
391             # Finally(!!) cross correlate signals and scale max -> 1
392             corrdb[ccd] = signal.correlate(*sig) if not alt else alt(*sig)
393             corrdb[ccd] /= np.max(corrdb[ccd])
394             # noinspection PyTypeChecker
395             lagsdb[ccd] = signal.correlation_lags(
396                 sig[0].shape[-1],
397                 sig[1].shape[-1]
398             ) * self.wav_cdel
399
400     return spec, wav, bpm, corrdb, lagsdb
401
402 # MARK: ftcs alternate
403 def ftcs(
404     self,
405     signal1: np.ndarray,
406     signal2: np.ndarray
407 ) -> np.ndarray:
408     """
409     Cross correlates the data using the Fourier Transform.
410
411     Parameters
412     -----
413     signal1 : np.ndarray
414         The first signal to cross correlate.
415     signal2 : np.ndarray
416         The second signal to cross correlate.
417
418     Returns
419     -----
420     np.ndarray
421         The correlation data using the Fourier Transform.
422
423     """
424     logging.debug(
425         f"ftcs - data shape:\n{tspec/wav/bpm: {signal1.shape}}"
426     )
427
428     # Invert BPM (and account for 2); zero bad pixels
429     ft_spec1 = np.fft.fft(signal1)
430     ft_spec2 = np.fft.fft(signal2)

```

```

431
432     if self.can_plot:
433         plt.plot(ft_spec1)
434         plt.plot(ft_spec2)
435         plt.show()
436
437     # Cross correlate signals
438     # ft_spectrum1 * np.conj(ft_spectrum2)
439     corr_entry = signal.correlate(ft_spec1, ft_spec2)
440
441     return np.fft.ifft(corr_entry)
442
443 # MARK: Plot
444 def plot(self, spec, wav, bpm, corrdb, lagsdb) -> None:
445     """
446     Plot the data.
447
448     Parameters
449     -----
450     spec : np.ndarray
451         The spectrum.
452     wav : np.ndarray
453         The wavelength.
454     bpm : np.ndarray
455         The bad pixel mask.
456     corrdb : np.ndarray
457         The cross correlation data.
458     lagsdb : np.ndarray
459         The `lags` data.
460
461     Returns
462     -----
463     None
464
465     """
466     plt.style.use([
467         Path(__file__).parent.resolve() / 'utils/STOPS.mplstyle',
468         Path(__file__).parent.resolve() / 'utils/STOPS_correlate.mplstyle',
469     ])
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         # noinspection PyTypeChecker
477         axs: np.ndarray[matplotlib.axes.Axes] = np.swapaxes(np.atleast_2d(axs), 0, 1)
478
479     # for ext, ccd in iters.product(range(2), range(self.ccds)):
480
481     for ccd in range(self.ccds):
482         axs[0, ccd].plot(
483             lagsdb[ccd],
484             corrdb[ccd] * 100,
485             color='C4',
486             label=f"max lag @ {lagsdb[ccd][corrdb[ccd].argmax()]} - (bounds[1, ccd, "
487             f"0] - bounds[0, ccd, 0])",
488         )
489
490         for ext in range(2):
491             lb, ub = bounds[ext, ccd]
492             logging.debug(f"fl-{ext}: {wav[ext, lb]}:{wav[ext, ub - 1]}")
493
494             axs[1, ccd].plot(
495                 wav[ext, lb:ub],
496                 spec[ext, lb:ub] * abs(bpm[ext, lb:ub] * -1 + 1) + OFFSET * ext,
497                 label=(
498                     f"${self.beams if self.beams != 'OE' else self.beams[ext]}"
499                     f"_-{ext + 1 if self.beams != 'OE' else 1}$"
500                     f"{'(' (+ str(OFFSET * ext) + ')') if ext > 0 else ''}"
501                 ),
502             )

```

```

503     axs[0, 0].set_ylabel("Normalised Correlation\n(\%)")
504     for ax in axs[1:, 0]:
505         ax.set_ylabel("Normalised Intensity\n(Counts)")
506     xcol = int(self.ccds != 1)
507     axs[0, xcol].set_xlabel(f"Signal Lag ({self.wav_unit})")
508     axs[-1, xcol].set_xlabel(f"Wavelength ({self.wav_unit})")
509     for ax in axs.flatten():
510         leg = ax.legend()
511         leg.set_draggable(True)
512
513     # plt.tight_layout()
514     # fig1 = plt.gcf()
515     # DPI = fig1.get_dpi()
516     # fig1.set_size_inches(700.0/float(DPI), 250.0/float(DPI))
517     plt.show()
518
519     # Handle do not save
520     if not self.save_prefix:
521         return
522
523     # Handle save
524     fig.savefig(fname=self.save_prefix)
525
526     return
527
528 # MARK: Process all listed images
529 def process(self) -> None:
530     """
531     Process the data.
532
533     Returns
534     -----
535     None
536
537     """
538     if self.beams != 'OE' and len(self.fits_list) == 1:
539         # change mode to OE with warning
540         logging.warning((
541             f"`{self.beams}` correlation not possible for "
542             "a single file. correlation `mode` changed to 'OE'."
543         ))
544         self.beams = 'OE'
545
546     # OE `mode` (same file, diff. ext.)
547     if self.beams == 'OE':
548         for fl in self.fits_list:
549             logging.info(f"'OE' correlation of {fl}.")
550             spec, wav, bpm, corr, lags = self.correlate(fl, alt=self.alt)
551             self.plot(spec, wav, bpm, corr, lags)
552
553     return
554
555     # O/E `mode` (diff. files, same ext.)
556     for fl1, fl2 in iters.combinations(self.fits_list, 2):
557         logging.info(f"{self.beams} correlation of {fl1} vs {fl2}.")
558         spec, wav, bpm, corr, lags = self.correlate(fl1, fl2, alt=self.alt)
559         self.plot(spec, wav, bpm, corr, lags)
560
561     return
562
563
564 # MARK: Main function
565 def main(argv) -> None:
566     return
567
568
569 if __name__ == "__main__":
570     main(sys.argv[1:])

```

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

```

1 #!/usr/bin/env python3
2 # -*- coding: utf-8 -*-
3
4 """
5 Module for analyzing the sky lines of a wavelength calibrated image.
6 """
7
8 # MARK: Imports
9 import sys
10 import logging
11 from pathlib import Path
12
13 import numpy as np
14 import matplotlib.pyplot as plt
15 import matplotlib.axes
16 from astropy.io import fits as pyfits
17 from scipy import signal
18
19 from STOPS.utils.SharedUtils import find_files
20 from STOPS.utils.Constants import SAVE_SKY, FIND_PEAK_PARAMS, ARC_FILE
21
22 # print(
23 #     [logging.getLogger(name) for name in logging.root.manager.loggerDict]
24 # )
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
30
31 # MARK: Skylines Class
32 class Skylines:
33
34     #-----sky0-----
35
36     """
37         Class representing the Skylines object.
38
39     Parameters
40     -----
41     data_dir : Path
42         The directory containing the data files.
43     filenames : list[str]
44         The list of filenames to be processed.
45     beam : str, optional
46         The beam mode, by default "OE".
47     plot : bool, optional
48         Flag indicating whether to plot the continuum, by default False.
49     save_prefix : Path / None, optional
50         The prefix for saving the data, by default None.
51     **kwargs
52         Additional keyword arguments.
53
54     Attributes
55     -----
56     data_dir : Path
57         The directory containing the data files.
58     fits_list : list[str]
59         The list of fits file paths.
60     beams : str
61         The beam mode.
62     can_plot : bool
63         Flag indicating whether to plot the continuum.
64     save_prefix : Path / None
65         The prefix for saving the data.
66     wav_unit : str
67         The unit of wavelength.
68
69     Methods
70     -----
71     checkLoad(self, path1: str) -> np.ndarray:

```

```

72     Checks and loads the data from the given path.
73     transform(self, wav_sol: np.ndarray, spec: np.ndarray) -> np.ndarray:
74         Transforms the input wavelength and spectral data based on
75         the given wavelength solution.
76     rmvCont(self) -> np.ndarray:
77         Removes the continuum from the spectrum.
78     process(self) -> None:
79         Placeholder method for processing the data.
80     """
81
82 #-----sky1-----
83
84 # MARK: Skylines init
85 def __init__(self,
86             data_dir: Path,
87             filenames: list[str],
88             beams: str = "OE",
89             split_ccd: bool = False,
90             cont_ord: int = 11,
91             plot: bool = False,
92             transform: bool = True,
93             save_prefix: Path | None = None,
94             **kwargs,
95             ) -> None:
96     self.data_dir = data_dir
97     self.fits_list, self.arc_list = find_files(
98         data_dir=self.data_dir,
99         filenames=filenames,
100        prefix="wmxgbp", # t[o/e]beam
101       ext="fits",
102       sep_arc=True,
103     )
104     self._beams = None
105     self.beams = beams
106     self.ccds = 1
107     if split_ccd:
108         # See cross_correlate for initial implementation
109         self.ccds = 3
110
111     self.cont_ord = cont_ord
112     self.can_plot = plot
113     self.must_transform = transform
114
115     self.save_prefix = save_prefix
116     # Handle directory save name
117     if self.save_prefix and self.save_prefix.is_dir():
118         self.save_prefix /= SAVE_SKY
119         logging.warning((
120             f"Skylines save name resolves to a directory. "
121             f"Saving under {self.save_prefix}"
122         ))
123
124     self.max_difference = 5
125
126     self.wav_unit = "$\AA$"
127
128     logging.debug("__init__ - \n", self.__dict__)
129
130     return
131
132
133 # MARK: Beams property
134 @property
135 def beams(self) -> str:
136     return self._beams
137
138 @beams.setter
139 def beams(self, mode: str) -> None:
140     if mode not in ['O', 'E', 'OE']:
141         err_msg = f"Correlation mode '{mode}' not recognized."
142         logging.error(err_msg)
143         raise ValueError(err_msg)
144

```

```

145     self._beams = mode
146
147     return
148
149     # MARK: Find Peaks
150     def find_peaks(
151         self,
152         spec: np.ndarray,
153         axis: int | None = None,
154         min_height: float = 0.5,
155         **kwargs,
156     ) -> tuple[list[np.ndarray], list[dict]]:
157         """
158             Finds the peaks in the given spectral data.
159
160             Parameters
161             -----
162             spec : np.ndarray
163                 The spectral data.
164             axis: int / None, optional
165                 The axis along which the peaks are found.
166             min_height : float, optional
167                 The minimum height of the peaks, by default 0.5.
168
169             Returns
170             -----
171             peaks, properties : tuple[list[np.ndarray], list[dict]]
172                 The peaks and their properties.
173
174         """
175         peaks = []
176         props = []
177         row_means = []
178
179         for ext in range(len(self.beams)):
180             row_mean = spec[ext] if axis is None else np.mean(spec[ext], axis=axis)
181
182             peak, prop = signal.find_peaks(
183                 row_mean,
184                 prominence=min_height * np.max(row_mean),
185                 width=0,
186                 **kwargs,
187             )
188             peaks.append(peak)
189             props.append(prop)
190             row_means.append(row_mean)
191
192         if self.can_plot:
193             fig, axs = plt.subplots(2, 1)
194             for ext in range(len(self.beams)):
195                 axs[ext].plot(
196                     row_means[ext],
197                     label=f"'E' if ext else 'O'")
198             )
199             axs[ext].plot(
200                 peaks[ext],
201                 row_means[peaks[ext]],
202                 "x",
203                 label=f"'E' if ext else 'O'" peaks"
204             )
205             axs[ext].legend()
206             plt.show()
207
208             logging.debug(f"find_peaks - peaks: {[len(i) for i in peaks]}")
209             logging.debug(f"find_peaks - props: {[key for key in props[0].keys()]}")
210
211         return peaks, props
212
213     # MARK: Min. of Diff. Matrix
214     @staticmethod
215     def min_diff_matrix(
216         a: np.ndarray,
217         b: np.ndarray,

```

```

218         max_diff: int = 100
219     ) -> tuple[np.ndarray, np.ndarray, np.ndarray]:
220     """
221     Find the minimum difference between the elements of two arrays.
222
223     Parameters
224     -----
225     a : np.ndarray
226         The first 1d array.
227     b : np.ndarray
228         The second 1d array.
229     max_diff : int, optional
230         The maximum difference allowed, by default 100.
231
232     Returns
233     -----
234     a : np.ndarray (len(a))
235         The elements of the first array.
236     min_vals : np.ndarray (len(a))
237         The minimum difference between the elements of the two arrays.
238     min_idxs : np.ndarray (len(a))
239         The indices of the minimum difference between
240         the elements of the two arrays.
241
242     """
243     # Compute the difference matrix using transpose
244     diff = a - b[:, np.newaxis]
245
246     # Find the minimum value in each row (A) of `diff`
247     min_idxs = np.abs(diff).argmin(axis=0)
248     print(min_idxs.shape, diff.shape)
249     min_vals = np.array([diff[j, i] for i, j in enumerate(min_idxs)])
250     # TODO: Recalculate min_val after selecting best min_val and
251     # TODO: removing the corresponding row/column
252
253     logging.debug(f"min_diff_matrix - min_vals: {np.round(min_vals, 2)}")
254     logging.debug(f"min_diff_matrix - min_idxs: {min_idxs}")
255
256     max_mask = (min_vals <= max_diff) & (min_vals >= -1 * max_diff)
257
258     return a[max_mask], min_vals[max_mask], min_idxs[max_mask]
259
260     # MARK: Load File Data
261     def load_file_data(
262         self,
263         filename: Path
264     ) -> tuple[np.ndarray, np.ndarray, np.ndarray]:
265     """
266     Loads the data from the given file.
267
268     Parameters
269     -----
270     filename : Path
271         The path to the file to be loaded.
272
273     Returns
274     -----
275     spec, wav, bpm : tuple[np.ndarray, np.ndarray, np.ndarray]
276         The wavelength, spectral, and bad pixel mask data.
277
278     """
279     # Load data from self.beams extension
280     with pyfits.open(filename) as hdul:
281         exts = [0, 1] if len(self.beams) == 2 else 0 + int(self.beams == '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(
287             f"load_file_data - {filename.name} - shape: {spec2d.shape}"
288         )
289
290     return spec2d, wav2d, bpm2d

```

```

291
292     # MARK: Load Sky or Arc Lines
293     @staticmethod
294     def load_lines(
295         filename: str | 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 : str / Path / None, optional
306                 The path to the file to be loaded.
307                 Defaults to loading the skylines from `utils/sky.salt`.
308             dtype : list[tuple], optional
309                 The data type of the sky lines.
310                 (Default is [('wav', float), ('flux', float)])
311             skip_header : int, optional
312                 The amount of lines to skip of the `filenames` header.
313                 (Default is 3)
314             skip_footer : int, optional
315                 The amount of lines to skip of the `filename`'s footer.
316                 (Default is 1)
317
318             Returns
319             -----
320             sky_lines : np.ndarray['wav', 'flux']
321                 The sky lines from the file.
322
323         """
324         usecols = None
325         if filename:
326             filename = Path(__file__).parent.resolve() / filename
327             usecols = (0, 1)
328         else:
329             filename = Path(__file__).parent.resolve() / 'utils/sky.salt'
330
331         lines = np.genfromtxt(
332             filename,
333             dtype=dtype,
334             skip_header=skip_header,
335             skip_footer=skip_footer,
336             usecols=usecols
337         )
338
339         logging.debug(
340             f"load_lines - {filename.name} - shape: {lines.shape}"
341         )
342
343         return lines
344
345     # MARK: Mask Traces
346     def mask_traces(
347         self,
348         spec: np.ndarray,
349         bpm: np.ndarray,
350         max_traces: int = 1,
351         tr_pad: int = 5,
352         bg_margin: int = 10,
353         lr_margins: list[int] = [10, 10],
354         h_min: float = 0.5,
355         h_rel: float = 1 - 0.05,
356     ) -> np.ndarray:
357         """
358             Masks the traces in the bad pixel mask.
359
360             Parameters
361             -----
362             spec : np.ndarray
363                 The spectral data.

```

```

364     bpm : np.ndarray
365         The bad pixel mask.
366     max_traces : int, optional
367         The maximum number of traces to be masked.
368         (Default is 1)
369     tr_pad : int, optional
370         The amount to pad traces by.
371         (Default is 5)
372     bg_margin : int, optional
373         The margin size for the background.
374         (Default is 10)
375     lr_margins : list[int, int], optional
376         The left and right background margins at the spectrum edge.
377         (Default is [10, 10])
378     h_min: float, optional
379         The minimum height of a detected peak.
380         (Default is 0.5)
381     h_rel: float, optional
382         The relative height for the properties of a detected peak.
383         (Default is 1)
384
385     Returns
386     -----
387     bpm : np.ndarray
388         The updated bad pixel mask.
389
390     """
391     # Base mask
392     bpm[:, :bg_margin] = True
393     bpm[:, -bg_margin:] = True
394     bpm[:, :, :lr_margins[0]] = True
395     bpm[:, :, -lr_margins[1]:] = True
396
397     # Get the traces
398     traces, tr_props = self.find_peaks(
399         spec,
400         axis=1,
401         min_height=h_min,
402         rel_height=h_rel
403     )
404
405     for ext in range(len(self.beams)):
406         # Mask the traces
407         for i in range(len(traces[ext])[:max_traces]):
408             lb = max(
409                 0,
410                 int(tr_props[ext]['left_ips'][i]) - tr_pad
411             )
412             ub = min(
413                 spec.shape[-1],
414                 int(tr_props[ext]['right_ips'][i]) + tr_pad
415             )
416             bpm[ext, lb: ub] = True
417             # TODO: Relocate targets after initial masking
418
419             logging.info(f"mask_traces - {min(max_traces, len(traces))} of {len(traces)}"
420                         "traces masked.")
421
422     return bpm
423
424     # MARK: Transform Spectra
425     def transform(
426         self,
427         spec: np.ndarray,
428         wav_sol: np.ndarray,
429         row_max: int | None = None,
430         res_plot: bool = False,
431     ) -> tuple[np.ndarray, np.ndarray]:
432         """
433             Transforms the input wavelength and spectral data
434             based on the given wavelength solution.
435
436             Parameters
437
438             Returns
439             -----
440             transformed_spec: np.ndarray
441                 The transformed spectral data.
442             transformed_wav: np.ndarray
443                 The transformed wavelength solution.
444
445             Raises
446             -----
447             ValueError
448                 If the input data is invalid or incompatible.
449
450             Notes
451             -----
452             This method performs several key operations:
453             1. It applies the wavelength solution (wav_sol) to the
454                 input spectrum (spec). This involves mapping the
455                 original wavelength grid to a new one defined by
456                 the solution.
457             2. It handles the case where the input spectrum has a
458                 different number of rows than the wavelength solution.
459                 If 'row_max' is specified, it truncates the spectrum
460                 to match the solution's length. Otherwise, it pads
461                 the spectrum to match the solution's length.
462             3. It applies any necessary transformations to the
463                 spectrum based on the 'res_plot' flag.
464
465             The resulting tuple contains the transformed spectrum and
466             the transformed wavelength solution.
467
468             Examples
469             -----
470             # Create a simple spectrum and wavelength solution
471             spec = np.random.rand(100, 100)
472             wav = np.linspace(400, 700, 100)
473
474             # Perform transformation
475             transformed_spec, transformed_wav = self.transform(spec, wav)
476
477             # Print results
478             print(transformed_spec.shape)  # (100, 100)
479             print(transformed_wav.shape)   # (100,)
```

```

436     -----
437     spec : np.ndarray
438         The spectral data.
439     wav_sol : np.ndarray
440         The wavelength solution.
441     row_max : int, optional
442         The row along which the spectral data is to be transformed.
443         (Default is None)
444     res_plot : bool, optional
445         Flag indicating whether to plot the results.
446         (Default is False)
447
448     Returns
449     -----
450     spec, wav : np.ndarray
451         The transformed wavelength and spectral data.
452
453     """
454     # Create arrays to return
455     cs = np.zeros_like(spec)
456     cw = np.zeros_like(wav_sol.mean(axis=1))
457
458     for ext in range(len(self.beams)):
459
460         if row_max:
461             avg_max = row_max
462         else:
463             # Get middle row (to interpolate the rest of the rows to)
464             avg_max = np.mean(spec[ext], axis=1).argmax()
465
466         # Correct extensions based on wavelength
467         # Get wavelength values at row with most trace
468         cw[ext] = wav_sol[ext, avg_max]
469
470         # Spec ext
471         for row in range(cs.shape[1]):
472             cs[ext, row] = np.interp(
473                 cw[ext],
474                 wav_sol[ext, row],
475                 spec[ext, row]
476             )
477             # f_2d = interpolate.interp2d(
478             #     wav_sol[ext, row],
479             #     np.arange(rows),
480             #     spec[ext],
481             # )
482             # cs[ext] = f_2d(cw[ext], np.arange(rows))
483
484         # Plot results
485         if res_plot:
486             fig, axs = plt.subplots(2, 1, figsize=[20, 4])
487             for ext in range(len(self.beams)):
488                 axs[ext].imshow(
489                     cs[ext],
490                     vmax=cs[ext].mean() + 2 * cs[ext].std(),
491                     vmin=cs[ext].mean() - 2 * cs[ext].std()
492                 )
493
494             logging.debug(f"{'E' if ext else '0'} Average continuum =
495             ↪ {np.median(np.median(cs[ext], axis=0)):4.3f}")
496
497             axx = axs[ext].twinx()
498             axx.hlines(
499                 np.median(np.median(cs[ext], axis=0)),
500                 0,
501                 cs[ext].shape[-1],
502                 colors='black',
503             )
504             axx.plot(
505                 cs[ext].mean(axis=0),
506                 "k",
507                 label=f"mean {'E' if ext else '0'}"
508             )

```

```

508         axx.plot(
509             np.median(cs[ext], axis=0),
510             "r",
511             label=f"median {'E' if ext else 'O'}"
512         )
513         axx.legend()
514     plt.show()
515
516     logging.info(f"transform - {cs.shape} transformed.")
517
518     return cs, cw
519
520 # MARK: Plot
521 def plot(
522     self,
523     spectra,
524     wavelengths,
525     peaks,
526     properties,
527     arc: bool = False,
528 ) -> None:
529     plt.style.use([
530         Path(__file__).parent.resolve() / 'utils/STOPS.mplstyle',
531         Path(__file__).parent.resolve() / 'utils/STOPS_skylines.mplstyle',
532     ])
533     plt.rcParams['figure.subplot.hspace'] *= len(self.beams)
534
535     def norm(vals):
536         return (vals - np.min(vals)) / (np.max(vals) - np.min(vals))
537
538     # Load known lines
539     if arc:
540         lines = self.load_lines(filename=f'utils/RSS_arc_files/{ARC_FILE}')
541     else:
542         lines = self.load_lines()
543
544     # noinspection PyTypeChecker
545     lines = lines[
546         (lines['wav'] > wavelengths[1][0][0].min()) &
547         (lines['wav'] < wavelengths[1][0][0].max())
548     ]
549
550     # Create plot for results
551     fig, axs = plt.subplots(2, self.ccds, sharex='col', sharey='row')
552
553     # Convert axs to a 2D array if ccd count is 1
554     if self.ccds == 1:
555         # noinspection PyTypeChecker
556         axs: np.ndarray[matplotlib.axes.Axes] = np.swapaxes(np.atleast_2d(axs), 0, 1)
557
558     for fl in range(len(self.arc_list if arc else self.fits_list)):
559
560         # set color cycle
561         color = next(axs[0, 0].get_lines.prop_cycler)['color']
562
563         for ext in range(len(self.beams)):
564
565             ccdrange = spectra[1][fl][ext].shape[-1] // self.ccds
566             for ccd in range(self.ccds):
567                 # MARK: plot spectrum
568                 # (transformed)
569                 axs[0, ccd].plot(
570                     wavelengths[1][fl][ext][
571                         ccdrange * ccd:ccdrange * (ccd + 1)
572                     ],
573                     norm(spectra[1][fl][ext][
574                         ccdrange * ccd:ccdrange * (ccd + 1)
575                     ]) * 100 + 10 * ext + 30 * fl,
576                     color=color,
577                     linestyle='dashed' if ext else 'solid',
578                     label=f"${{{self.beams[ext]}}}_{{{fl + 1}}}^{{{10 * ext + 30 * fl}}}$" if ccd == 0 else None,
579                 )

```

```

580
581     # MARK: plot dev
582     # noinspection PyTypeChecker
583     sky_wavs, dev, peak_idx = self.min_diff_matrix(
584         lines['wav'],
585         wavelengths[1][fl][ext][peaks[1][fl][ext]],
586         max_diff=self.max_difference,
587     )
588
589     # # MARK: width/width_init
590     # width = properties[1][fl][ext]['widths'][peak_idx]
591     # width_i = np.zeros_like(width)
592
593     # sky_i, i_dev, i_idx = self.min_diff_matrix(
594     #     lines['wav'],
595     #     wavelengths[0][fl][ext][peaks[0][fl][ext]],
596     #     max_diff=self.max_difference,
597     # )
598
599     # width_i = np.array([
600     #     properties[0][fl][ext]['widths'][
601     #         np.where(wav == sky_i)[0][0]
602     #     ]
603     #     if wav in sky_i else 1000
604     #     for wav in sky_wavs
605     # ])
606     # width_ratio = (width / width_i) - 1
607     # width_ratio[width_ratio < 0] = 0
608
609     # ylolims = width_ratio > self.max_difference
610     # width_ratio[
611     #     width_ratio > self.max_difference
612     # ] = self.max_difference // 2
613
614     ok = np.where(
615         (sky_wavs >= wavelengths[1][fl][ext].data[ccdrange * ccd]) &
616         (sky_wavs <= wavelengths[1][fl][ext].data[ccdrange * (ccd + 1)])
617     )
618     axs[1, ccd].plot(
619         sky_wavs[ok],
620         dev[ok],
621         # yerr=(width_ratio[ok] * 0, width_ratio[ok]),
622         # lolims=ylolims[ok],
623         "."
624         if ext else "x",
625         # fmt="."
626         if ext else "x",
627         alpha=0.8,
628         color=color,
629         # markeredgecolor='white',
630         # markeredgewidth=0.5,
631         # label=f"${self.beams[ext]}_{{{fl + 1}}}$",
632     )
633
634     logging.debug(f"plot - RMS: {np.sqrt(np.mean(dev[ok] ** 2)):.2f}")
635
636     for ccd in range(self.ccds):
637         ccdrange = spectra[1][0][0].shape[-1] // self.ccds
638
639         # spectrum
640         # noinspection PyTypeChecker
641         ok = np.where(
642             (lines['wav'] >= wavelengths[1][0][0].data[ccdrange * ccd]) &
643             (lines['wav'] <= wavelengths[1][0][0].data[ccdrange * (ccd + 1)])
644         )
645         # noinspection PyTypeChecker
646         axs[0, ccd].plot(
647             lines['wav'][ok],
648             lines['flux'][ok] * 0,
649             'x',
650             color='C4',
651             label="\textsc{salt}\nModel" if ccd == 0 else None,
652         )
653         # noinspection PyTypeChecker
654         for x in lines['wav'][ok]:

```

```

653         axs[0, ccd].axvline(x, ls='dashed', c='0.7')
654
655     axs[0, 0].set_ylabel("Rel. Intensity ($\%$)")
656     axs[1, 0].set_ylabel(
657         "Closest Peak ($\Delta\lambda$)")
658     )
659     # for ax in axs[:, 0]:
660     #     ax.legend(loc='upper left', ncols=(fl + 1) * (ext + 1) + 1)
661     leg = fig.legend(
662         loc='center',
663         ncol=min(8, len(spectra[0]) + 1),
664         columnspacing=0.5,
665         bbox_to_anchor=(
666             np.mean((
667                 plt.rcParams['figure.subplot.left'],
668                 plt.rcParams['figure.subplot.right']
669             )),
670             np.mean((
671                 plt.rcParams['figure.subplot.bottom'],
672                 plt.rcParams['figure.subplot.top']
673             )))
674     ),
675     )
676     leg.set_draggable(True)
677     for ax in axs[1, :]:
678         ax.grid(axis='y')
679
680     # fig.add_subplot(111, frameon=False)
681     # # hide tick and tick label of the big axis
682     # plt.tick_params(
683     #     labelcolor='none',
684     #     which='both',
685     #     top=False,
686     #     bottom=False,
687     #     left=False,
688     #     right=False
689     # )
690     axs[-1, 0 if self.ccds == 1 else 1].set_xlabel(
691         f"Wavelength ({self.wav_unit})"
692     )
693
694     # plt.tight_layout()
695
696     plt.show()
697
698     # Save results
699     if self.save_prefix:
700         fig.savefig(fname=self.save_prefix)
701
702     return
703
704     # MARK: Process all listed images
705
706 def process(self, arc: bool = False) -> None:
707     files = self.fits_list
708     if arc:
709         files = self.arc_list
710
711     logging.info(f"Processing '{self.beams}' lines.")
712
713     spectra = [[], []]
714     wavs = [[], []]
715     peaks = [[], []]
716     peak_props = [[], []]
717
718     for fl in files:
719         # Load data
720         spec2d, wav2d, bpm2d = self.load_file_data(fl)
721
722         # Mask traces in BPM
723         bpm2d = self.mask_traces(
724             spec2d,
725             bpm2d,

```

```

726         max_traces=0,
727         bg_margin=15,
728         h_min=0.05
729     )
730     m_spec2d = np.ma.masked_array(spec2d, mask=bpm2d) # spec2d
731     m_wav2d = np.ma.masked_array(wav2d, mask=bpm2d) # wav2d
732
733     # Initial spectra
734     spec_i = np.mean(m_spec2d, axis=-2)
735     wav_i = np.mean(m_wav2d, axis=-2)
736
737     # Transform data
738     t_spec2d, t_wav = self.transform(
739         m_spec2d,
740         m_wav2d,
741         res_plot=self.can_plot
742     )
743
744     # Final spectra
745     spec_f = np.mean(t_spec2d, axis=-2)
746     wav_f = t_wav
747
748     # Find peaks
749     peaks_i, props_i = self.find_peaks(
750         spec_i,
751         **FIND_PEAK_PARAMS
752     )
753     peaks_f, props_f = self.find_peaks(
754         spec_f,
755         **FIND_PEAK_PARAMS
756     )
757
758     spectra[0].append([*spec_i])
759     spectra[1].append([*spec_f])
760     wavs[0].append([*wav_i])
761     wavs[1].append([*wav_f])
762     peaks[0].append([*peaks_i])
763     peaks[1].append([*peaks_f])
764     peak_props[0].append([*props_i])
765     peak_props[1].append([*props_f])
766
767     # Plot results
768     self.plot(spectra, wavs, peaks, peak_props, arc=arc)
769
770     if arc:
771         return
772     elif self.arc_list:
773         self.process(arc=True)
774
775     return
776
777
778 # MARK: Main function
779 def main(argv) -> None:
780     return
781
782
783 if __name__ == "__main__":
784     main(sys.argv[1:])

```


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Glossary

FITS extensions Extensions used in FITS files to store different types of data.

‘**BPM**’ The Bad Pixel Map extension in a FITS file.

‘**Primary**’ The Primary extension of a FITS file which contains the file Header.

‘**SCI**’ The Science data extension in a FITS file.

‘**VAR**’ The Variance data extension in a FITS file.

‘**WAV**’ The Wavelength extension in a FITS file.

Johnson-Cousins photometric system A widely-used system of broad-band photometry that uses a set of standard filters to measure the magnitudes of stars and other astronomical objects.

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.

Development of tools for the SALT/RSS spectropolarimetry reductions: application to the blazar 3C 279

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Blazars represent a subset of AGN with relativistic jets, where the direction of the jet lies very close to our line of sight. The highly Doppler boosted emission from the blazar's jet results in high apparent luminosities, and blazars display variability on periods from less than one day up to years. At optical wavelengths, the observed emission of the blazar is a superposition of the polarised non-thermal synchrotron emission, arising from the jet, and the unpolarised thermal emission, arising from the accretion disc, broad line region, torus and host galaxy. Polarimetry observations can serve as an important tool for diagnosing the emission from blazars. The RSS spectrograph, on SALT, can operate in spectropolarimetry mode and is currently being used to undertake spectropolarimetric observations of transient blazar sources. We present additional tools developed to work in conjunction with the current SALT spectropolarimetry reduction pipeline, POLSALT, that aims to streamline the reduction of the SALT polarisation data, including the testing of the wavelength calibration of the individual O and E beams. This was applied to observations of 3C 279 during 2017.

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1. Introduction

Active Galactic Nuclei (AGN) are the centres of galaxies powered by accretion onto a supermassive black hole. The accretion can power relativistic jets which produce non-thermal emission over multiple wavelengths [1]. Blazars are a subclass of AGN where the direction of the jet lies very close to our line of sight. The highly Doppler boosted emission from the jet results in high apparent luminosities.

At optical wavelengths the observed emission is a superposition of polarised non-thermal synchrotron emission, arising from the jet, and unpolarised thermal emission, arising from the disc, broad line region, torus, and host galaxy [2].

The Robert Stobie Spectrograph (RSS) on the Southern African Large Telescope (SALT) [3] [4] is capable of long-slit spectropolarimetry and has been used to observe blazars in flaring and quiescent states. Data reduction of these observations is processed using the SALT spectropolarimetry reduction package `POLSALT`.¹ `POLSALT` allows for the full reduction, from pre-reduction to the extraction of the target spectra, and the measuring of the polarisation. However, it does not allow for much flexibility with the wavelength calibrations, nor does it provide tools to confirm that the wavelength calibrations lead to similar wavelength calibrated spectra for the O and E beams.

In order to streamline the data reduction we are developing additional tools to work in conjunction with `POLSALT`. We present the overview of this pipeline and demonstrate its application to an observation of 3C 279 taken in 2017.

2. Pipeline Overview

The tools being developed are designed to work in conjunction with `POLSALT` and provide a method to perform the wavelength calibrations using conventional `IRAF` methods [5]. They also allow easy comparisons to be made between the wavelength solutions of the O and E beam, to determine their quality and reliability.

The workflow for reductions is depicted in figure 1. It summarises the steps followed to reduce spectropolarimetric data. Steps that are performed using `POLSALT` are indicated in blue; steps performed by the new tools are shown in orange, while the `IRAF` calibration is shown in green.

If the wavelength solutions are found with `IRAF`, the tools split the multi-extension FITS files into the correct format for `IRAF` and the `IRAF` wavelength calibration is performed. The files are then written back into multi-extension FITS files in the correct format for `POLSALT` to complete the extraction and measurement of polarisation.

The cross-correlation between the O and E beam spectra, named correlation in figure 1, and relative flux calibrations are optional, though correlation is suggested. Relative flux calibrations may be performed assuming a standard and published standard spectra can be acquired. We performed the relative flux calibrations using the `ASTROPY` [6, 7] and `SCIPY`² packages.

¹<https://github.com/saltastro/polsalt>

²<http://www.scipy.org/>

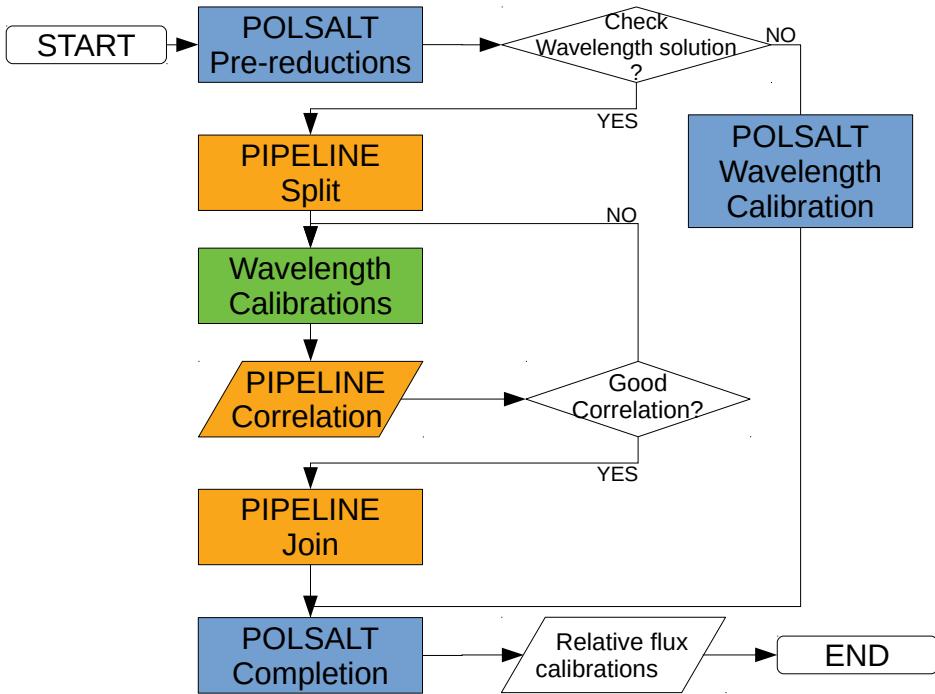


Figure 1: The flow diagram of the SALT RSS spectropolarimetry reductions steps.

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2.1 Pre-reduction

The first step in the pipeline uses **POLSLT** and this performs the pre-reductions, the over-scan subtraction, gain and cross talk corrections, and mosaicing. After the pre-reduction is performed, the next step is to either undertake the wavelength calibration with **POLSLT**, or to split the files into the correct format for **IRAF**.

2.2 FITS split

Once all pre-reductions are complete, the tool **SPLIT** converts the multi-extension FITS files into multiple, single extension O or E beam FITS files. This is done as some **IRAF** tasks do not handle multi-extension FITS files well. The O and E beam frames are cropped to remove any non-exposed rows to accommodate the standard **IRAF** tasks and the FITS files saved with updated header information.

2.3 Wavelength calibration

If the **POLSLT** pipeline is used, the wavelength calibration is performed using the wavelength calibration tools which form part of **PYSALT** [8].

If the files have been formatted for **IRAF**, standard wavelength calibration methods are followed, using the **NOAO** package and the **identify**, **re-identify**, and **fitcoords** tasks. This allows greater control of the resultant wavelength solution.

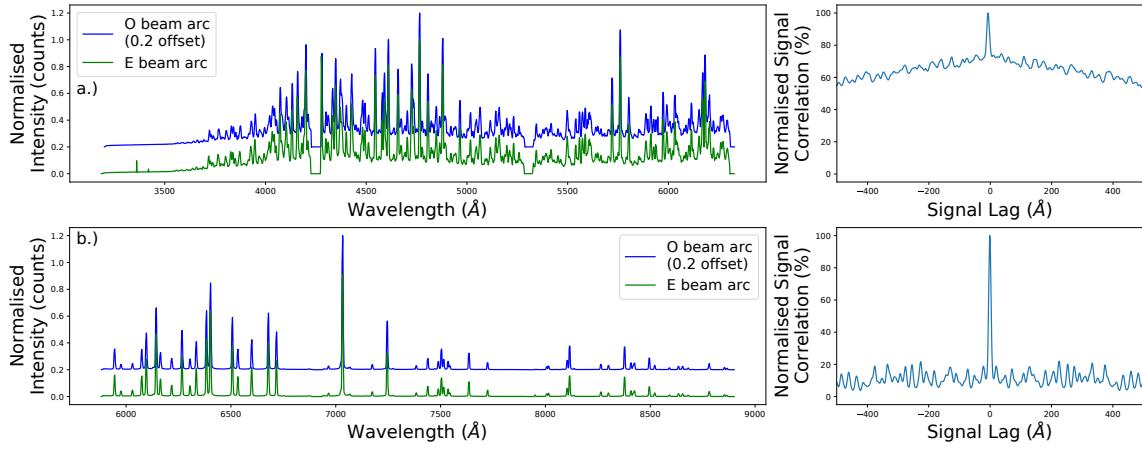


Figure 2: Comparison of the O and E beams for a.) ThAr and b.) Ne arc lamp spectra as well as the cross-correlation of their O and E beams.

2.4 Correlation

Our tool CORRELATE allows a comparison to be made between the O and E beam solutions, by performing a cross-correlation between the two arc or target observations, after the wavelength solution as been applied by `IRAF`. This is important as the polarisation is calculated from the difference between the O and E beam and, therefore, accurate wavelength solutions are required. The comparison between the O and E beams for a ThAr and Ne arc spectra and their cross-correlations, with a near zero lag, are shown in figure 2.a) and figure 2.b), respectively. Figure 2's Signal Lag plots show a clear peak at zero lag but also show an important distinction between noisy and quiet spectra in the non-peaking region.

2.5 FITS join

Once the `IRAF` wavelength calibrations are complete, the tool JOIN performs cosmic-ray cleaning using the LACOSMIC package [9], applies a wollaston correction which accounts for the physical shift of the spectra on the CCD, and then formats the single extension O and E beam FITS files into the multi-extension format required by `POLSALT`. This includes saving the wavelength solution found in `IRAF` as an additional extension. Currently only wavelength solutions fit with a Chebychev function are recognised but further development is planned to recognise Legendre functions.

2.6 Completion - extraction and polarisation measurement

After the wavelength solution is found, the final step is performed using `POLSALT`, which performs the curvature corrections, background subtraction, spectral extraction, and the raw and final stokes calculations. The binning and plotting also form part of the `POLSALT` completion.

3. Application to 3C 279

The blazar 3C 279 was observed in linear spectropolarimetry mode, on 2017 May 17, using the the PG0900 grating with two different grating angles (12.5° and 19.5°). The spectrophotometric

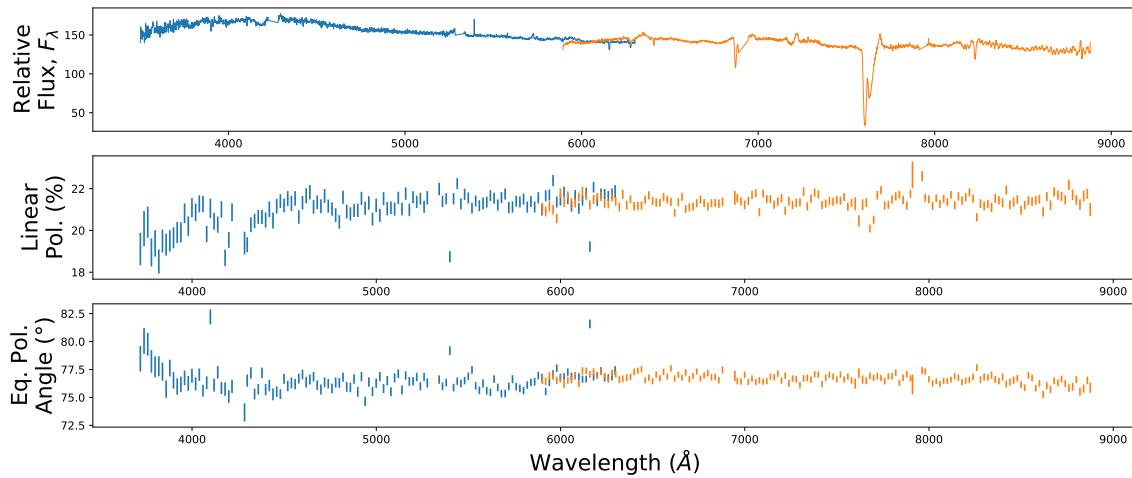


Figure 3: Reduced observations of 3C 279, taken with grating angle 12.5° (blue line) and 19.5° (orange line). Top: relative flux calibrated spectra. Middle: degree of linear polarisation. Bottom: Polarisation angle (relative to instrument).

standard star Hiltner 600 was observed on 2017 February 24, using the same configuration and was used for relative flux calibrations.

The target and standard were reduced following the steps discussed about. The flux correction was performed using `ASTROPY` and `SCIPY` python packages to correct the flux shape.

The results are shown in figure 3, indicating a good overlap between the observations taken at two different grating angles, with the polarisation measurements generally agree well where the observations overlap.

Figure 2 shows the comparison of the O and E beams for this observations. The cross-correlation is very close to zero lag, indicating the wavelength solution is similar for both the O and E beams.

4. Discussion and Conclusions

Creating an independent 2D wavelength solution for the O and E beams using `IRAF` allows for more flexibility in obtaining the wavelength solutions and provides a tool to directly compare the O and E beam solutions. This is useful for difficult cases, such as arc line identification for the PG0300 spectral grating, because there are fewer arc lines in some parts of the spectra and it is more complicated to create a consistent solution across the full wavelength range covered.

The cross-correlation plot cannot only be considered when deciding on whether to proceed onward with the reductions or to return to wavelength calibrations as depicted in figure 1. The comparison of the spectra is as important since the cross-correlation may show zero lag but lines in the spectra could still be mis-identified in both beams. The cross-correlation serves as a method to check the similarity of the wavelength solutions but not the accuracy of said solutions.

The tools developed create an alternative to the `POLSALT` wavelength calibration and add a method to check the consistency of the wavelength solutions, as can be seen with the application to 3C 279. These assist with the wavelength calibration, in particular for observations taken with

the PG0300 and PG0900 RSS gratings, that have been used for numerous observations of blazar sources.

Acknowledgments

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SALT Spectropolarimetric Pipeline Comparisons

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Blazars are active galactic nuclei (AGN) with jets aligned very closely to our line of sight. The optical emission of blazars is often dominated by the polarised, non-thermal emission arising in the jets, with an underlying unpolarised, thermal emission component arising from the host galaxy, dusty torus, and accretion disk components.

Coupled with multi-wavelength observations, optical spectropolarimetry of blazars during both flaring and quiescent states can be used to disentangle the polarised and unpolarised components in their spectral energy distributions, providing better constraints for the non-thermal particle distribution. To this end, spectropolarimetry of blazars during different states of activity was taken with the Southern African Large Telescope (SALT) using the Robert Stobie Spectrograph (RSS). For RSS spectropolarimetry, reductions are performed using the POLSALT pipeline. In order to streamline the spectropolarimetric reductions, we have implemented supplementary interactive tools which provides additional wavelength calibration to improve the accuracy of the wavelength calibration for the O & E beam.

Here we present a brief overview of the tools and the results for Hiltner 652, a spectropolarimetric standard, as well as results for the blazars 3C 279. The reduced, P_Q and P_U , Stokes parameters of Hiltner 652 show no major deviation from previously published results which reassures us that there is no interference introduced into the Stokes parameter calculations when wavelength calibrations are handled by our supplementary tools. The $\sim 6000 - 9000 \text{ \AA}$ range of 3C 279 shows a notable dip in the normalized spectrum during a period of flaring when compared to epochs of enhanced activity. The degree of polarisation for 3C 279 of 13.2%, 9.5%, and 21.2% for the epochs 2017 March 28, 2017 March 31, and 2017 May 17, respectively, remains fairly constant across the observed wavelength ranges while still varying with the blazars' state of quiescence or flaring.

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1. Introduction

Blazars are a radio-loud sub-set of Active Galactic Nuclei (AGN), where the jet is aligned very closely to our line of sight and whose observed emission varies over time scales from hours to decades [1]. The optical emission observed from blazars is often dominated by the polarised, non-thermal emission arising in the jets, but there is also underlying non-polarised, thermal emission arising from the host galaxy, dusty torus, and accretion disk components [2]. When a blazar varies between flaring and quiescent states, the relative strength of the thermal component to the non-thermal component changes.

The Spectral Energy Distribution (SED) of blazars shows two clear components: a lower energy component produced through leptonic synchrotron processes (covering the radio to the UV/soft X-ray regimes) and a higher energy component (covering the X-ray to the γ -ray regimes) which can be produced through either leptonic or hadronic processes [3]. Optical spectropolarimetry observations, coupled with multi-wavelength observations during both flaring and quiescent states, can be used to disentangle the polarised and non-polarised components in the blazar's SED, providing better constraints for the non-thermal particle distribution [4, 5].

To this end, spectropolarimetric observations of blazars during different states of activity were taken using SALT [6] and the RSS [7]. RSS spectropolarimetry data is reduced with the dedicated POLSALT pipeline [8]. In order to facilitate the blazar observations we have developed supplementary tools to provide a more interactive approach to the wavelength calibration, allowing for improved accuracy for the O & E beam wavelength solutions [9]. Furthermore, spectropolarimetric standards, which were also observed with SALT and the RSS, were reduced alongside the blazar observations to test that the developed tools correctly performed the wavelength calibration. Here we present an overview of the pipeline as well as the preliminary results of a spectropolarimetric standard, namely Hiltner 652, and for the blazar 3C 279.

2. Pipeline Overview

RSS spectropolarimetry data is currently reduced using the POLSALT pipeline [8]. This python package allows for a full reduction from pre-reduction to extracted spectrum, and measured polarisation. However, the wavelength calibration component of the package does not allow for flexibility, nor provide a tool to confirm that the wavelength calibrations of the O & E beams are in agreement. This flexibility is most notably missed when performing calibrations of observations taken using the PG0300 grating¹ due to the very sparse spectral features of the Argon arc lamp used by SALT as well as second order contamination which differs between the O & E beams.

The developed tools work in conjunction with the existing pipeline and provide a method to perform the wavelength calibrations using conventional IRAF [10] methods. Figure 1 shows the typical workflow for data reductions of spectropolarimetric SALT data. Items in blue refer to processing steps completed entirely using POLSALT while items in orange refer to processing steps completed using the developed tools. The single green item refers to the wavelength calibration

¹This grating has been decommissioned and replaced by the PG0700, and is not available for general use as of November 2022.

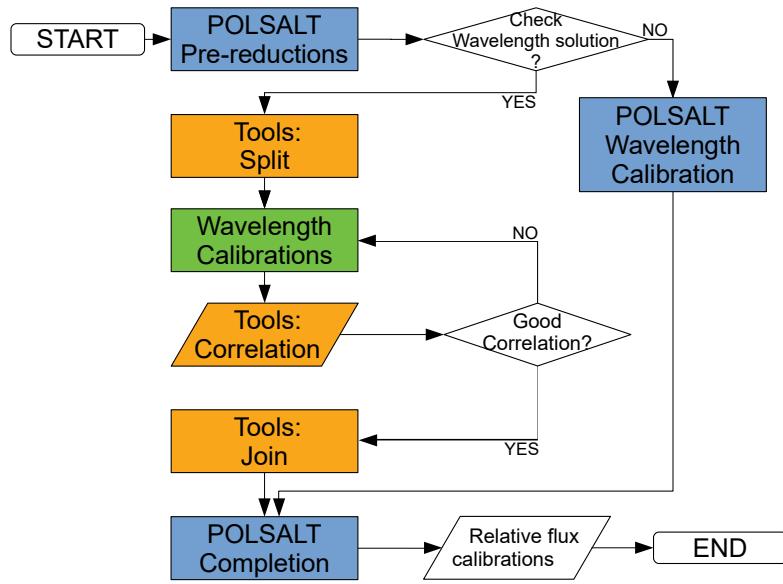


Figure 1: A general workflow for data reductions using a combination of **POLSALT** and our developed tools.

Source	Observation date	Grating angle (°)	Slit width (")	Exposure time (sec)	Wavelength range (Å)
Hiltner 652	2022 June 10	12.878	2	48.5	3350 - 6440
3C 279	2017 March 28	12.5	1.5	480.8	3300 - 6300
3C 279	2017 March 28	19.625	1.5	480.8	5800 - 8800
3C 279	2017 March 31	12.5	1.5	480.8	3300 - 6300
3C 279	2017 March 31	19.625	1.5	480.8	5800 - 8800
3C 279	2017 May 17	12.5	1.5	720.8	3300 - 6300
3C 279	2017 May 17	19.625	1.5	720.8	5800 - 8800

Table 1: All spectropolarimetric observations taken with SALT and the RSS and used as part of development and testing of the supplementary tools.

done in **IRAF**. Additional tools to cross-check that the wavelength calibration is consistent across both beams have also been implemented.²

3. Observations

The spectropolarimetric observations were taken using the RSS mounted on SALT, in **LINEAR** mode. The spectropolarimetric standard, Hiltner 652, was observed in 2022 and the blazar 3C 279, was observed in 2017, as summarized in Table 1. All observations presented here were observed using the PG0900 and were reduced following the reduction workflow as described in Figure 1.

²A further, in-depth, discussion of the developed tools can be found at [9].

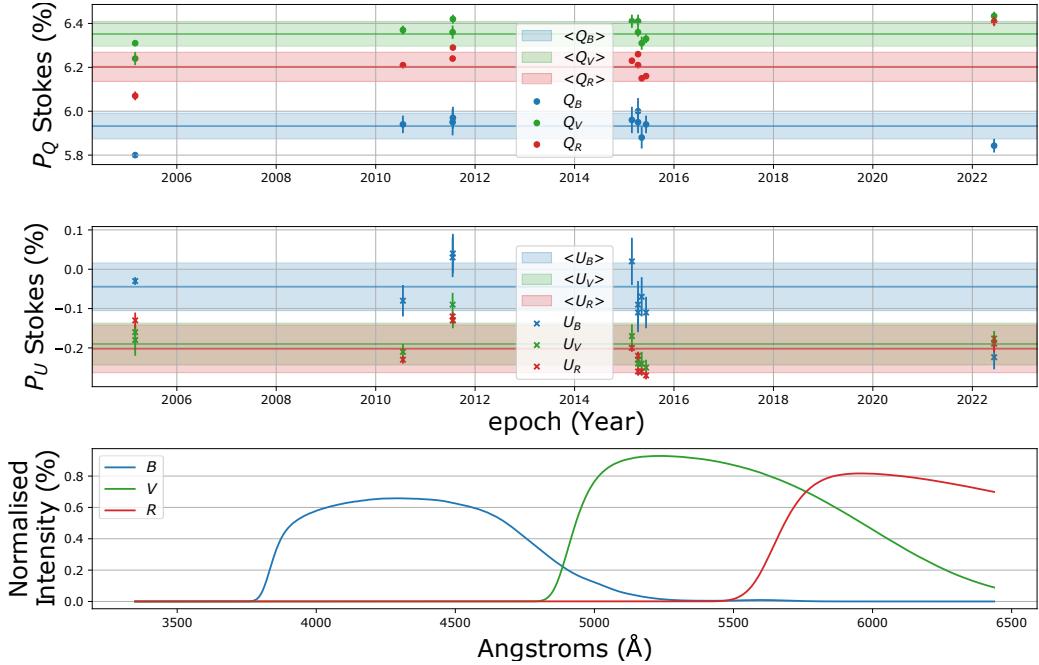


Figure 2: The reduced Q and U Stokes parameters for Hiltner 652 obtained with SALT in 2022 (post 2020) calculated by convolving the spectropolarimetry with the Johnson-Cousins filter pass-bands. This is compared to the published FORS1 [11] and FORS2 [12] observation results (top and middle panels). The average of the FORS reduced Stokes parameters as well as their standard deviation are plotted as the horizontal lines and shaded regions, respectively. Hiltner 652 was observed by SALT in 2022, by FORS1 from 1999 to 2006 (shown as average value at March 2005), and by FORS2 from 2010 to 2016. Finally, the Johnson-Cousins filter pass-band's used by POLSALT to calculate the stokes parameters in the different filters are shown in the bottom panel.

4. Results

The linear Stokes parameters, Q & U , normalized to the total intensity, referred to henceforth as the reduced Stokes parameters, P_Q & P_U , are relative quantities which are used to calculate the polarisation properties, and from which the fraction of linear polarisation may be easily calculated as $P_L = \sqrt{P_Q^2 + P_U^2}$ [13]. The reduced Stokes parameters of Hiltner 652, convolved against the Johnson-Cousins filter pass-bands, as performed by POLSALT, are shown in Figure 2 and are compared against published filtered reduced Stokes parameters obtained with FORS1 [11] and FORS2 [12]. The bottom panel of Figure 2 also shows the filter band-passes for the wavelength range covered by the SALT spectropolarimetry; note that the full R band is not covered by the observation setup.

The reduced Stokes parameters of Hiltner 652 fall within or near the 1σ level of the previously published reduced Stokes parameters over the course of multiple years. This shows that Hiltner 652 is not only a good standard for spectropolarimetric observations but also that using POLSALT with the supplementary wavelength calibrations correctly calculated the Stokes parameters.

The blazar 3C 279 was observed during periods of enhanced and flaring γ -ray activity for energies of 0.1 – 100 GeV and were sourced from the Fermi Light Curve Repository (Fermi LCR)

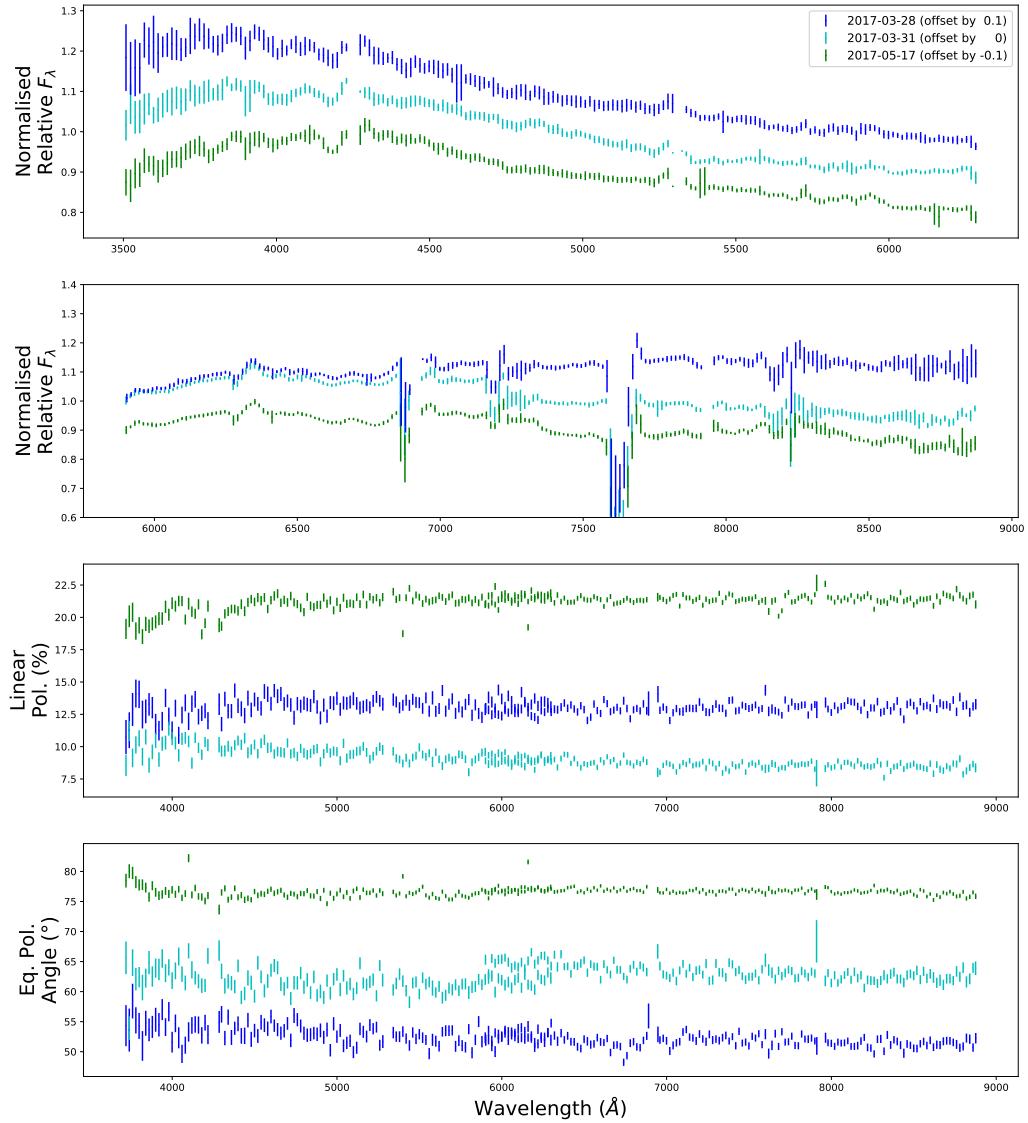


Figure 3: Optical spectropolarimetric observations of 3C 279 during two different periods of flaring. The relative flux calibrated spectra for the grating angles 12.5° (top), observed first at each epoch, and 19.625° (second from top), the degree of polarisation (third from top), and the polarisation angle (bottom).

[14]. 3C 279 was observed at fluxes of 1.58×10^{-6} , 2.87×10^{-6} , and 2.00×10^{-6} ph cm $^{-2}$ s $^{-1}$ as compared to a ‘quiescent’ median flux of 4.59×10^{-7} ph cm $^{-2}$ s $^{-1}$.

Figure 3 shows the relative flux calibrated spectra normalized to the spectrum’s mean (and offset as indicated), degree of polarisation, and polarisation angle for 3C 279. The relative flux was normalized to better compare how the shape of the spectrum changes during the differing γ -ray states. 3C 279 showed variable flux and polarisation during the three observations, with the polarisation changing by $\sim 12.23\%$ and the angle changing by $\sim 24.22^\circ$. The relative spectral shape remains similar over all three observations, however the second observation (2017-03-31) appears to show a slightly brighter spectrum in the blue. There is also a relatively good agreement

in the polarisation at the wavelength overlap for the different grating angles. The difference of the polarisation and degree of polarisation is on the order of 0.25 % and 1.25°, respectively.

5. Discussion and Conclusions

In this paper we have considered the observations of a spectropolarimetric standard, Hiltner 652, and a flaring blazar, 3C 279, to test our supplementary tools used for the reduction of spectropolarimetric data obtained with the RSS. The results serve to confirm that the supplementary tools' wavelength reductions, in combination with POLSALT, produces the correct polarisation behavior. Our results for Hiltner 652 agree well with the historical results obtained using the FOcal Reducer and low dispersion Spectrograph (FORS1 and FORS2) mounted at the Very Large Telescope (VLT).

For 3C 279, there is similarly good agreement between the polarisation for the observations taken at two grating angles where the wavelength ranges overlap. Some disagreement is found which may be due to the inherent nature of flaring blazars which cause the polarisation angle to drastically vary and the two observations at different grating angles are not taken simultaneously. Additionally, the disagreement may be due to a lower Signal-to-Noise Ratio (SNR) at the edges of the RSS, which would introduce a larger systematic error. The lower SNR could originate from either blaze effects, or from the extraction of the trace, which is currently limited to a rectangular aperture in the current POLSALT pipeline.

The results show that our supplementary wavelength calibrations for POLSALT increase the efficiency of the data reduction and produce acceptable results. This reduction procedure has been used for the reduction of a number of blazar observations undertaken as part of a long term monitoring campaign [15].

Acknowledgments

All observations taken in this study were obtained using the RSS mounted on SALT under the programme ID 2016-2-LSP-001 (PI DAH Buckley).

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