Supplementary wavelength calibration methods for SALT/RSS spectropolarimetric observations

Justin Cooper

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Department of Physics

University of the Free State

South Africa

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

Abstract

TODO:

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

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

TODO:

- **Add Keywords $\rightarrow$ look up the astronomy journal keywords**
- **Look up keywords for pipeline development and data reduction.**

Acknowledgements

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

- **TODO: Add acknowledgements!**

Contents

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
HET	Hobby-Eberly Telescope
HgAr	Mercury-Argon
HRS	High Resolution Spectrograph
IRAF	*Image Reduction and Analysis Facility*
L+45°	Linear +45° Polarized
L−45°	Linear −45° Polarized
LCP	Left Circularly Polarized
LHP	Linear Horizontally Polarized
LVP	Linear Vertically Polarized
Ne	Neon-Argon
NIR	Near Infra-Red
NIRWALS	Near Infra-Red Washburn Labs Spectrograph
POLSALT	*Polarimetric reductions for SALT*
RCP	Right Circularly Polarized
RMS	Root Mean Square
RSS	Robert Stobie Spectrograph
S/N	Signal-to-Noise Ratio
SAAO	South African Astronomical Observatory
SAC	Spherical Aberration Corrector
SALT	Southern African Large Telescope
SALTICAM	SALT Imaging Camera
STOPS	*Supplementary Tools for POLSALT Spectropolarimetry*
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.

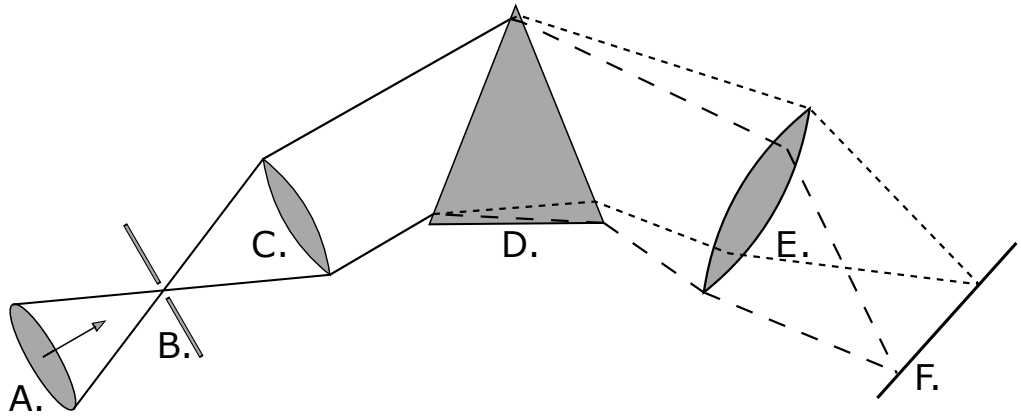


Figure 2.1: Layout depicting the light path through a spectrometer. Diagram adapted from Birney et al. (2006).

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 miniscule 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:

$$R = \frac{\lambda}{FWHM}\,, \tag{2.1}$$

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:

$$\frac{\partial\theta}{\partial\lambda} = \frac{B}{a}\frac{dn}{d\lambda}\,, \tag{2.2}$$

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

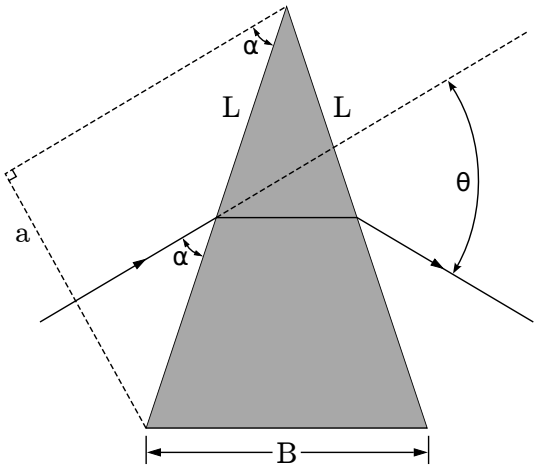


Figure 2.2: Geometry of a prism refracting an incident monochromatic beam at a minimum deviation angle. Diagram adapted from Birney et al. (2006).

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:

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

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,

$$\begin{aligned} \frac{\partial\theta}{\partial\lambda} &= -\frac{B}{a}\frac{2B_C}{\lambda^3} \\ &\propto -\lambda^{-3} , \end{aligned} \tag{2.4}$$

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]

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

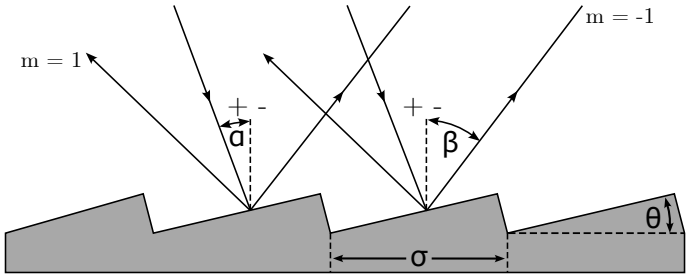


Figure 2.3: Geometry of a reflective blazed grating refracting an incident monochromatic beam. Diagram adapted from Birney et al. (2006).

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 $m \in Z$, 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:

$$m\lambda = \sigma(\sin(\alpha) \pm \sin(\beta))\,, \tag{2.5}$$

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:

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

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,

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

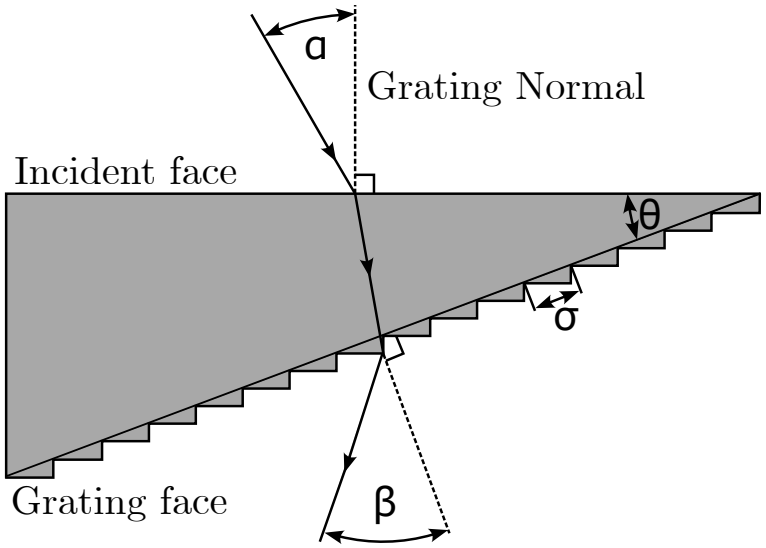


Figure 2.4: Diagram of a grism for an incident monochromatic beam of light and a diffracted beam of order $m = 1$. Diagram adapted from Birney et al. (2006).

Substituting m/σ with the grating equation results in

$$\begin{aligned} \frac{\partial \beta}{\partial \lambda} &= \frac{\sin(\alpha) + \sin(\beta)}{\lambda \cos(\beta)} \\ &\propto \lambda^{-1} . \end{aligned} \tag{2.8}$$

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

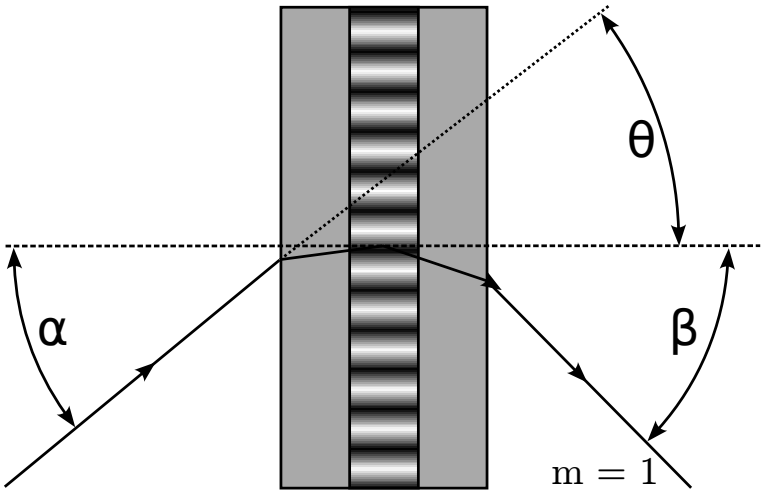


Figure 2.5: Diagram of a VPH grating for an incident monochromatic beam of light. Diagram adapted from Birney et al. (2006).

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.

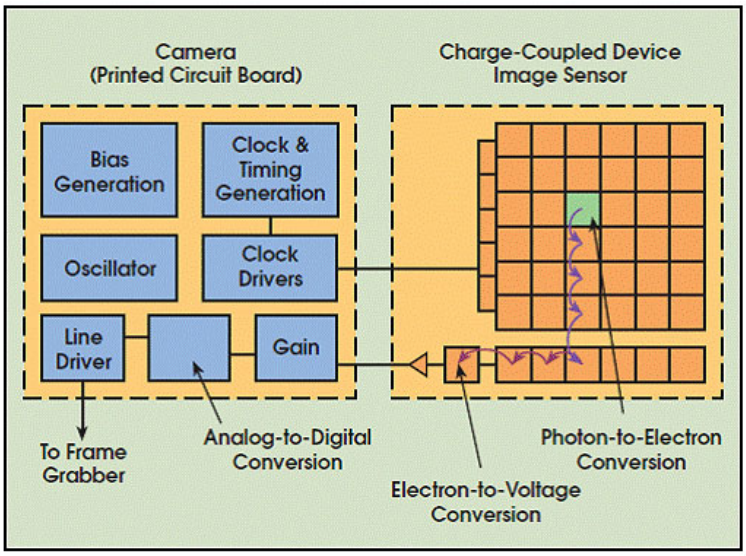


Figure 2.6: Diagram of the inner logic of a CCD. Figure adapted from Litwiller (2001).

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 telescopes dome, and are used in both photometry and spectroscopy. The surface is uniformly and indirectly illuminated by a projector lamp, ideal for flat-field images. Alternate flat-fielding methods, such as night sky and twilight flats, are available but are suited solely for photometry.

Night sky flats are produced from science images containing mostly sky. The science images are combined using the 'mode' statistic which removes any celestial objects at the cost of a low Signal-to-Noise Ratio (S/N) flat-field.

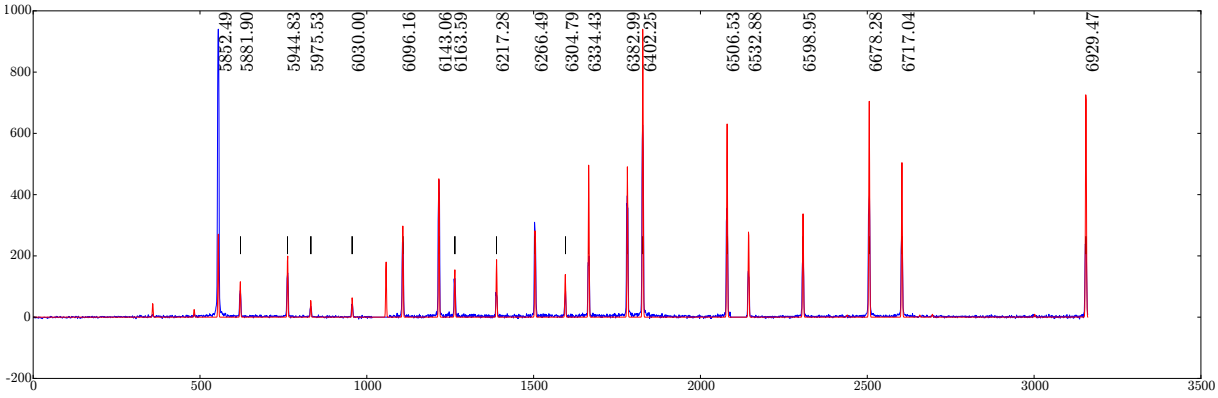


Figure 2.7: Example of an arc spectrum for NeAr taken with SALT's RSS using the PG1800 grating at a grating angle of 34.625°, an articulation angle of 69.258°, and covering a wavelength range of $\sim 5600 - 6900$ Å. Plot adapted from SALT's published Longslit Line Atlases, (2023).[2]

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 $\sim 20°$ 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, $F^n_\lambda(x, y)$, can be calculated as:

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

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:

$$S^*_\lambda(x,y) = \frac{S_\lambda(x,y) - B(x,y) - (\frac{t_S}{t_D})D(x,y)}{F^n_\lambda(x,y)}\,. \tag{2.10}$$

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.

[2]NeAr plot sourced from `https://astronomers.salt.ac.za/data/salt-longslit-line-atlas/`

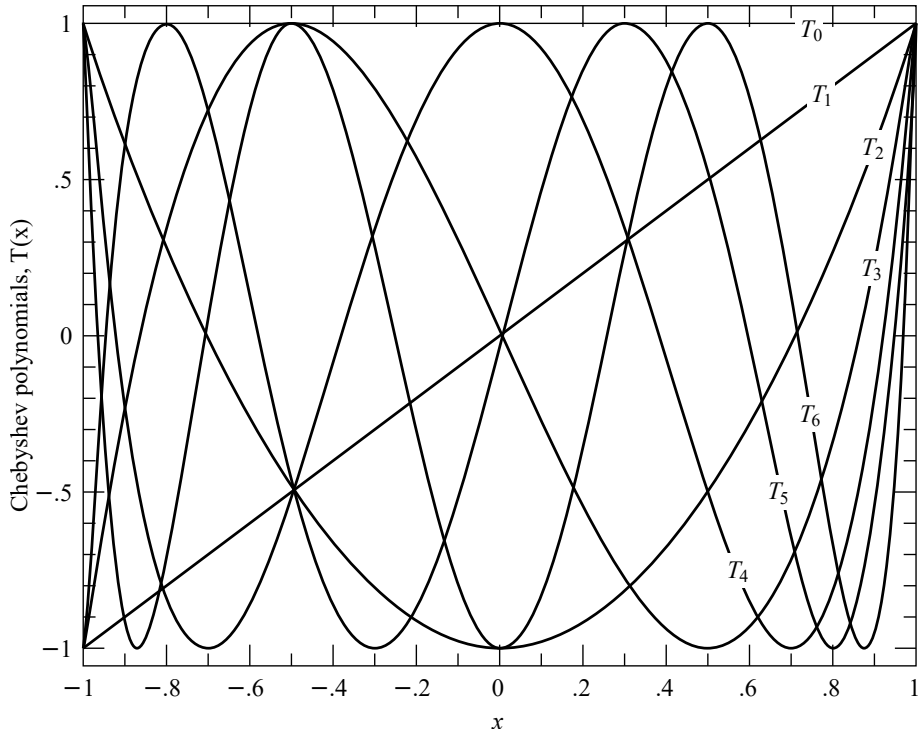


Figure 2.8: The first seven Chebyshev polynomials (T_0 through T_6) as defined by Equation 2.12 over the region $[-1, 1]$ for which they are orthogonal. Plot adapted from (Press et al., 2007) (2023)[3]

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.

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

Chebyshev Polynomials The Chebyshev polynomials are defined explicitly as:

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

or recursively as:

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

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:

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

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:

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

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

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:

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

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).

[4] Chebyshev polynomials are denoted T as a hold-over from the alternate spelling of 'Tchebycheff'.

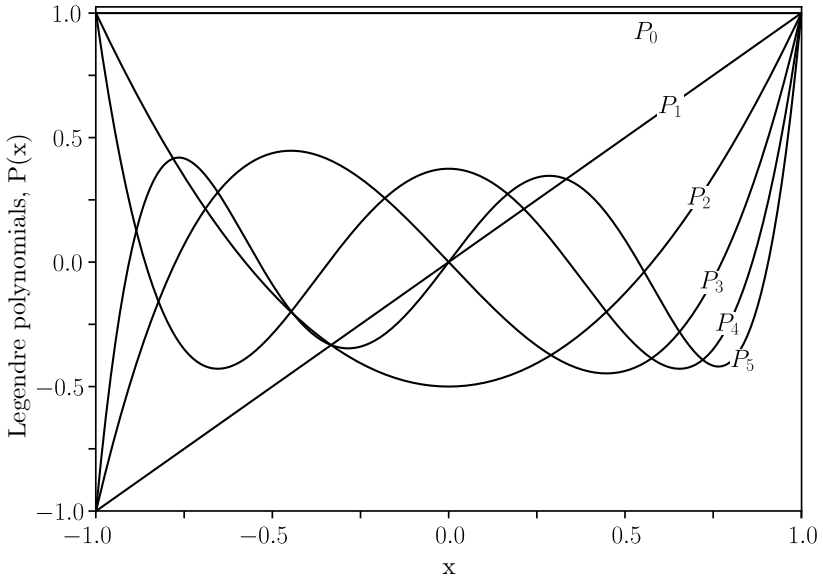


Figure 2.9: The first six Legendre polynomials (P_0 through P_5) as defined by Equation 2.20 over the region $[-1, 1]$ for which they are orthogonal. Plot adapted from Geek3, CC BY-SA 3.0, via Wikimedia Commons (2023).

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

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

or recursively as:

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

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:

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

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:

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

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

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.

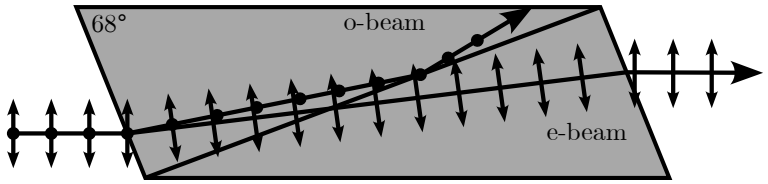


Figure 2.10: Diagram of a Nicol prism for incident non-polarized light. Diagram adapted from Fred the Oyster, CC BY-SA 4.0, via Wikimedia Commons (2023).

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:

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

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:

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

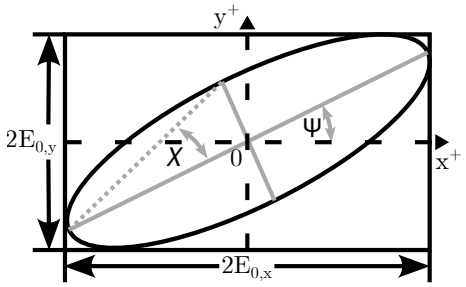


Figure 2.11: The polarization ellipse for an electric field vector propagating through free space. Diagram adapted from Inductiveload, PDM 1.0, via Wikimedia Commons (2023).

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:

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

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:

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

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:

$$(E_{0x}^2 + E_{0y}^2)^2 - (E_{0x}^2 - E_{0y}^2)^2 - (2E_xE_y\cos\Phi)^2 = (2E_xE_y\sin\Phi)^2\,. \tag{2.29}$$

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

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

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 $+45°$ Polarized (L$+45°$) to Linear $-45°$ Polarized (L$-45°$) light; and S_3, ratio of the Right Circularly Polarized (RCP) (clockwise) to Left Circularly Polarized (LCP)

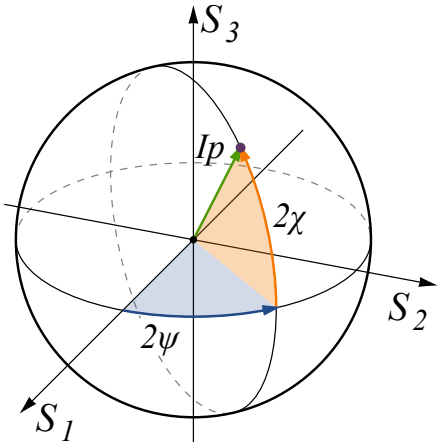


Figure 2.12: The Poincaré sphere describing the polarization properties of a wave-packet propagating through free space. Diagram adapted from Inductiveload, PDM 1.0, via Wikimedia Commons (2023).

(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:

$$I^2 = Q^2 + U^2 + V^2 \,, \tag{2.31}$$

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:

$$I^2 \geq Q^2 + U^2 + V^2 \,, \tag{2.32}$$

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

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

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:

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

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.

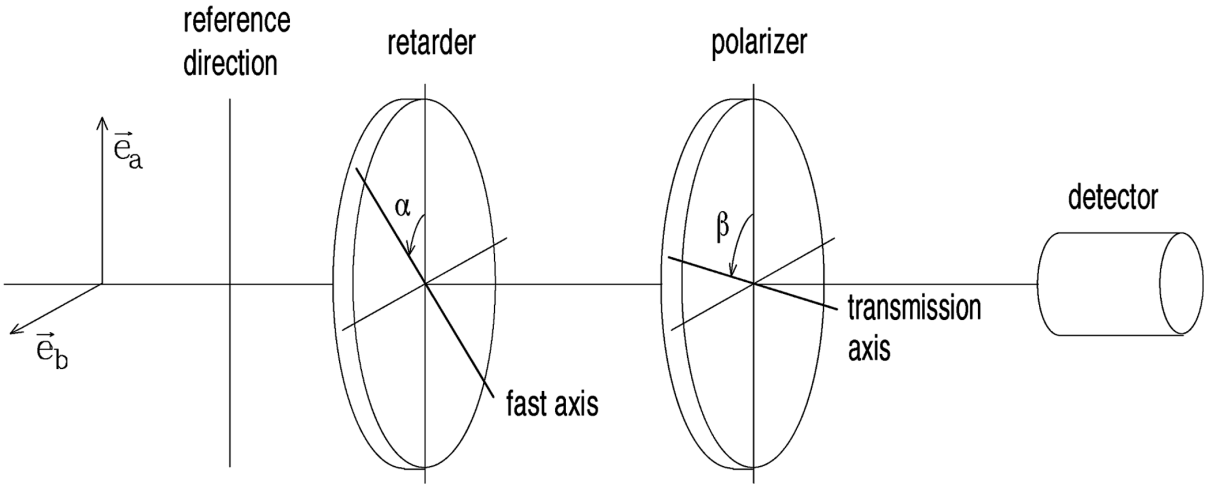


Figure 2.13: A diagram of an ideal polarimeter. Diagram adapted from Degl'Innocenti and Landolfi (2004).

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 $(\mathbf{M}_0, \ldots, \mathbf{M}_N)$ results in an outgoing beam $\mathbf{S}'$ such that:

$$\mathbf{S}' = \mathbf{M}_N \ldots \mathbf{M}_0 \mathbf{S} \,. \tag{2.35}$$

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,

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

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 retandance 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

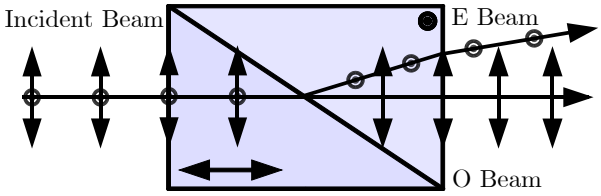


Figure 2.14: Diagram of a Rochon prism. Included in the diagram are the optical axes of the differing sections of the birefringent material as well as polarizing directions of the incident beam, denoted using the ↔ and ⊙ symbols, for the *O*- and *E*-beams, respectively. Figure adapted from ChrisHodgesUK, 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:

$$\gamma = \frac{2\pi\Delta n L}{\lambda_0} \tag{2.40}$$

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 $m \in Z^+$, 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

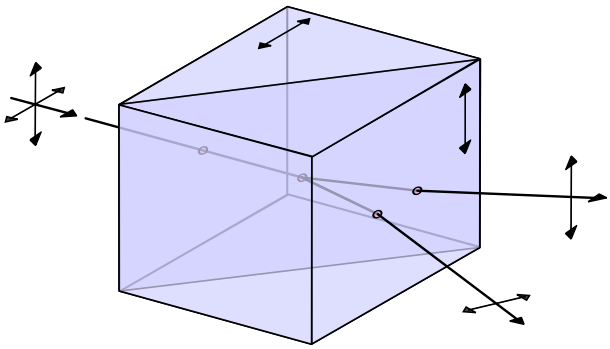


Figure 2.15: Diagram of a Wollaston prism. Included in the diagram are the optical axes of the differing sections of the birefringent material as well as polarizing directions of the incident beam, denoted using the ↔ and ↕ symbols, for the *O*- and *E*-beams, respectively. Diagram adapted from fgalore, 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 Romaniello, 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

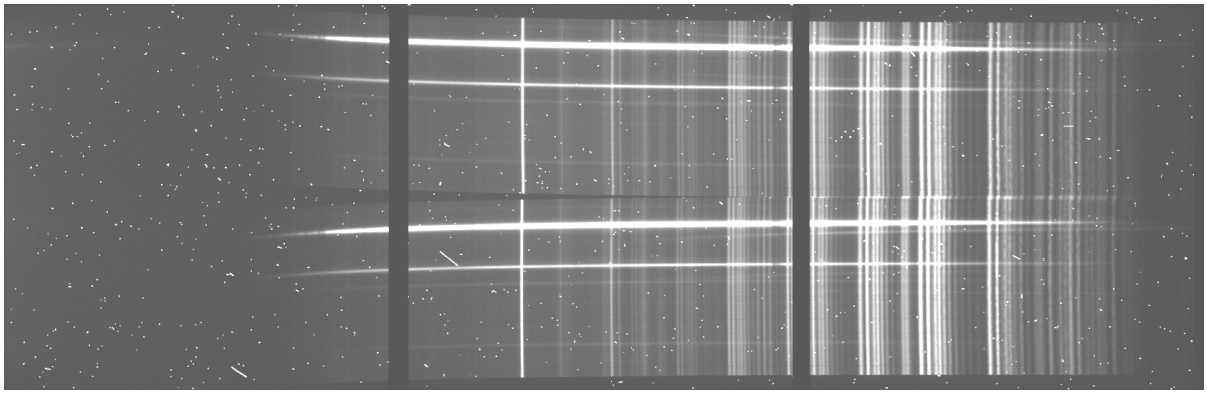


Figure 2.16: A spectropolarimetric target exposure as observed by the SALT RSS in spectropolarimetry mode.

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:

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

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

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

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:

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

which allows Equation 2.41 to be written, as

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

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:

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

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.

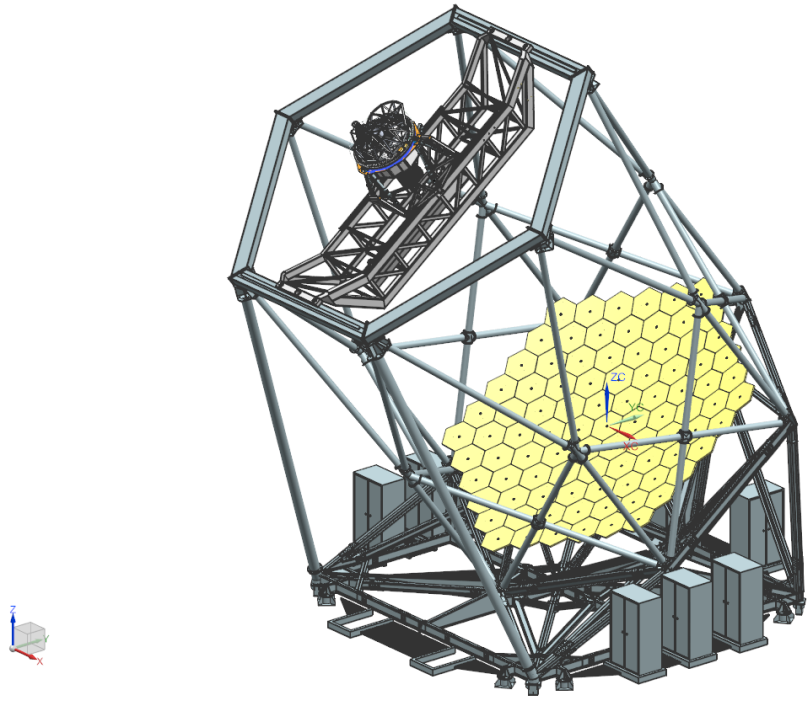


Figure 2.17: The tracker, supporting structure, and primary mirror of SALT. Figure adapted from the SALT call for proposals (2022).[5]

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).

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

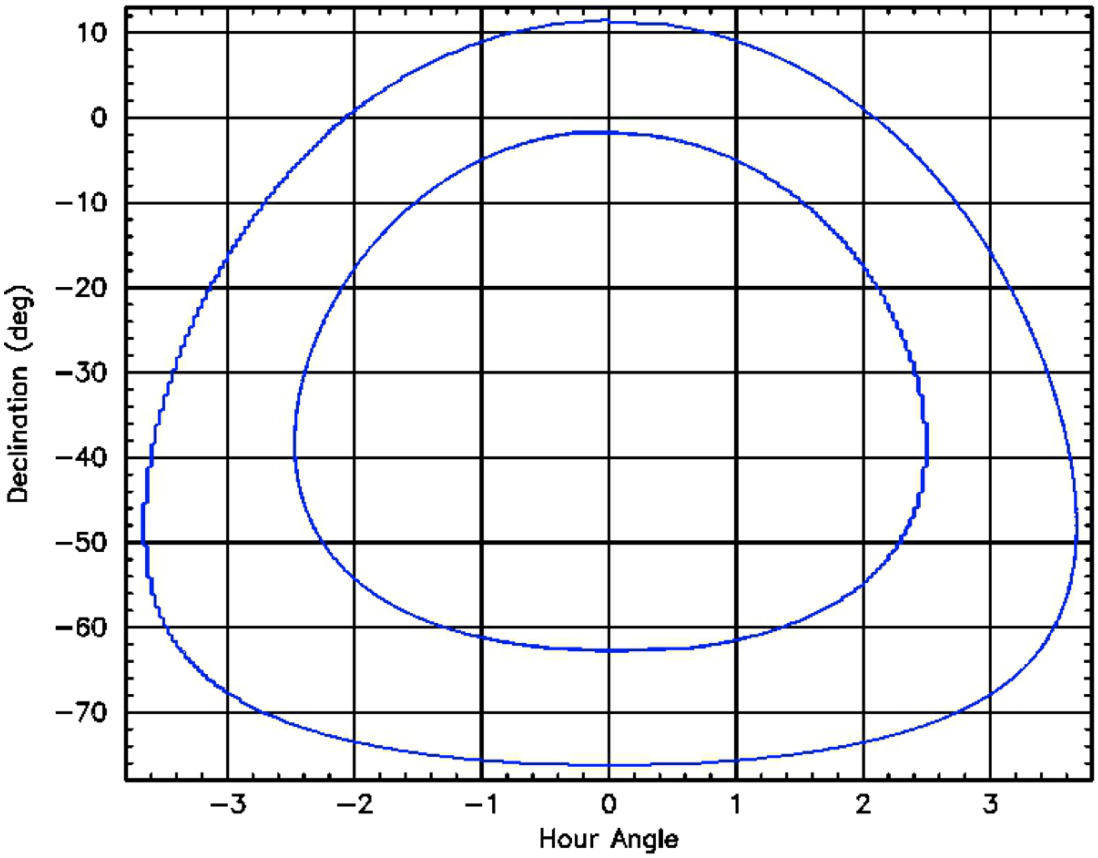


Figure 2.18: The visibility annulus of objects observable by SALT. Figure adapted from the SALT call for proposals (2013).[6]

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 μm and is capable of tracking $\pm 6°$ 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 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 Å. These return a corrected flat focal plane with an $8'$ diameter field of view at prime focus on to the science instruments, with a $1'$ annulus around it used by the tracker in a closed-loop guidance system. The tracker also houses the calibration system which contains the Ar, CuAr, HgAr, Ne, ThAr, and Xe wavelength calibration lamps (Buckley et al., 2008).

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

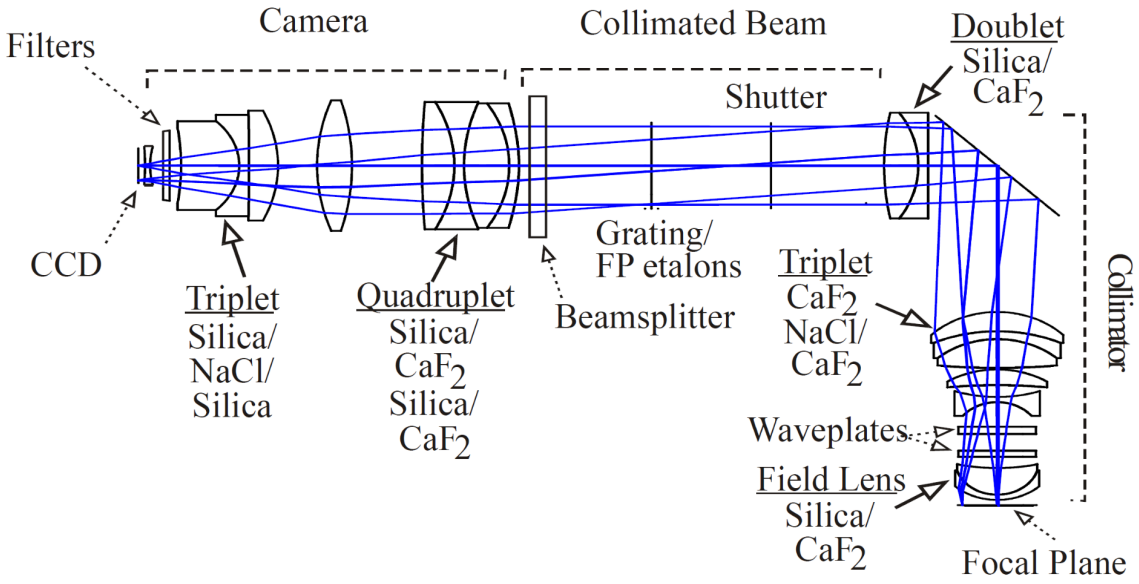


Figure 2.19: The optical path of the SALT RSS. Figure adapted from the SALT call for proposals (2023).[7]

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.

[7] `https://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]

[8]The 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.

[9]Commission status sourced from the latest 'Polarimetry Observers Guide' (2024).

Linear (°)		Linear-Hi (°)		Circular (°)		Circular-Hi (°)		All Stokes (°)	
$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$
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 basic CCD reductions, wavelength calibrations, background subtraction and spectral extraction, raw Stokes calculations, final Stokes calculations, and visualization of the results. Accurate reductions at each step are crucial for accurate results and are thus briefly discussed below. Further details for the reduction process may be found at the POLSALT GitHub wiki.[3]

[1] POLSALT 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.

[2] Installation files and instructions for the 'beta version' utilizing the GUI are available at `http://www.saao.ac.za/~ejk/polsalt/code/` in a TAR GZIP file.

[3] The GitHub wiki for POLSALT is available at `https://github.com/saltastro/polsalt/wiki`.

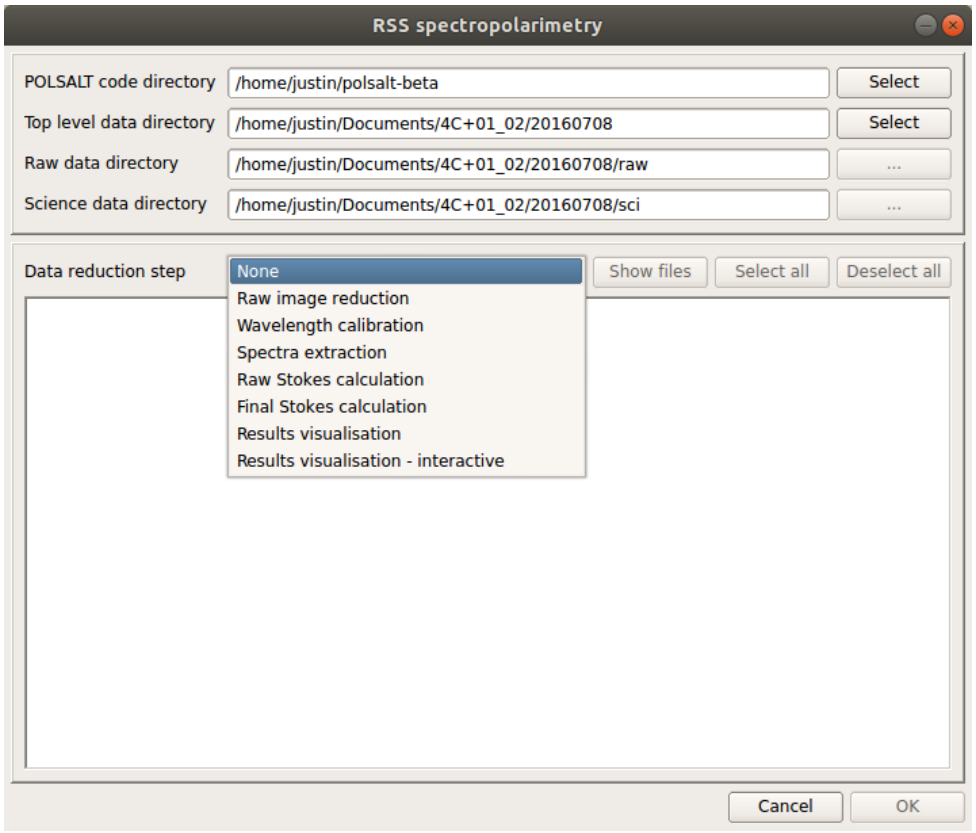


Figure 3.1: The layout of the POLSALT Graphical User Interface (GUI), including the contents of the reduction steps accessible via the dropdown menu. Note that there is no trailing forward slash after the 'Top level data directory'. Figure created from a local instance of the POLSALT GUI.

3.1.1 Basic CCD Reductions

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

3.1.2 Wavelength Calibrations

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

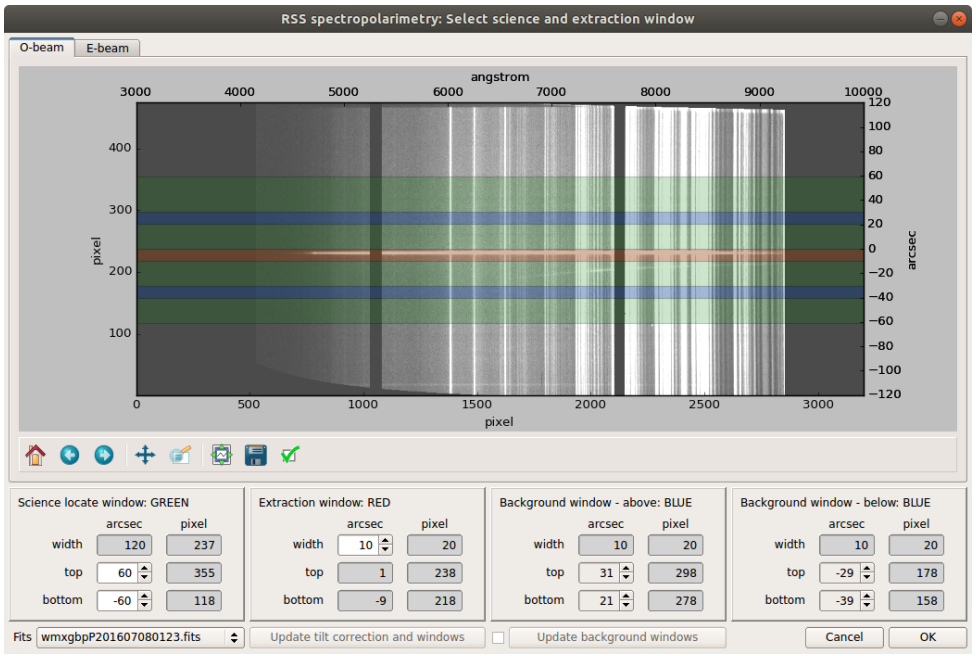


Figure 3.2: The layout of the interactive POLSALT `spectra extraction` GUI after selecting the 'update tilt correction and windows' button along the bottom border of the window. Figure created from a local instance of the POLSALT GUI.

3.1.3 Spectral Extraction

Background subtraction and spectral extraction is run via **specpolextract_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:

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

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

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.

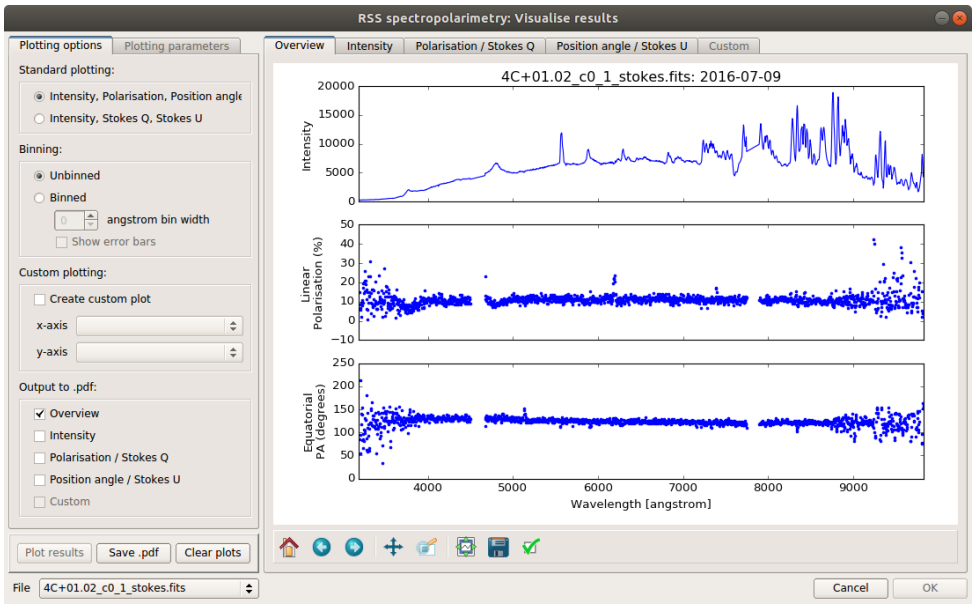


Figure 3.3: The layout of the interactive POLSALT `visualization` GUI after selecting the 'Plot results' button along the bottom border of the window. Figure created from a local instance of the POLSALT GUI.

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 (°) 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.

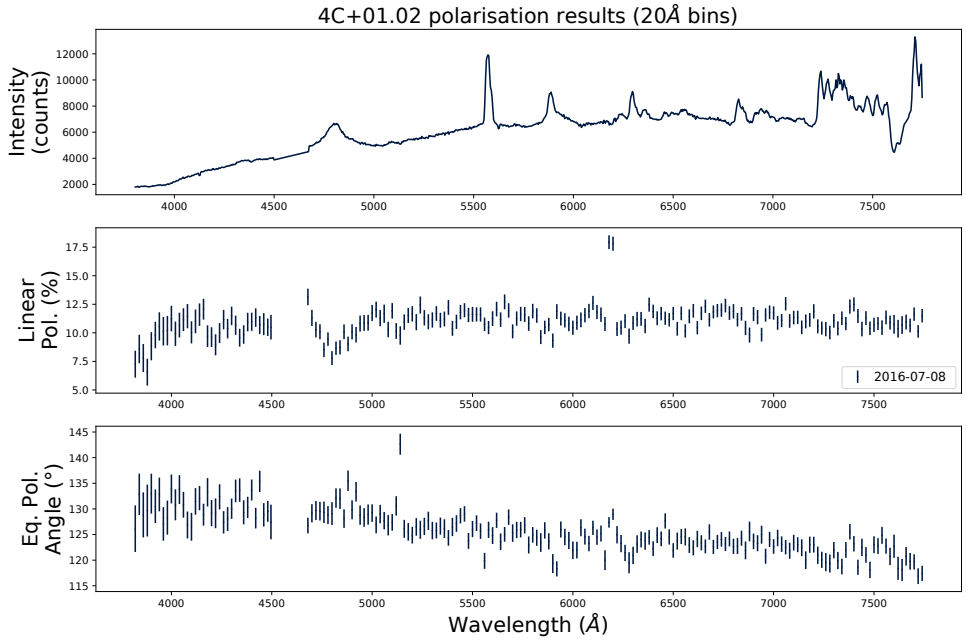


Figure 3.4: A typical plot resulting from the reduction process. Figure adapted from (Cooper et al., 2022).

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 ($\sim 10.68°$ and $\sim 5.38°$, 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,

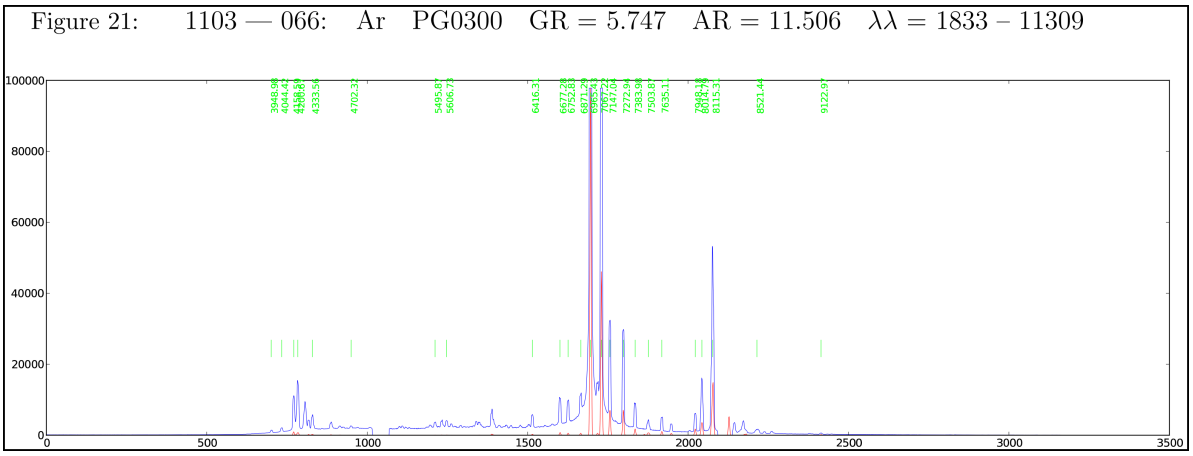


Figure 3.5: One of many Ar arc lamp spectra as provided by SALT for line identification. Plot adapted from SALT's published Longslit Line Atlases (as of 2024), resized to fit within the document margins but otherwise unchanged.[4]

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

[4]The 'low resolution' Ar plot sourced from `https://astronomers.salt.ac.za/data/salt-longslit-line-atlas/`

[5]Online 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`.

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

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

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

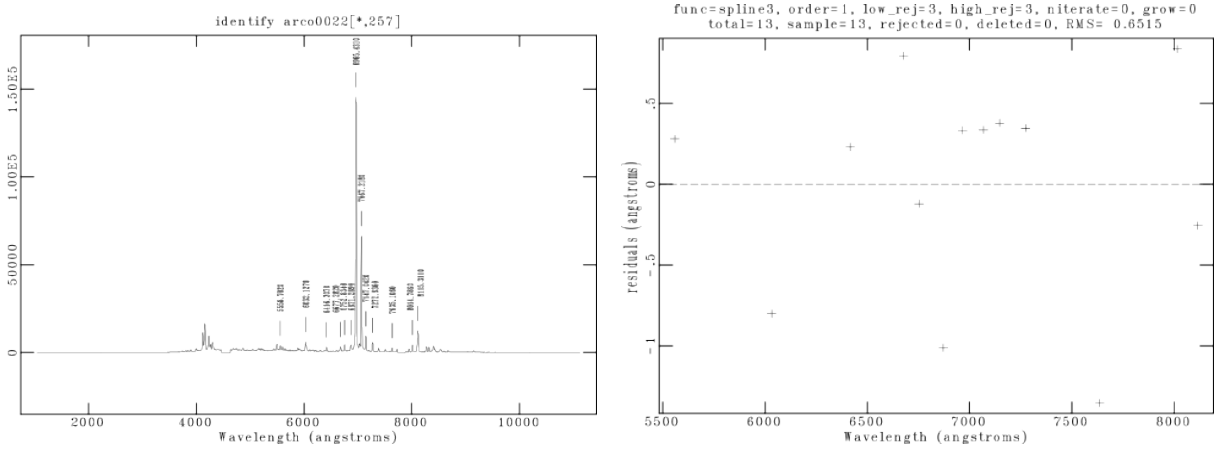
[9] Help documentation for the `identify` task may be found at `https://astro.uni-bonn.de/~sysstw/lfa_html/iraf/noao.onedspec.identify.html`.

[10] See also `https://iraf.net/irafdocs/formats/identify.php` for an explanation of the database contents.

[11] Help 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
```



(a) Identified features.

(b) Root Mean Square (RMS) of the identified features.

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.

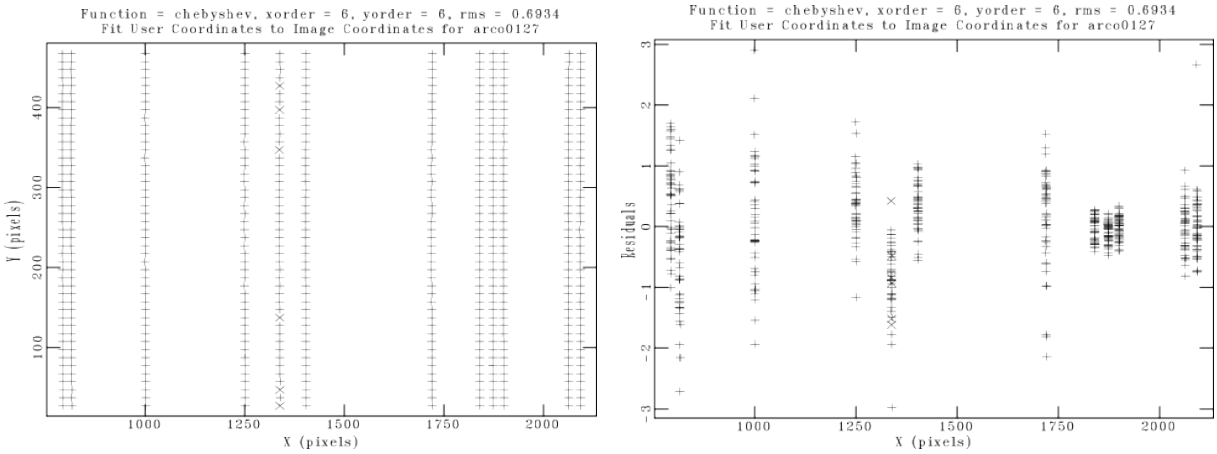
3.2.3 Fitcoords

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.

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

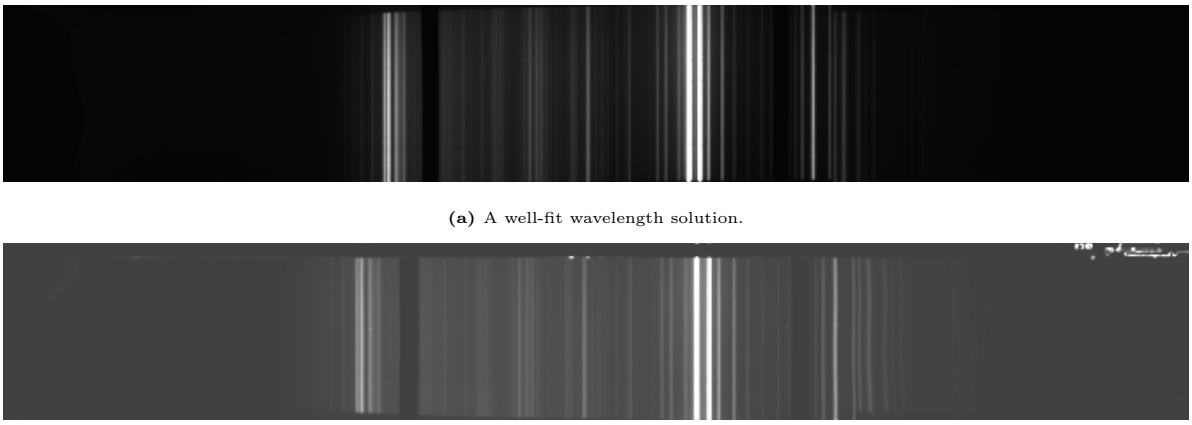
[13]See also `https://iraf.net/irafdocs/formats/fitcoords.php` for an explanation of the database contents.



(a) Features identified across an exposure.

(b) RMS of the identified features.

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



(a) A well-fit wavelength solution.

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

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

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.

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

```
25
26  """
27  The `Split` class allows for the splitting of `polsalt` FITS files
28  based on the polarization beam. The FITS files must have basic
29  `polsalt` pre-reductions already applied (`mxgbp...` FITS files).
30
31  Parameters
32  ----------
33  data_dir : str | Path
34      The path to the data to be split
35  fits_list : list[str], optional
36      A list of pre-reduced `polsalt` FITS files to be split within `data_dir`.
37      (The default is None, `Split` will search for `mxgbp*.fits` files)
38  split_row : int, optional
39      The row along which to split the data of each extension in the FITS file.
40      (The default is SPLIT_ROW (See Notes), the SALT RSS CCD's middle row)
41  no_arc : bool, optional
42      Decides whether the arc frames should be recombined.
43      (The default is False, `polsalt` has no use for the arc after wavelength calibrations)
44  save_prefix : dict[str, list[str]], optional
45      The prefix with which to save the  O & E beams.
46      Setting `save_prefix` = ``None`` does not save the split O & E beams.
47      (The default is SAVE_PREFIX (See Notes))
48
49  Attributes
50  ----------
51  arc : str
52      Name of arc FITS file within `data_dir`.
53      `arc` = `""` if `no_arc` or not detected in `data_dir`.
54  o_files, e_files : list[str]
55      A list of the `O`- and `E`-beam FITS file names.
56      The first entry is the arc file if `arc` defined.
57  data_dir
58  fits_list
59  split_row
60  save_prefix
61
62  Methods
63  -------
64  split_file(file: os.PathLike)
65      -> tuple[astropy.io.fits.HDUList]
66      Handles creation and saving the separated FITS files
67  split_ext(hdulist: astropy.io.fits.HDUList, ext: str = 'SCI')
68      -> astropy.io.fits.HDUList
69      Splits the data in the `ext` extension along the `split_row`
70  crop_file(hdulist: astropy.io.fits.HDUList, crop: int = CROP_DEFAULT (See Notes))
71      -> tuple[numpy.ndarray]
72      Crops the data along the edge of the frame, that is,
73      `O`-beam cropped as [crop:], and
74      `E`-beam cropped as [:-crop].
75  update_beam_lists(o_name: str, e_name: str)
76      -> None
77      Updates `o_files` and `e_files`.
78  save_beam_lists(file_suffix: str = 'frames')
79      -> None
80      Creates (Overwrites if exists) and writes the `o_files` and `e_files` to files named
81      `o_{file_suffix}` and `e_{file_suffix}`, respectively.
82  process()
83      -> None
84      Calls `split_file` and `save_beam_lists` on each file in `fits_list` for automation.
85
86  Other Parameters
87  ----------------
88  **kwargs : dict
89      keyword arguments. Allows for passing unpacked dictionary to the class constructor.
90
91  Notes
92  -----
93  Constants Imported (See utils.Constants):
94      SAVE_PREFIX
95      CROP_DEFAULT
96      SPLIT_ROW
97
98  """
```

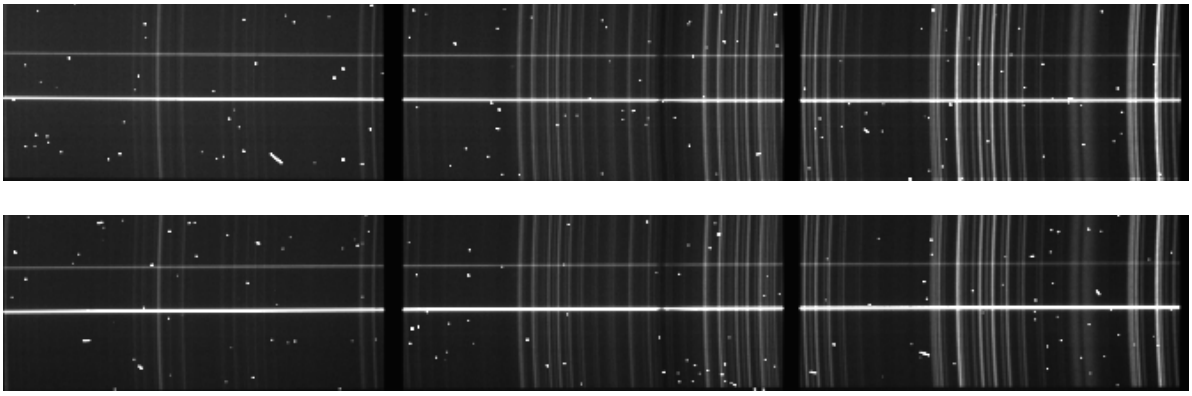


Figure 3.9: The split *O*- and *E*-beams as handed to IRAF. Figure created from the STOPS `split` method output.

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**

```
31
32  """
33  The `Join` class allows for the joining of previously split files and the
34  appending of an external wavelength solution in the `polsalt` FITS file format.
35
36  Parameters
37  ----------
38  data_dir : str | Path
39      The path to the data to be joined
40  database : str, optional
41      The name of the `IRAF` database folder.
42      (The default is "database")
43  fits_list : list[str], optional
44      A list of pre-reduced `polsalt` FITS files to be joined within `data_dir`.
45      (The default is ``None``, `Join` will search for `mxgbp*.fits` files)
46  solutions_list: list[str], optional
47      A list of solution filenames from which the wavelength solution is created.
48      (The default is ``None``, `Join` will search for `fc*` files within the `database` directory)
49  split_row : int, optional
50      The row along which the data of each extension in the FITS file was split.
51      Necessary when Joining cropped files.
52      (The default is 517, the SALT RSS CCD's middle row)
53  save_prefix : dict[str, list[str]], optional
54      The prefix with which the previously split `O`- & `E`-beams were saved.
55      Used for detecting if cropping was applied during the splitting procedure.
56      (The default is SAVE_PREFIX (See Notes))
57  verbose : int, optional
58      The level of verbosity to use for the Cosmic ray rejection
59      (The default is 30, I.E. logging.INFO)
60
61  Attributes
62  ----------
63  fc_files : list[str]
64      Valid solutions found from `solutions_list`.
65  custom : bool
66      Internal flag for whether `solutions_list` uses the `IRAF` or a custom format.
67      See Notes for custom solution formatting.
68      (Default (inherited from `solutions_list`) is False)
69  arc : str
70      Deprecated. Name of arc FITS file within `data_dir`.
71  data_dir
72  database
73  fits_list
74  split_row
75  save_prefix
76
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 astroscrappy [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 """
```

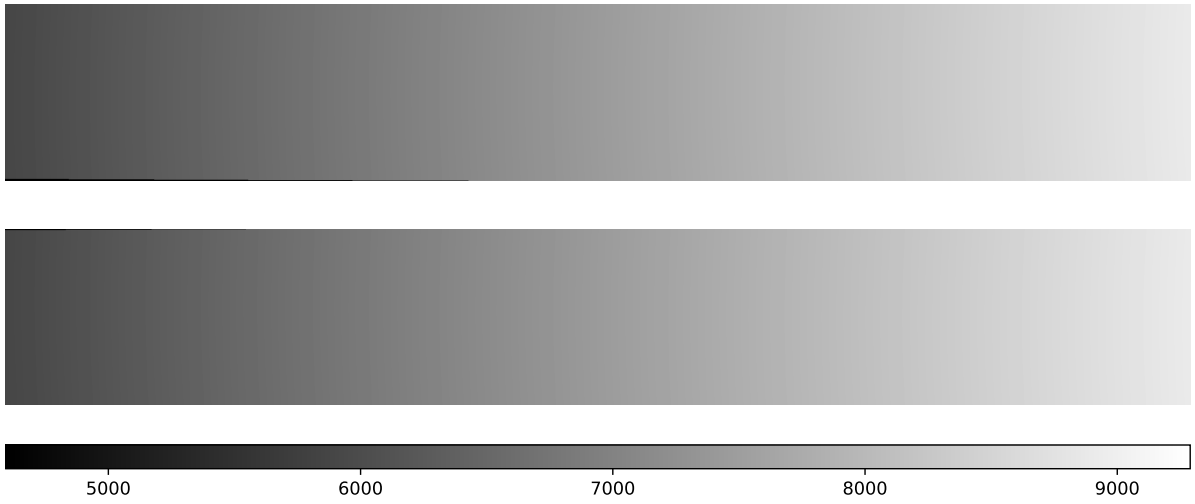


Figure 3.10: A representative 'WAV' extension of a FITS file, for the *O*- (top) and *E*-beam (bottom), ready to be processed by the POLSALT pipeline. The color bar shows the wavelength in Å. Note that regions which fall outside the exposed region are masked by setting the corresponding pixel values 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 suggestions[15] 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**

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

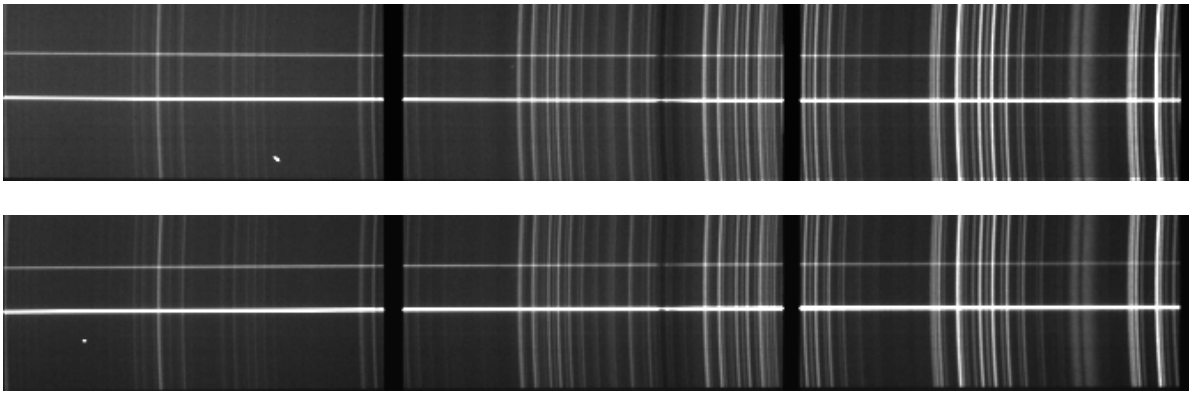


Figure 3.11: A representative 'SCI' extension of a FITS file, for the *O*- (top) and *E*-beam (bottom), ready to be processed by the POLSALT pipeline. The observed intensity is displayed via the grayscale value at each pixel. Figure created from the STOPSjoin method output.

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 (Å, 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.

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

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

[17]The 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**

```
35
36  """
37  Cross correlate allows for comparing the extensions of multiple
38  FITS files, or comparing the O and E beams of a single FITS file.
39
40  Parameters
41  ----------
42  data_dir : str | Path
43      The path to the data to be cross correlated
44  filenames : list[str]
45      The ecwmxgbp*.fits files to be cross correlated.
46      If only one filename is defined, correlation is done against the two polarization beams.
47  split_ccd : bool, optional
48      Decides whether the CCD regions should each be individually cross correlated.
49      (The default is True, which splits the spectrum up into its separate CCD regions)
50  cont_ord : int, optional
51      The degree of a chebyshev to fit to the continuum.
52      (The default is 11)
53  plot : bool, optional
54      Decides whether the continuum fitting should be plotted
55      (The default is False, so no continua plots are displayed)
56  save_prefix : str, optional
57      The name or directory to save the figure produced to.
58      "." saves a default name to the current working. A default name is also used when save_prefix is a directory.
59      (The default is None, I.E. The figure is not saved, only displayed)
60
61  Attributes
62  ----------
63  data_dir
64  fits_list
65  beams : str
66      The mode of correlation.
67      'OE' for same file, and 'O' or 'E' for different files but same extension.
68  ccds : int
69      The number of CCD's in the data. Used to split the CCD's if split_ccd is True.
70  cont_ord : int
71      The degree of the chebyshev to fit to the continuum.
72  can_plot : bool
73      Decides whether the continuum fitting should be plotted
74  offset : int
75      The amount the spectrum is shifted, mainly to test the effect of the cross correlation
76      (The default is 0, I.E. no offset introduced)
77  save_prefix
78  wav_unit : str
79      The units of the wavelength axis.
80      (The default is Angstroms)
81  wav_cdelt : int
82      The wavelength increment.
83      (The default is 1)
84  alt : Callable
85      An alternate method of cross correlating the data.
86      (The default is None)
87
88  Methods
89  -------
90  load_file(filename: Path) -> tuple[np.ndarray, np.ndarray, np.ndarray]
91      Loads the data from a FITS file.
92  get_bounds(bpm: np.ndarray) -> np.ndarray
93      Finds the bounds for the CCD regions.
94  remove_cont(spec: list, wav: list, bpm: list, plot_cont: bool) -> None
95      Removes the continuum from the data.
96  correlate(filename1: Path, filename2: Path | None = None) -> None
97      Cross correlates the data.
98  ftcs(filename1: Path, filename2: Path | None = None) -> None
99      Cross correlates the data using the Fourier Transform.
100 plot(spec, wav, bpm, corrdb, lagsdb) -> None
101     Plots the data.
102 process() -> None
103     Processes the data.
104
105 Other Parameters
106 ----------------
107 offset : int, optional
108     The amount the spectrum is shifted, mainly to test the effect of the cross correlation
109     (The default is 0, I.E. no offset introduced)
110 **kwargs : dict
111     keyword arguments. Allows for passing unpacked dictionary to the class constructor.
112     ftcs : bool, optional
113         Decides whether the Fourier Transform should be used for cross correlation.
114
115 See Also
116 --------
117 scipy
118     https://docs.scipy.org/doc/scipy/reference/generated/
119     correlation: scipy.signal.correlate.html
120
121
122 Notes
123 -----
124 Constants Imported (See utils.Constants):
125     SAVE_CORR
126
127 """
```

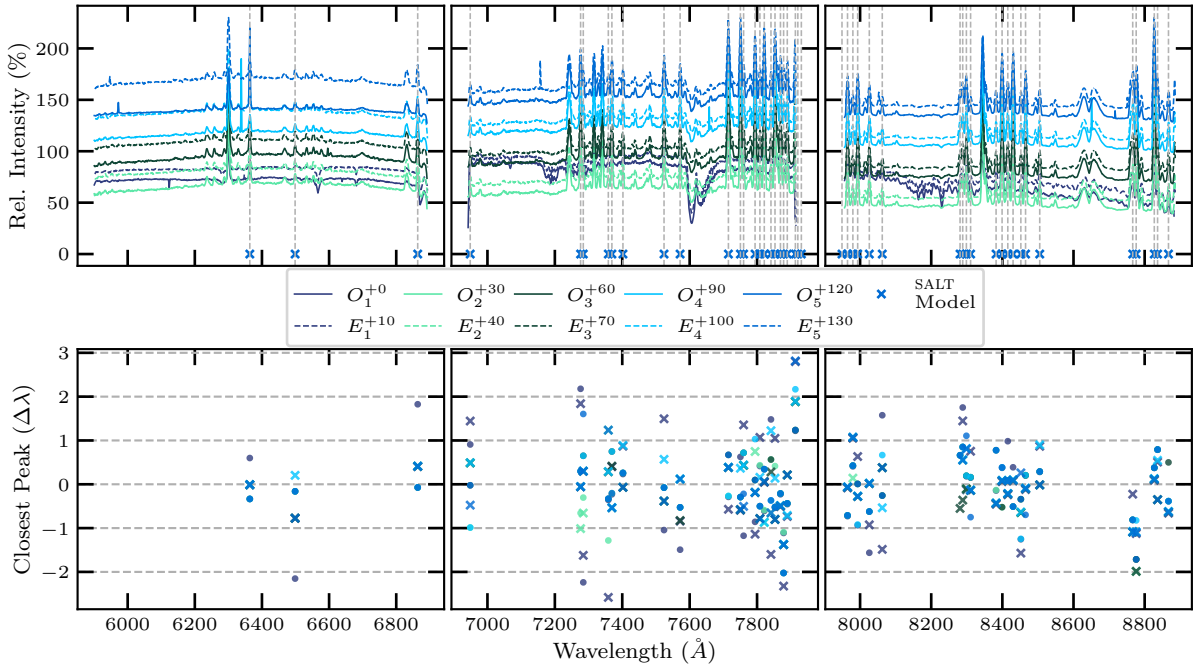


Figure 3.12: An example of a well calibrated wavelength solution, specifically shown for science images. Figure created via the STOPS `skyline` method.

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.

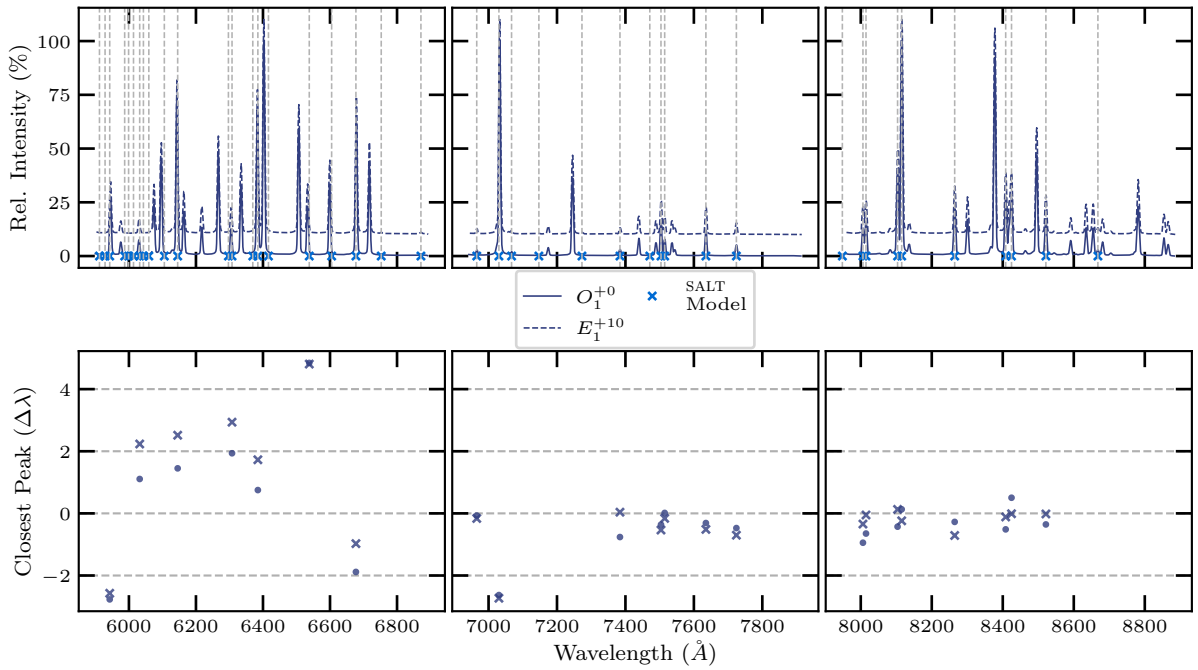


Figure 3.13: An example of a wavelength solution with a poor fit at shorter wavelengths (bottom left), specifically shown for an arc image. Arc lines are Figure created via the STOPS `skyline` method.

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.

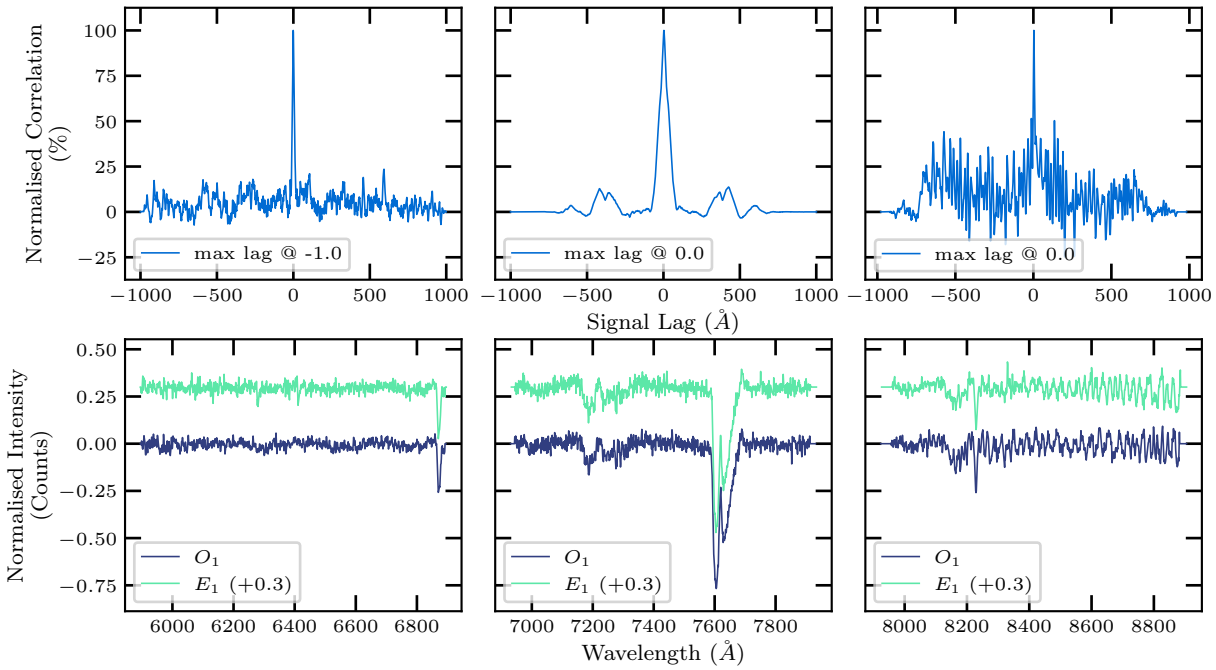


Figure 3.14: The resultant output plot of the STOPS `correlate` method. Figure created via the STOPS `correlate` method.

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.

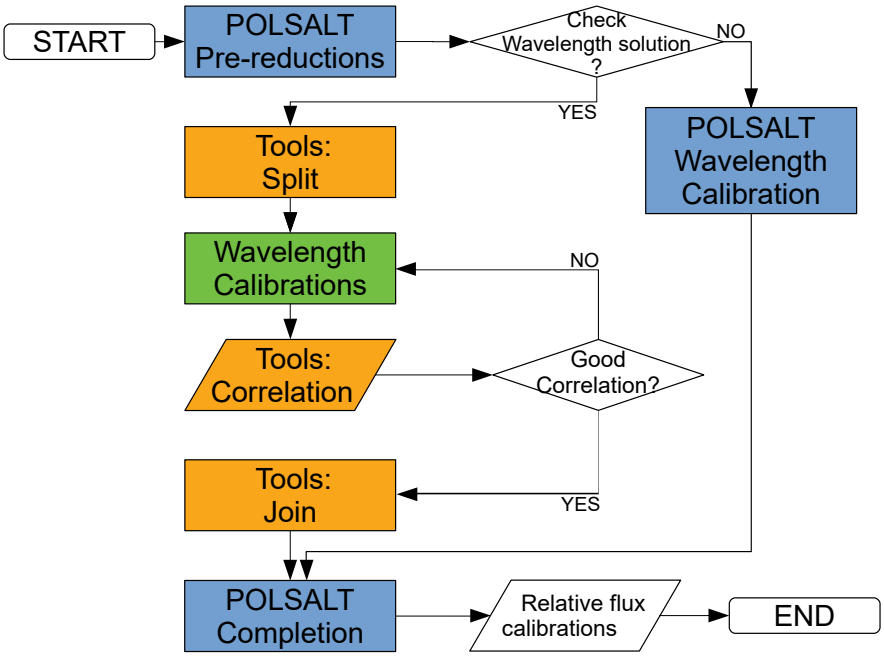


Figure 3.15: A general workflow for data reductions using a combination of POLSALT, IRAF, and the developed supplementary tools. Diagram adapted from Cooper et al. (2022).

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 `identify`, `reidentify`, `fitcoords`, and optionally `transform`. In general, these tasks are run directly in the IRAF terminal using:[18]

[18]Please 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.

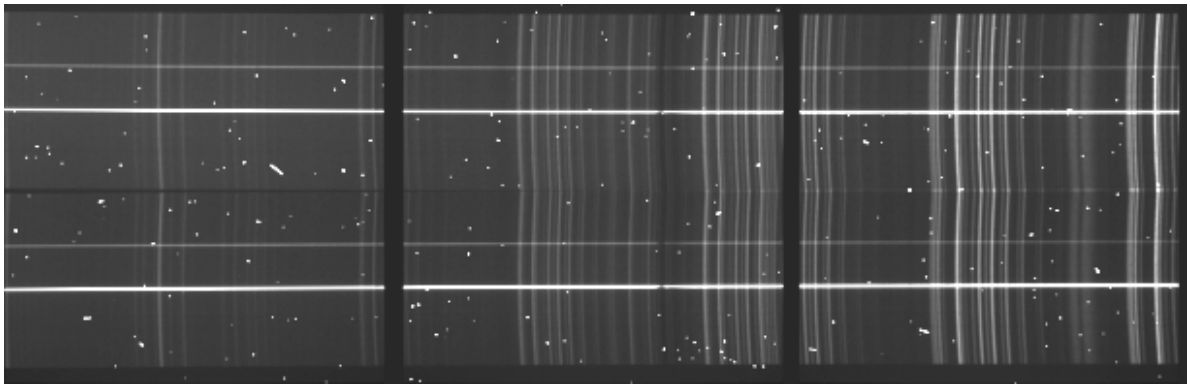


Figure 3.16: The 'SCI' extension of a typical spectropolarimetric FITS file taken with the SALT RSS, after basic POLSALT CCD reductions have been completed. Figure created from the STOPS `split` output.

```
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.

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.

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. 68 onwards).[19]

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

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

```
import os, sys, glob, shutil
poldir = '/home/justin/polsalt-beta/'                              # Will differ according to user

reddir=poldir+'polsalt/'
scrdir=poldir+'scripts/'
sys.path.extend((reddir,scrdir,poldir))

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

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]

[20]Please 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) and its application in publications (§ 4.4).

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 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` methods 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 'beam*.fits' files contain the split 'SCI' extension data as well as the same header as the pre-reduced file. The only changes to the data of each file is the exclusion of the opposing perpendicular polarization beam, as well as a cropping which defaults to 40 pixels (see § 3.3.1), introduced to the top- and bottom-most rows of the data. This

Filename	No.	Name	Type	Cards	Dimensions	Format
POLSALT	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
STOPS `split` 'O'	0	'Primary'	PrimaryHDU	162	(3199, 474)	float32
STOPS `split` 'E'	0	'Primary'	PrimaryHDU	162	(3199, 474)	float32

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

accounts for the discrepancy in the 'Dimensions' between the input and output files in Table 4.1.

The header is left mostly untouched, and only updated to represent the new data 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 input and output file header entries in Table 4.1.

This output file shape was chosen for IRAF compatibility, and was tested for robustness 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 POLSALT pre-reduced files as input and outputs POLSALT `spectra extraction` compatible ('wmxgbp-' prefixed) FITS file structures. Ensuring that the output format was correct was paramount as the POLSALT `spectra extraction` method is unable to process the files otherwise, thus halting the reduction process.

Table 4.2 shows the FITS file information for the files with both POLSALT and IRAF wavelength calibrations.

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 consistent with those created by POLSALT. This was achieved through the `correlate` and `skylines` methods, which were designed to validate the wavelength solutions produced by IRAF.

Before the POLSALT wavelength calibrations were replaced with the IRAF wavelength

[1] The '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
POLSALT	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 POLSALT wavelength calibrated FITS file to the (IRAF wavelength calibrated) STOPS `join` FITS file. Table created using the `Astropy fitsinfo` CLI tool.

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.

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` method output files as input.

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.

4.3 Application of STOPS

4.3.1 Polarization Parameters

4.3.2 Spectropolarimetric Standards

4.4 Application in Publications

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 '`cl>`' 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, $<OBSDATE>$ (formatted 'YYYYMMDD'), the split science FITS files, $<O\text{-}beam\ FILES>$ or $<E\text{-}beam\ FILES>$, the split arc FITS files, $<O\text{-}beam\ ARC>$ or $<E\text{-}beam\ ARC>$, and a wildcard symbol, $<*>$.

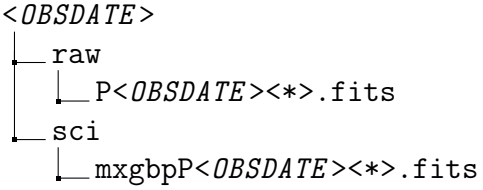


Figure A.1: The typical minimal file structure of data provided by SALT.

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 $<OBSDATE>$.
- 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` task[1] 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$idhenear.dat", units="", nsum="10", match=-3.,
>>> maxfeatures=50, zwidth=100., ftype="emission", fwidth=8.,
>>> cradius=5., threshold=0., minsep=2., function="spline3", order=2,
>>> sample="*", niterate=0, low_reject=3., high_reject=3., grow=0.,
>>> autowrite=no, graphics="stdgraph", cursor="", aidpars="")
```

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

The `reidentify` task may be run using the commands in Listing 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$idhenear.dat",
>>> match=-3., maxfeatures=50, minsep=2., database="database",
>>> logfiles="logfile", plotfile="", verbose=yes, graphics="stdgraph",
>>> cursor="", aidpars="")
```

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

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

[3] See `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 <*O-beam ARC*> with <*E-beam ARC*> 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 <*O-beam ARC*> with <*E-beam ARC*>.

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 <*O-beam FILES*> and <*O-beam ARC*> with <*E-beam FILES*> and <*E-beam ARC*> 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

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

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

[6] See `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'.

[7]The 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.

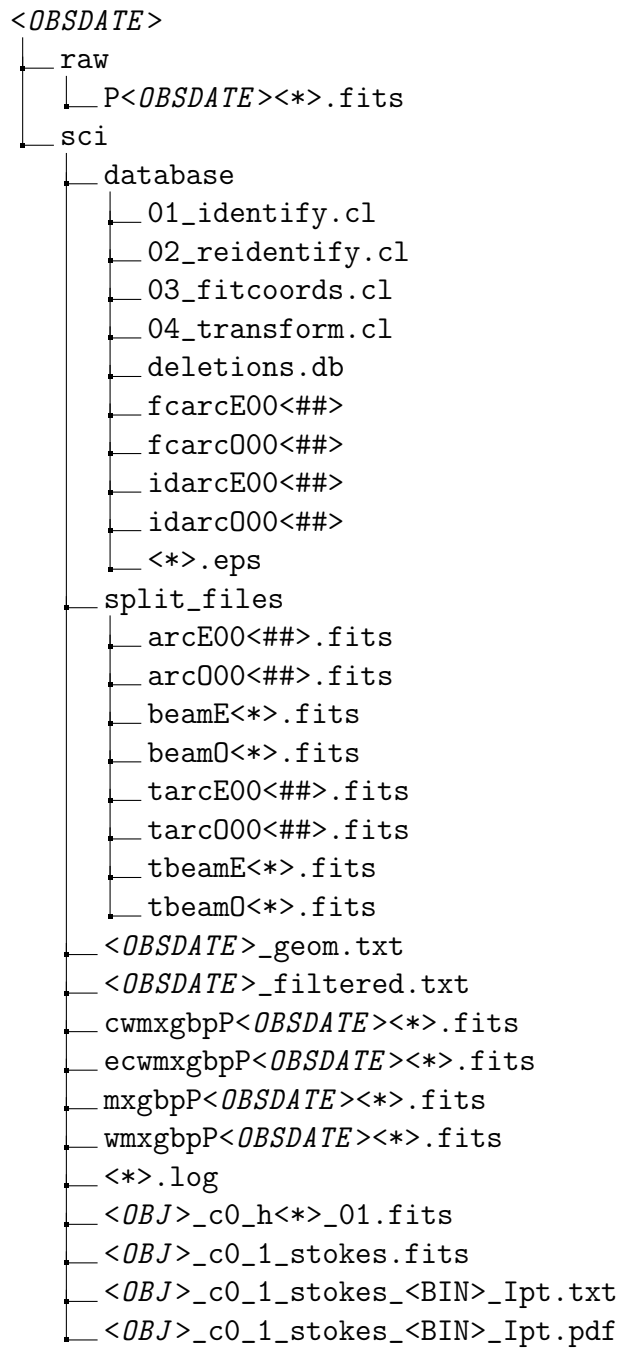


Figure A.2: The typical file structure after completing the reduction process.

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**

```
"""Argument parser for STOPS."""

#!/usr/bin/env python3
# -*- coding: utf-8 -*-

from __init__ import __version__, __author__, __email__

# MARK: Imports
import os
import sys
import argparse
import logging
from pathlib import Path

from split import Split
from join import Join
from cross_correlate import CrossCorrelate
from skylines import Skylines

from utils import ParserUtils as pu
from utils.Constants import SPLIT_ROW, PREFIX, PARSE, SAVE_CORR,
↪ SAVE_SKY

# MARK: Constants
PROG = "STOPS"
DESCRIPTION = """
Supplementary TOols for Polsalt Spectropolarimetry (STOPS) is a
collection of supplementary tools created for SALT's POLSALT pipeline,
allowing for wavelength calibrations with IRAF. The tools provide
support for splitting and joining polsalt formatted data as well as
cross correlating complementary polarimetric beams.

DOI: 10.22323/1.401.0056
```

```
"""


# MARK: Universal Parser
parser = argparse.ArgumentParser(
    prog=PROG,
    description=DESCRIPTION,
    formatter_class=argparse.RawDescriptionHelpFormatter,
)
parser.add_argument(
    "-V",
    "--version",
    action="version",
    version=f"%(prog)s as of {__version__}",
)
parser.add_argument(
    "-v",
    "--verbose",
    action="count",
    default=PARSE['VERBOSE'],
    help=(
        "Counter flag which enables and increases verbosity. "
        "Use -v or -vv for greater verbosity levels."
    ),
)
parser.add_argument(
    "-l",
    "--log",
    action="store",
    type=pu.parse_logfile,
    help=(
        "Filename of the logging file. "
        "File is created if it does not exist. Defaults to None."
    ),
)
parser.add_argument(
    "data_dir",
    action="store",
    nargs="?",
    default=PARSE['DATA_DIR'],
    type=pu.parse_path,
    help=(
        "Path of the directory which contains the working data. "
        f"Defaults to the cwd -> `{PARSE['DATA_DIR']}` (I.E. '.')."
    ),
)


# MARK: Split\Join Parent
split_join_args = argparse.ArgumentParser(add_help=False)
split_join_args.add_argument(
    "-n",
    "--no_arc",
    action="store_true",
    help="Flag to exclude arc files from processing.",
)
split_join_args.add_argument(
    "-s",
```

```
    "--split_row",
    default=SPLIT_ROW,
    type=int,
    help=(
        "Row along which the O and E beams are split. "
        f"Defaults to polsalt's default -> {SPLIT_ROW}."
    ),
)
split_join_args.add_argument(
    "-p",
    "--save_prefix",
    nargs=2,
    default=PREFIX,
    help=(
        "Prefix appended to the filenames, "
        "with which the O and E beams are saved. "
        f"Defaults to {PREFIX}."
    ),
)


# MARK: Correlate\Skylines Parent
corr_sky_args = argparse.ArgumentParser(add_help=False)
corr_sky_args.add_argument(
    "filenames",
    action="store",
    nargs="+",
    type=pu.parse_file,
    help=(
        "File name(s) of FITS file(s) to be processed."
        "A minimum of one filename is required."
    ),
)
corr_sky_args.add_argument(
    "-b",
    "--beams",
    choices=["O", "E", "OE"],
    type=str.upper,
    default=PARSE['BEAMS'],
    help=(
        "Beams to process. "
        f"Defaults to {PARSE['BEAMS']}, but "
        "may be given 'O', 'E', or 'OE' to "
        "determine which beams are processed."
    ),
)
corr_sky_args.add_argument(
    "-ccd",
    "--split_ccd",
    action="store_false",
    help=(
        "Flag to NOT split CCD's. "
        "Recommended to leave off unless the chip gaps "
        "have been removed from the data."
    ),
)
corr_sky_args.add_argument(
    "-c",
```

```
    "--continuum_order",
    type=int,
    default=PARSE['CONT_ORD'],
    dest="cont_ord",
    help=(
        "Order of continuum to remove from spectra. "
        "Higher orders recommended to remove most variation, "
        "leaving only significant features."
    ),
)
corr_sky_args.add_argument(
    "-p",
    "--plot",
    action="store_true",
    help="Flag for additional plot outputs.",
)
corr_sky_args.add_argument(
    "-s",
    "--save_prefix",
    action="store",
    nargs="?",
    type=lambda path: Path(path).expanduser().resolve(),
    const=SAVE_CORR,
    help=(
        "Prefix used when saving plot. "
        "Excluding flag does not save output plot, "
        f"flag usage of option uses default prefix, "
        "and a provided prefix overwrites default prefix."
    ),
)


# MARK: Create subparser modes
subparsers = parser.add_subparsers(
    dest="mode",
    help="Operational mode of supplementary tools",
)


# MARK: Split Subparser
split_parser = subparsers.add_parser(
    "split",
    aliases=["s"],
    help="Split mode",
    parents=[split_join_args],
)
# 'children' split args here
# Change defaults here
split_parser.set_defaults(
    mode="split",
    func=Split,
)


# MARK: Join Subparser
join_parser = subparsers.add_parser(
    "join",
    aliases=["j"],
```

```
    help="Join mode",
    parents=[split_join_args],
)
# 'children' join args here
join_parser.add_argument(
    "-c",
    "--coefficients",
    dest="solutions_list",
    nargs='*',
    type=pu.parse_file,
    help=(
        "Custom coefficients to use instead of the `IRAF` fitcoords "
        "database. Use as either '-c <o_solution> <e_solution>' or "
        "a regex descriptor '-c <*solution*extention>'."
    ),
)
# Change defaults here
join_parser.set_defaults(
    mode="join",
    func=Join,
)


# MARK: Correlate Subparser
corr_parser = subparsers.add_parser(
    "correlate",
    aliases=["x"],
    help="Cross correlation mode",
    parents=[corr_sky_args],
)
# 'children' join args here
corr_parser.add_argument(
    "-o",
    "--offset",
    type=int,
    default=PARSE['OFFSET'],
    help=(
        "Introduces an offset when correcting for "
        "known offset in spectra or for testing purposes. "
        f"Defaults to {PARSE['OFFSET']}. "
        "(For testing, not used during regular operation.)"
    ),
)
# Change defaults here
corr_parser.set_defaults(
    mode="correlate",
    func=CrossCorrelate,
)


# MARK: Skyline Subparser
sky_parser = subparsers.add_parser(
    "skylines",
    aliases=["sky"],
    help="Sky line check mode",
    parents=[corr_sky_args],
)
# 'children' skyline args here
```

```
sky_parser.add_argument(
    "-t",
    "--transform",
    action="store_false",
    help=(
        "Flag to force transform images. "
        "Recommended to use only when input image(s) "
        "are prefixed 't' but are not yet transformed."
    ),
)
# Change defaults here
sky_parser.set_defaults(
    mode="skyline",
    func=Skylines,
)


# MARK: Keyword Clean Up
args = parser.parse_args()

if len(sys.argv) == 1:
    parser.print_help(sys.stderr)
    sys.exit(2)

args.verbose = pu.parse_loglevel(args.verbose)

if 'log' in args and args.log not in ["", None]:
    args.log = args.data_dir / args.log

if "filenames" in args:
    args.filenames = pu.flatten(args.filenames)

if "solutions_list" in args and type(args.solutions_list) == list:
    args.solutions_list = pu.flatten(args.solutions_list)

# MARK: Begin logging
logging.basicConfig(
    filename=args.log,
    format="%(asctime)s - %(module)s - %(levelname)s - %(message)s",
    datefmt="%Y-%m-%d %H:%M:%S",
    level=args.verbose,
)

# MARK: Call Relevant Class(Args)
logging.debug(f"Argparse namespace: {args}")
logging.info(f"Mode:{args.mode}")
args.func(**vars(args)).process()


# Confirm all processes completed and exit without error
logging.info("All done! Come again!\n")
```

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

```
#!/usr/bin/env python3
# -*- coding: utf-8 -*-

"""Module for splitting ``polsalt`` FITS files."""

from __init__ import __author__, __email__, __version__

# MARK: Imports
import os
import sys
import logging
from copy import deepcopy
from pathlib import Path

import numpy as np
from astropy.io import fits as pyfits

from utils.SharedUtils import find_files, find_arc
from utils.Constants import SAVE_PREFIX, CROP_DEFAULT, SPLIT_ROW


# MARK: Split Class
class Split:
    #----------split0----------

    """
    The `Split` class allows for the splitting of `polsalt` FITS files
    based on the polarization beam. The FITS files must have basic
    `polsalt` pre-reductions already applied (`mxgbp...` FITS files).

    Parameters
    ----------
    data_dir : str | Path
        The path to the data to be split
    fits_list : list[str], optional
        A list of pre-reduced `polsalt` FITS files to be split within `
        ↪ data_dir`.
        (The default is None, `Split` will search for `mxgbp*.fits`
        ↪ files)
    split_row : int, optional
        The row along which to split the data of each extension in the
        ↪ FITS file.
        (The default is SPLIT_ROW (See Notes), the SALT RSS CCD's
        ↪ middle row)
    no_arc : bool, optional
        Decides whether the arc frames should be recombined.
        (The default is False, `polsalt` has no use for the arc after
        ↪ wavelength calibrations)
    save_prefix : dict[str, list[str]], optional
        The prefix with which to save the  O & E beams.
        Setting `save_prefix` = ``None`` does not save the split O & E
        ↪ beams.
        (The default is SAVE_PREFIX (See Notes))

    Attributes
    ----------
```

```
    arc : str
        Name of arc FITS file within `data_dir`.
        `arc` = `""` if `no_arc` or not detected in `data_dir`.
    o_files, e_files : list[str]
        A list of the `O`- and `E`-beam FITS file names.
        The first entry is the arc file if `arc` defined.
    data_dir
    fits_list
    split_row
    save_prefix

    Methods
    -------
    split_file(file: os.PathLike)
        -> tuple[astropy.io.fits.HDUList]
        Handles creation and saving the separated FITS files
    split_ext(hdulist: astropy.io.fits.HDUList, ext: str = 'SCI')
        -> astropy.io.fits.HDUList
        Splits the data in the `ext` extension along the `split_row`
    crop_file(hdulist: astropy.io.fits.HDUList, crop: int =
    ↪ CROP_DEFAULT (See Notes))
        -> tuple[numpy.ndarray]
        Crops the data along the edge of the frame, that is,
        `O`-beam cropped as [crop:], and
        `E`-beam cropped as [:-crop].
    update_beam_lists(o_name: str, e_name: str)
        -> None
        Updates `o_files` and `e_files`.
    save_beam_lists(file_suffix: str = 'frames')
        -> None
        Creates (Overwrites if exists) and writes the `o_files` and `
        ↪ e_files` to files named
        `o_{file_suffix}` and `e_{file_suffix}`, respectively.
    process()
        -> None
        Calls `split_file` and `save_beam_lists` on each file in `
        ↪ fits_list` for automation.

    Other Parameters
    ----------------
    **kwargs : dict
        keyword arguments. Allows for passing unpacked dictionary to
        ↪ the class constructor.

    Notes
    -----
    Constants Imported (See utils.Constants):
        SAVE_PREFIX
        CROP_DEFAULT
        SPLIT_ROW

    """

    #----------split1----------

    # MARK: Split init
    def __init__(
            self,
```

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

```
            # o_beam[0].data = raw_split['SCI'].data[1]
            # e_beam[0].data = raw_split['SCI'].data[0]
            o_beam[0].data, e_beam[0].data = self.crop_file(raw_split)

            # Handle prefix and names
            pref = "arc" if file == self.arc else "beam"
            o_name = self.save_prefix[pref][0] + file.name[-9:]
            e_name = self.save_prefix[pref][1] + file.name[-9:]

            # Add split data to O & E beam lists
            self.update_beam_lists(o_name, e_name, pref == "arc")

            # Handle don't save case
            if self.save_prefix is None:
                return o_beam, e_beam

            # Handle save case
            o_beam.writeto(o_name, overwrite=True)
            e_beam.writeto(e_name, overwrite=True)

            return o_beam, e_beam

    # MARK: Split extensions
    def split_ext(
            self,
            hdulist: pyfits.HDUList,
            ext: str = "SCI"
    ) -> pyfits.HDUList:
        """
        Split the data of the specified extension of `hdulist` into
        its `O`- and `E`- beams.

        Parameters
        ----------
        hdulist : astropy.io.fits.HDUList
            The FITS HDUList to be split.
        ext : str, optional
            The name of the extension to be split.
            (Defaults to 'SCI')

        Returns
        -------
        astropy.io.fits.HDUList
            The HDUList with the split applied.

        """
        hdu = deepcopy(hdulist)
        rows, cols = hdu[ext].data.shape

        # if odd number of rows, strip off the last one
        rows = int(rows / 2) * 2

        # how far split is from center of detector
        offset = int(self.split_row - rows / 2)

        # split arc into o/e images
        ind_rc = np.indices((rows, cols))[0]
        padbins = (ind_rc < offset) | (ind_rc > rows + offset)
```

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

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

Listing B.3: The source code for **join.py**

```
#!/usr/bin/env python3
# -*- coding: utf-8 -*-

"""Module for joining the split FITS files with an external wavelength solution."""

from __init__ import __author__, __email__, __version__

# MARK: Imports
import os
import sys
import logging
import re
from pathlib import Path

import numpy as np
from numpy.polynomial.chebyshev import chebgrid2d as chebgrid2d
from numpy.polynomial.legendre import leggrid2d as leggrid2d
from astropy.io import fits as pyfits

# from lacosmic import lacosmic # Replaced: ccdproc is ~6x faster
from ccdproc import cosmicray_lacosmic as lacosmic

from utils.specpolpy3 import read_wollaston, split_sci
from utils.SharedUtils import find_files, find_arc
from utils.Constants import DATADIR, SAVE_PREFIX, SPLIT_ROW, CR_PARAMS


# MARK: Join Class
class Join:
    #----------join0----------

    """
    The `Join` class allows for the joining of previously split files and the
    appending of an external wavelength solution in the `polsalt` FITS file format.

    Parameters
    ----------
    data_dir : str | Path
        The path to the data to be joined
    database : str, optional
        The name of the `IRAF` database folder.
        (The default is "database")
    fits_list : list[str], optional
        A list of pre-reduced `polsalt` FITS files to be joined within `data_dir`.
        (The default is ``None``, `Join` will search for `mxgbp*.fits` files)
    solutions_list: list[str], optional
        A list of solution filenames from which the wavelength solution is created.
        (The default is ``None``, `Join` will search for `fc*` files within the `database` directory)
    split_row : int, optional
```

```
        The row along which the data of each extension in the FITS file
        ↪ was split.
        Necessary when Joining cropped files.
        (The default is 517, the SALT RSS CCD's middle row)
    save_prefix : dict[str, list[str]], optional
        The prefix with which the previously split `O`- & `E`-beams
        ↪ were saved.
        Used for detecting if cropping was applied during the splitting
        ↪ procedure.
        (The default is SAVE_PREFIX (See Notes))
    verbose : int, optional
        The level of verbosity to use for the Cosmic ray rejection
        (The default is 30, I.E. logging.INFO)

    Attributes
    ----------
    fc_files : list[str]
        Valid solutions found from `solutions_list`.
    custom : bool
        Internal flag for whether `solutions_list` uses the `IRAF` or a
        ↪ custom format.
        See Notes for custom solution formatting.
        (Default (inherited from `solutions_list`) is False)
    arc : str
        Deprecated. Name of arc FITS file within `data_dir`.
    data_dir
    database
    fits_list
    split_row
    save_prefix


    Methods
    -------
    get_solutions(wavlist: list | None, prefix: str = "fc") ->
    ↪ (fc_files, custom): tuple[list[str], bool]
        Parse `solutions_list` and return valid solution files and if
        ↪ they are non-`IRAF` solutions.
    parse_solution(fc_file: str, x_shape: int, y_shape: int) ->
    ↪ tuple[dict[str, int], np.ndarray]
        Loads the wavelength solution file and parses keywords
        ↪ necessary for creating the wavelength extension.
    join_file(file: os.PathLike) -> None
        Joins the files,
        attaches the wavelength solutions,
        performs cosmic ray cleaning,
        masks the extension,
        and checks cropping performed in `Split`.
        Writes the FITS file in a `polsalt` valid format.
    check_crop(hdu: pyfits.HDUList, o_file: str, e_file: str) -> int
        Opens the split `O`- and `E`-beam FITS files and returns the
        ↪ amount of cropping that was performed.
    process() -> None
        Calls `join_file` on each file in `fits_list` for automation.


    Other Parameters
    ----------------
```

```
    no_arc : bool, optional
        Deprecated. Decides whether the arc frames should be processed.
        (The default is False, `polsalt` has no use for the arc after
        ↪ wavelength calibrations)
    **kwargs : dict
        keyword arguments. Allows for passing unpacked dictionary to
        ↪ the class constructor.

    Notes
    -----
    Constants Imported (See utils.Constants):
        DATADIR, SAVE_PREFIX, SPLIT_ROW, CR_PARAMS

    Custom wavelength solutions must be formatted containing:
        `x`, `y`, *coefficients...
    where a solution are of order (`x` by `y`) and must contain x*y
    ↪ coefficients,
    all separated by newlines. The name of the custom wavelength
    ↪ solution file
    must contain either "cheb" or "leg" for Chebyshev or Legendre
    wavelength solutions, respectively.

    Cosmic ray rejection is performed using lacosmic [1]_ implemented
    ↪ in ccdproc via astroscrappy [2]_.

    References
    ----------
    .. [1] van Dokkum 2001, PASP, 113, 789, 1420 (article :
    ↪ https://adsabs.harvard.edu/abs/2001PASP..113.1420V)
    .. [2] https://zenodo.org/records/1482019

    """

    #----------join1----------

    # MARK: Join init
    def __init__(
            self,
            data_dir: Path,
            database: str = "database",
            fits_list: list[str] = None,
            solutions_list: list[Path] = None,
            split_row: int = SPLIT_ROW,
            no_arc: bool = True,
            save_prefix: Path | None = None,
            verbose: int = 30,
            **kwargs,
    ) -> None:
        self.data_dir = data_dir
        self.database = Path(data_dir) / database
        self.fits_list = find_files(
            data_dir=self.data_dir,
            filenames=fits_list,
            prefix="mxgbp",
            ext="fits",
        )
        self.fc_files, self.custom = self.get_solutions(solutions_list)
        self.split_row = split_row
```

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

```
                    f"dir.: {self.database}"
                )
                logging.error(msg)
                raise FileNotFoundError(msg)

            sols = {
                i: j for i, j in zip(['O', 'E'], sorted(ws,
                ↪ reverse=reverse))
            }
            logging.debug(f"get_solutions - Found {sols} in
            ↪ {self.database}")

            return sorted(ws, reverse=reverse), False

        # Custom solution
        if len(wavlist) >= 2:
            if len(wavlist) > 2:
                logging.warning(f" Too many solutions, only
                ↪ {wavlist[:2]} are considered")
                wavlist = wavlist[:2]

            for fl in wavlist:
                if not os.path.isfile(os.path.join(self.data_dir, fl)):
                    msg = (
                        f"{fl} not found in the "
                        f"data directory {self.data_dir}"
                    )
                    logging.error(msg)
                    raise FileNotFoundError(msg)

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

            return sorted(wavlist, reverse=reverse), True

    # MARK: Parse 2D WAV Function
    def parse_solution(
            self,
            fc_file: str,
            x_shape: int,
            y_shape: int
    ) -> tuple[dict[str, int], np.ndarray]:
        """
        Parse the 2D wavelength solution function from `fc_file`.

        Parameters
        ----------
        fc_file : str
            The filename of the wavelength solutions file.
        x_shape : int
            The x-order of the 2D solution.
        y_shape : int
            The y-order of the 2D solution.

```

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

```
316             coeff = np.reshape(
317                 coeff,
318                 (fit_params["xorder"], fit_params["yorder"])
319             )
320 
321             return fit_params, coeff
322 
323         # MARK: Join Files
324         def join_file(self, file: os.PathLike) -> None:
325             """
326             Join the `O`- and `E`-beams, attach the wavelength solutions,
327             perform cosmic ray cleaning, mask the extensions,
328             and checks cropping performed by `Split`.
329             Write the FITS file in a `polsalt` valid format.
330 
331             Parameters
332             ----------
333             file : os.PathLike
334                 The path of the FITS file to be joined.
335 
336             See Also
337             --------
338             IRAF - `fitcoords` task
339                 https://iraf.net/irafdocs/formats/fitcoords.php,
340             numpy 2D grid functions
341                 https://numpy.org/doc/stable/reference/generated/numpy
342                 Chebyshev: + '.polynomial.chebyshev.chebgrid2d.html'
343                 Legendre: + '.polynomial.legendre.leggrid2d.html'
344 
345             """
346             # Create empty wavelength appended hdu list
347             whdu = pyfits.HDUList()
348 
349             # Handle prefix and names
350             pref = "arc" if file == self.arc else "beam"
351             o_file = self.save_prefix[pref][0] + file.name[-9:]
352             e_file = self.save_prefix[pref][1] + file.name[-9:]
353 
354             # Open file
355             with pyfits.open(file) as hdu:
356                 # Check if file has been cropped
357                 cropsize = self.check_crop(hdu, o_file, e_file)
358 
359                 y_shape = int(hdu["SCI"].data.shape[0] / 2) - cropsize
360                 x_shape = hdu["SCI"].data.shape[1]
361 
362                 # No differences in "PRIMARY" extention header
363                 primary_ext = hdu["PRIMARY"]
364                 whdu.append(primary_ext)
365 
366                 for ext in ["SCI", "VAR", "BPM"]:
367                     whdu.append(pyfits.ImageHDU(name=ext))
368                     whdu[ext].header = hdu[ext].header.copy()
369                     whdu[ext].header["CTYPE3"] = "O,E"
370 
371                     # Create empty extentions with correct order and format
372                     if ext == "BPM":
373                         whdu[ext].data = np.zeros(
```

```
                        (2, y_shape, x_shape),
                        dtype="uint8"
                    )
                    whdu[ext].header["BITPIX"] = "-uint8"
                else:
                    whdu[ext].data = np.zeros(
                        (2, y_shape, x_shape),
                        dtype=">f4"
                    )
                    whdu[ext].header["BITPIX"] = "-32"

                # Fill in empty extentions
                if cropsize:
                    temp_split = split_sci(
                        hdu,
                        self.split_row,
                        ext=ext
                    )[ext].data
                    whdu[ext].data[0] = temp_split[0, cropsize:]
                    whdu[ext].data[1] = temp_split[1, 0:-cropsize]

                else:
                    whdu[ext].data = split_sci(
                        hdu,
                        self.split_row,
                        ext=ext
                    )[ext].data
        # End of hdu calls, close hdu

        # MARK: Join (Wav. Ext.)
        whdu.append(pyfits.ImageHDU(name="WAV"))
        wav_header = whdu["SCI"].header.copy()
        wav_header["EXTNAME"] = "WAV"
        wav_header["CTYPE3"] = "0,E"
        whdu["WAV"].header = wav_header

        whdu["WAV"].data = np.zeros(
            whdu["SCI"].data.shape,
            dtype=">f4"
        )

        for num, fname in enumerate(self.fc_files):
            params, coeffs = self.parse_solution(
                fname,
                x_shape,
                y_shape
            )

            if params["function"] == 1:  # Function type (1 = chebyshev)
                # Set wavelength extention values to function
                whdu["WAV"].data[num] = chebgrid2d(
                    x=np.linspace(-1, 1, params["ymax"]),
                    y=np.linspace(-1, 1, params["xmax"]),
                    c=coeffs,
                )

            elif params["function"] == 2:  # Function type (2 =
            ↪ legendre)
```

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

```
                whdu["WAV"].data[1, int(col) + cropsize:, c] = 0.0

        # MARK: BPM masking
        whdu["BPM"].data[0] = np.where(
            whdu["WAV"].data[0] == 0,
            1,
            whdu["BPM"].data[0]
        )
        whdu["BPM"].data[1] = np.where(
            whdu["WAV"].data[1] == 0,
            1,
            whdu["BPM"].data[1]
        )

        whdu.writeto(f"w{os.path.basename(file)}", overwrite="True")

        return

    # MARK: Check Crop
    @staticmethod
    def check_crop(
            hdu: pyfits.HDUList,
            o_file: str,
            e_file: str
    ) -> int:
        """
        Check if cropping is necessary when joining `O`- and `E`-beams.

        Parameters
        ----------
        hdu : astropy.io.fits.HDUList
            The HDUList to check for cropping.
        o_file : str
            The name of the previously split `O`-beam FITS file.
        e_file : str
            The name of the previously split `E`-beam FITS file.

        Returns
        -------
        int
            The number of rows which were cropped by `Split`.

        """
        cropsize = 0

        with pyfits.open(o_file) as o, \
                pyfits.open(e_file) as e:
            o_y = o[0].data.shape[0]
            e_y = e[0].data.shape[0]

        if hdu["SCI"].data.shape[0] != (o_y + e_y):
            # Get crop size, assuming crop same on both sides
            cropsize = int((hdu["SCI"].data.shape[0] - o_y - e_y) / 2)

        return cropsize

    # MARK: Process all Listed Images
    def process(self) -> None:
```

```
547         """Process all FITS images stored in the `fits_list`
        ↪ attribute"""
548         for target in self.fits_list:
549             logging.debug(f"Processing {target}")
550             self.join_file(target)
551 
552         return
553 
554 
555 def main(argv) -> None:
556     """Main function."""
557 
558     return
559 
560 
561 if __name__ == "__main__":
562     main(sys.argv[1:])
```

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

```
#!/usr/bin/env python3
# -*- coding: utf-8 -*-

"""Module for cross correlating polarization beams."""

from __init__ import __author__, __email__, __version__

# MARK: Imports
import sys
import logging
import itertools as iters
from pathlib import Path
from typing import Callable

import numpy as np
from numpy.polynomial import chebyshev
import matplotlib.pyplot as plt
import matplotlib.axes
from astropy.io import fits as pyfits
from scipy import signal

from utils.SharedUtils import find_files, continuum
from utils.Constants import SAVE_CORR

OFFSET = 0.3

mpl_logger = logging.getLogger('matplotlib')
mpl_logger.setLevel(logging.INFO)


# MARK: Correlate class
class CrossCorrelate:

    #----------corr0----------

    """
    Cross correlate allows for comparing the extensions of multiple
    FITS files, or comparing the O and E beams of a single FITS file.

    Parameters
    ----------
    data_dir : str | Path
        The path to the data to be cross correlated
    filenames : list[str]
        The ecwmxgbp*.fits files to be cross correlated.
        If only one filename is defined, correlation is done against
        ↪ the two polarization beams.
    split_ccd : bool, optional
        Decides whether the CCD regions should each be individually
        ↪ cross correlated.
        (The default is True, which splits the spectrum up into its
        ↪ separate CCD regions)
    cont_ord : int, optional
        The degree of a chebyshev to fit to the continuum.
        (The default is 11)
    plot : bool, optional
```

```
54          Decides whether the continuum fitting should be plotted
55          (The default is False, so no continua plots are displayed)
56      save_prefix : str, optional
57          The name or directory to save the figure produced to.
58          "." saves a default name to the current working. A default name
            ↪ is also used when save_prefix is a directory.
59          (The default is None, I.E. The figure is not saved, only
            ↪ displayed)
60
61      Attributes
62      ----------
63      data_dir
64      fits_list
65      beams : str
66          The mode of correlation.
67          'OE' for same file, and 'O' or 'E' for different files but same
            ↪ extension.
68      ccds : int
69          The number of CCD's in the data. Used to split the CCD's if
            ↪ split_ccd is True.
70      cont_ord : int
71          The degree of the chebyshev to fit to the continuum.
72      can_plot : bool
73          Decides whether the continuum fitting should be plotted
74      offset : int
75          The amount the spectrum is shifted, mainly to test the effect
            ↪ of the cross correlation
76          (The default is 0, I.E. no offset introduced)
77      save_prefix
78      wav_unit : str
79          The units of the wavelength axis.
80          (The default is Angstroms)
81      wav_cdelt : int
82          The wavelength increment.
83          (The default is 1)
84      alt : Callable
85          An alternate method of cross correlating the data.
86          (The default is None)
87
88      Methods
89      -------
90      load_file(filename: Path) -> tuple[np.ndarray, np.ndarray,
        ↪ np.ndarray]
91          Loads the data from a FITS file.
92      get_bounds(bpm: np.ndarray) -> np.ndarray
93          Finds the bounds for the CCD regions.
94      remove_cont(spec: list, wav: list, bpm: list, plot_cont: bool) ->
        ↪ None
95          Removes the continuum from the data.
96      correlate(filename1: Path, filename2: Path | None = None) -> None
97          Cross correlates the data.
98      ftcs(filename1: Path, filename2: Path | None = None) -> None
99          Cross correlates the data using the Fourier Transform.
100     plot(spec, wav, bpm, corrdb, lagsdb) -> None
101         Plots the data.
102     process() -> None
103         Processes the data.
104
```

```
    Other Parameters
    ----------------
    offset : int, optional
        The amount the spectrum is shifted, mainly to test the effect
        ↪ of the cross correlation
        (The default is 0, I.E. no offset introduced)
    **kwargs : dict
        keyword arguments. Allows for passing unpacked dictionary to
        ↪ the class constructor.
        ftcs : bool, optional
            Decides whether the Fourier Transform should be used for
            ↪ cross correlation.

    See Also
    --------
    scipy
        https://docs.scipy.org/doc/scipy/reference/generated/
        correlation: scipy.signal.correlate.html


    Notes
    -----
    Constants Imported (See utils.Constants):
        SAVE_CORR

    """

    #----------corr1----------

    # MARK: Correlate init
    def __init__(
            self,
            data_dir: Path,
            filenames: list[str],
            beams: str = "OE",
            split_ccd: bool = True,
            cont_ord: int = 11,
            plot: bool = False,
            offset: int = 0,
            save_prefix: Path | None = None,
            **kwargs
    ) -> None:
        self.data_dir = data_dir
        self.fits_list = find_files(
            data_dir=self.data_dir,
            filenames=filenames,
            prefix="ecwmxgbp",
            ext="fits",
        )
        self._beams = None
        self.beams = beams
        self.ccds = 1
        if split_ccd:
            # BPM == 2 near center of CCD if CCD count varies
            with pyfits.open(self.fits_list[0]) as hdu:
                self.ccds = sum(hdu["BPM"].data.sum(axis=1)[0] == 2)

        self.cont_ord = cont_ord
```

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

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

```
                min(mid + bpm.shape[-1] // ccds, bpm.shape[-1])
            )

        return bounds.astype(int)

    # MARK: Remove Continua
    def remove_cont(
            self,
            spec: np.ndarray,
            wav: np.ndarray,
            bpm: np.ndarray,
            plot_cont: bool
    ) -> np.ndarray:
        """
        Remove the continuum from the data.

        Parameters
        ----------
        spec : np.ndarray
            The spectrum to remove the continuum from.
        wav : np.ndarray
            The wavelength of the spectrum.
        bpm : np.ndarray
            The bad pixel mask.
        plot_cont : bool
            Decides whether the continuum fitting should be plotted

        Returns
        -------
        spec : np.ndarray

        """
        # Mask out the bad pixels for fitting continua
        okwav = np.where(bpm != 1)

        # Define continua
        ctm = continuum(
            wav[okwav],
            spec[okwav],
            deg=self.cont_ord,
            plot=plot_cont,
        )

        # Normalise spectra
        spec /= chebyshev.chebval(wav, ctm)
        spec -= 1

        return spec

    # MARK: Correlate
    def correlate(
            self,
            filename1: Path,
            filename2: Path | None = None,
            alt: Callable = None
    ) -> tuple[np.ndarray, np.ndarray, np.ndarray, list[list],
    ↪ list[list]]:
        """
```

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

```
                # Invert BPM (and account for 2); zero bad pixels
                sig.append((
                        spec[ext, lb:ub]
                        * abs(bpm[ext, lb:ub] * -1 + 1)
                ))

            # Finally(!!!) cross correlate signals and scale max -> 1
            corrdb[ccd] = signal.correlate(*sig) if not alt else
            ↪ alt(*sig)
            corrdb[ccd] /= np.max(corrdb[ccd])
            # noinspection PyTypeChecker
            lagsdb[ccd] = signal.correlation_lags(
                sig[0].shape[-1],
                sig[1].shape[-1]
            ) * self.wav_cdelt

        return spec, wav, bpm, corrdb, lagsdb

    # MARK: ftcs alternate
    def ftcs(
            self,
            signal1: np.ndarray,
            signal2: np.ndarray
    ) -> np.ndarray:
        """
        Cross correlates the data using the Fourier Transform.

        Parameters
        ----------
        signal1 : np.ndarray
            The first signal to cross correlate.
        signal2 : np.ndarray
            The second signal to cross correlate.

        Returns
        -------
        np.ndarray
            The correlation data using the Fourier Transform.

        """
        logging.debug(
            f"ftcs - data shape:\n\tspec/wav/bpm: {signal1.shape}"
        )

        # Invert BPM (and account for 2); zero bad pixels
        ft_spec1 = np.fft.fft(signal1)
        ft_spec2 = np.fft.fft(signal2)

        if self.can_plot:
            plt.plot(ft_spec1)
            plt.plot(ft_spec2)
            plt.show()

        # Cross correlate signals
        # ft_spectrum1 * np.conj(ft_spectrum2)
        corr_entry = signal.correlate(ft_spec1, ft_spec2)

        return np.fft.ifft(corr_entry)
```

```
446
447     # MARK: Plot
448     def plot(self, spec, wav, bpm, corrdb, lagsdb) -> None:
449         """
450         Plot the data.
451
452         Parameters
453         ----------
454         spec : np.ndarray
455             The spectrum.
456         wav : np.ndarray
457             The wavelength.
458         bpm : np.ndarray
459             The bad pixel mask.
460         corrdb : np.ndarray
461             The cross correlation data.
462         lagsdb : np.ndarray
463             The `lags` data.
464
465         Returns
466         -------
467         None
468
469         """
470         plt.style.use([
471             Path(__file__).parent.resolve() / 'utils/STOPS.mplstyle',
472             Path(__file__).parent.resolve() /
                ↪ 'utils/STOPS_correlate.mplstyle'
473         ])
474         bounds = self.get_bounds(bpm)
475
476         fig, axs = plt.subplots(2, self.ccds, sharey="row")
477
478         if self.ccds == 1:
479             # Convert axs to a 2D array
480             # noinspection PyTypeChecker
481             axs: np.ndarray[matplotlib.axes.Axes] =
                ↪ np.swapaxes(np.atleast_2d(axs), 0, 1)
482
483         # for ext, ccd in iters.product(range(2), range(self.ccds)):
484
485         for ccd in range(self.ccds):
486             axs[0, ccd].plot(
487                 lagsdb[ccd],
488                 corrdb[ccd] * 100,
489                 color='C4',
490                 label=f"max lag @ {lagsdb[ccd][corrdb[ccd].argmax()] -
                    ↪ (bounds[1, ccd, 0] - bounds[0, ccd, 0])}",
491             )
492
493             for ext in range(2):
494                 lb, ub = bounds[ext, ccd]
495                 logging.debug(f"fl-{ext}: {wav[ext, lb]}:{wav[ext, ub -
                    ↪ 1]}")
496
497                 axs[1, ccd].plot(
498                     wav[ext, lb:ub],
499                     spec[ext, lb:ub] * abs(bpm[ext, lb:ub] * -1 + 1) +
```

```
                    ↪ OFFSET * ext,
                    label=(
                        f"${self.beams if self.beams != 'OE' else
                        ↪ self.beams[ext]}"
                        f"_{ext + 1 if self.beams != 'OE' else 1}$"
                        f"{(' (+' + str(OFFSET * ext) + ')') if ext > 0
                        ↪ else ''}"
                    ),
                )

        axs[0, 0].set_ylabel("Normalised Correlation\n(\%)")
        for ax in axs[1:, 0]:
            ax.set_ylabel("Normalised Intensity\n(Counts)")
        xcol = int(self.ccds != 1)
        axs[0, xcol].set_xlabel(f"Signal Lag ({self.wav_unit})")
        axs[-1, xcol].set_xlabel(f"Wavelength ({self.wav_unit})")
        for ax in axs.flatten():
            leg = ax.legend()
            leg.set_draggable(True)

        # plt.tight_layout()
        # fig1 = plt.gcf()
        # DPI = fig1.get_dpi()
        # fig1.set_size_inches(700.0/float(DPI), 250.0/float(DPI))
        plt.show()

        # Handle do not save
        if not self.save_prefix:
            return

        # Handle save
        fig.savefig(fname=self.save_prefix)

        return

    # MARK: Process all listed images
    def process(self) -> None:
        """
        Process the data.

        Returns
        -------
        None

        """
        if self.beams != 'OE' and len(self.fits_list) == 1:
            # change mode to OE with warning
            logging.warning((
                f"`{self.beams}` correlation not possible for "
                "a single file. correlation `mode` changed to 'OE'."
            ))
            self.beams = 'OE'

        # OE `mode` (same file, diff. ext.)
        if self.beams == 'OE':
            for fl in self.fits_list:
                logging.info(f"'OE' correlation of {fl}.")
                spec, wav, bpm, corr, lags = self.correlate(fl,
```

```
                ↪ alt=self.alt)
555             self.plot(spec, wav, bpm, corr, lags)
556
557         return
558
559     # O|E `mode` (diff. files, same ext.)
560     for fl1, fl2 in iters.combinations(self.fits_list, 2):
561         logging.info(f"{self.beams} correlation of {fl1} vs {fl2}.")
562         spec, wav, bpm, corr, lags = self.correlate(fl1, fl2,
            ↪ alt=self.alt)
563         self.plot(spec, wav, bpm, corr, lags)
564
565     return
566
567
568 # MARK: Main function
569 def main(argv) -> None:
570     return
571
572
573 if __name__ == "__main__":
574     main(sys.argv[1:])
```

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

```python
#!/usr/bin/env python3
# -*- coding: utf-8 -*-

"""
Module for analyzing the sky lines of a wavelength calibrated image.
"""

from __init__ import __author__, __email__, __version__

# MARK: Imports
import sys
import logging
from pathlib import Path

import numpy as np
import matplotlib.pyplot as plt
import matplotlib.axes
from astropy.io import fits as pyfits
from scipy import signal

from utils.SharedUtils import find_files
from utils.Constants import SAVE_SKY, FIND_PEAK_PARAMS, ARC_FILE

# print(
#  [logging.getLogger(name) for name in logging.root.manager.loggerDict]
# )
mpl_logger = logging.getLogger('matplotlib')
mpl_logger.setLevel(logging.INFO)
pil_logger = logging.getLogger('PIL')
pil_logger.setLevel(logging.INFO)


# MARK: Skylines Class
class Skylines:

    #----------sky0----------

    """
    Class representing the Skylines object.

    Parameters
    ----------
    data_dir : Path
        The directory containing the data files.
    filenames : list[str]
        The list of filenames to be processed.
    beam : str, optional
        The beam mode, by default "OE".
    plot : bool, optional
        Flag indicating whether to plot the continuum, by default False.
    save_prefix : Path | None, optional
        The prefix for saving the data, by default None.
    **kwargs
        Additional keyword arguments.

    Attributes
```

```
    ----------
    data_dir : Path
        The directory containing the data files.
    fits_list : list[str]
        The list of fits file paths.
    beams : str
        The beam mode.
    can_plot : bool
        Flag indicating whether to plot the continuum.
    save_prefix : Path | None
        The prefix for saving the data.
    wav_unit : str
        The unit of wavelength.

    Methods
    -------
    checkLoad(self, path1: str) -> np.ndarray:
        Checks and loads the data from the given path.
    transform(self, wav_sol: np.ndarray, spec: np.ndarray) ->
    ↪ np.ndarray:
        Transforms the input wavelength and spectral data based on
        the given wavelength solution.
    rmvCont(self) -> np.ndarray:
        Removes the continuum from the spectrum.
    process(self) -> None:
        Placeholder method for processing the data.
    """

    #----------sky1----------

    # MARK: Skylines init
    def __init__(
            self,
            data_dir: Path,
            filenames: list[str],
            beams: str = "OE",
            split_ccd: bool = False,
            cont_ord: int = 11,
            plot: bool = False,
            transform: bool = True,
            save_prefix: Path | None = None,
            **kwargs,
    ) -> None:
        self.data_dir = data_dir
        self.fits_list, self.arc_list = find_files(
            data_dir=self.data_dir,
            filenames=filenames,
            prefix="wmxgbp",  # t[o|e]beam
            ext="fits",
            sep_arc=True,
        )
        self._beams = None
        self.beams = beams
        self.ccds = 1
        if split_ccd:
            # See cross_correlate for initial implementation
            self.ccds = 3

```

```
        self.cont_ord = cont_ord
        self.can_plot = plot
        self.must_transform = transform

        self.save_prefix = save_prefix
        # Handle directory save name
        if self.save_prefix and self.save_prefix.is_dir():
            self.save_prefix /= SAVE_SKY
            logging.warning((
                f"Skylines save name resolves to a directory. "
                f"Saving under {self.save_prefix}"
            ))

        self.max_difference = 5

        self.wav_unit = "$\AA$"

        logging.debug("__init__ - \n", self.__dict__)

        return

    # MARK: Beams property
    @property
    def beams(self) -> str:
        return self._beams

    @beams.setter
    def beams(self, mode: str) -> None:
        if mode not in ['O', 'E', 'OE']:
            err_msg = f"Correlation mode '{mode}' not recognized."
            logging.error(err_msg)
            raise ValueError(err_msg)

        self._beams = mode

        return

    # MARK: Find Peaks
    def find_peaks(
            self,
            spec: np.ndarray,
            axis: int | None = None,
            min_height: float = 0.5,
            **kwargs,
    ) -> tuple[list[np.ndarray], list[dict]]:
        """
        Finds the peaks in the given spectral data.

        Parameters
        ----------
        spec : np.ndarray
            The spectral data.
        axis: int | None, optional
            The axis along which the peaks are found.
        min_height : float, optional
            The minimum height of the peaks, by default 0.5.

        Returns
```

```
        -------
        peaks, properties : tuple[list[np.ndarray], list[dict]]
            The peaks and their properties.

        """
        peaks = []
        props = []
        row_means = []

        for ext in range(len(self.beams)):
            row_mean = spec[ext] if axis is None else
            ↪ np.mean(spec[ext], axis=axis)

            peak, prop = signal.find_peaks(
                row_mean,
                prominence=min_height * np.max(row_mean),
                width=0,
                **kwargs,
            )
            peaks.append(peak)
            props.append(prop)
            row_means.append(row_mean)

        if self.can_plot:
            fig, axs = plt.subplots(2, 1)
            for ext in range(len(self.beams)):
                axs[ext].plot(
                    row_means[ext],
                    label=f"{'E' if ext else 'O'}"
                )
                axs[ext].plot(
                    peaks[ext],
                    row_means[peaks[ext]],
                    "x",
                    label=f"{'E' if ext else 'O'} peaks"
                )
                axs[ext].legend()
                plt.show()

        logging.debug(f"find_peaks - peaks: {[len(i) for i in peaks]}")
        logging.debug(f"find_peaks - props: {[key for key in
        ↪ props[0].keys()]}")

        return peaks, props

    # MARK: Min. of Diff. Matrix
    @staticmethod
    def min_diff_matrix(
            a: np.ndarray,
            b: np.ndarray,
            max_diff: int = 100
    ) -> tuple[np.ndarray, np.ndarray, np.ndarray]:
        """
        Find the minimum difference between the elements of two arrays.

        Parameters
        ----------
        a : np.ndarray
```

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

```
283             exts = [0, 1] if len(self.beams) == 2 else 0 +
                ↪ int(self.beams == 'E')
284             spec2d = np.atleast_3d(hdul["SCI"].data[exts])
285             wav2d = np.atleast_3d(hdul["WAV"].data[exts])
286             bpm2d = np.atleast_3d(hdul["BPM"].data[exts].astype(bool))
287
288             logging.info(
289                 f"load_file_data - {filename.name} - shape:
                    ↪ {spec2d.shape}"
290             )
291
292             return spec2d, wav2d, bpm2d
293
294     # MARK: Load Sky or Arc Lines
295     @staticmethod
296     def load_lines(
297             filename: str | Path | None = None,
298             dtype: list[tuple] = [('wav', float), ('flux', float)],
299             skip_header: int = 3,
300             skip_footer: int = 1
301     ) -> np.ndarray:
302         """
303         Loads the sky or arc lines from the given file.
304
305         Parameters
306         ----------
307         filename : str | Path | None, optional
308             The path to the file to be loaded.
309             Defaults to loading the skylines from `utils/sky.salt`
310         dtype : list[tuple], optional
311             The data type of the sky lines.
312             (Default is [('wav', float), ('flux', float)])
313         skip_header : int, optional
314             The amount of lines to skip of the `filenames` header.
315             (Default is 3)
316         skip_footer : int, optional
317             The amount of lines to skip of the `filename`s footer.
318             (Default is 1)
319
320         Returns
321         -------
322         sky_lines : np.ndarray['wav', 'flux']
323             The sky lines from the file.
324
325         """
326         usecols = None
327         if filename:
328             filename = Path(__file__).parent.resolve() / filename
329             usecols = (0, 1)
330         else:
331             filename = Path(__file__).parent.resolve() /
                ↪ 'utils/sky.salt'
332
333         lines = np.genfromtxt(
334             filename,
335             dtype=dtype,
336             skip_header=skip_header,
337             skip_footer=skip_footer,
```

```
            usecols=usecols
        )

        logging.debug(
            f"load_lines - {filename.name} - shape: {lines.shape}"
        )

        return lines

    # MARK: Mask Traces
    def mask_traces(
            self,
            spec: np.ndarray,
            bpm: np.ndarray,
            max_traces: int = 1,
            tr_pad: int = 5,
            bg_margin: int = 10,
            lr_margins: list[int] = [10, 10],
            h_min: float = 0.5,
            h_rel: float = 1 - 0.05,
    ) -> np.ndarray:
        """
        Masks the traces in the bad pixel mask.

        Parameters
        ----------
        spec : np.ndarray
            The spectral data.
        bpm : np.ndarray
            The bad pixel mask.
        max_traces : int, optional
            The maximum number of traces to be masked.
            (Default is 1)
        tr_pad : int, optional
            The amount to pad traces by.
            (Default is 5)
        bg_margin : int, optional
            The margin size for the background.
            (Default is 10)
        lr_margins : list[int, int], optional
            The left and right background margins at the spectrum edge.
            (Default is [10, 10])
        h_min: float, optional
            The minimum height of a detected peak.
            (Default is 0.5)
        h_rel: float, optional
            The relative height for the properties of a detected peak.
            (Default is 1)

        Returns
        -------
        bpm : np.ndarray
            The updated bad pixel mask.

        """
        # Base mask
        bpm[:, :bg_margin] = True
        bpm[:, -bg_margin:] = True
```

```
396         bpm[:, :, :lr_margins[0]] = True
397         bpm[:, :, -lr_margins[1]:] = True
398 
399         # Get the traces
400         traces, tr_props = self.find_peaks(
401             spec,
402             axis=1,
403             min_height=h_min,
404             rel_height=h_rel
405         )
406 
407         for ext in range(len(self.beams)):
408             # Mask the traces
409             for i in range(len(traces[ext][:max_traces])):
410                 lb = max(
411                     0,
412                     int(tr_props[ext]['left_ips'][i]) - tr_pad
413                 )
414                 ub = min(
415                     spec.shape[-1],
416                     int(tr_props[ext]['right_ips'][i]) + tr_pad
417                 )
418                 bpm[ext, lb: ub] = True
419                 # TODO: Relocate targets after initial masking
420 
421         logging.info(f"mask_traces - {min(max_traces, len(traces))} of
            ↪ {len(traces)} traces masked.")
422 
423         return bpm
424 
425     # MARK: Transform Spectra
426     def transform(
427             self,
428             spec: np.ndarray,
429             wav_sol: np.ndarray,
430             row_max: int | None = None,
431             res_plot: bool = False,
432     ) -> tuple[np.ndarray, np.ndarray]:
433         """
434         Transforms the input wavelength and spectral data
435         based on the given wavelength solution.
436 
437         Parameters
438         ----------
439         spec : np.ndarray
440             The spectral data.
441         wav_sol : np.ndarray
442             The wavelength solution.
443         row_max : int, optional
444             The row along which the spectral data is to be transformed.
445             (Default is None)
446         res_plot : bool, optional
447             Flag indicating whether to plot the results.
448             (Default is False)
449 
450         Returns
451         -------
452         spec, wav : np.ndarray
```

```
453             The transformed wavelength and spectral data.
454
455         """
456         # Create arrays to return
457         cs = np.zeros_like(spec)
458         cw = np.zeros_like(wav_sol.mean(axis=1))
459
460         for ext in range(len(self.beams)):
461
462             if row_max:
463                 avg_max = row_max
464             else:
465                 # Get middle row (to interpolate the rest of the rows
                    ↪ to)
466                 avg_max = np.mean(spec[ext], axis=1).argmax()
467
468             # Correct extensions based on wavelength
469             # Get wavelength values at row with most trace
470             cw[ext] = wav_sol[ext, avg_max]
471
472             # Spec ext
473             for row in range(cs.shape[1]):
474                 cs[ext, row] = np.interp(
475                     cw[ext],
476                     wav_sol[ext, row],
477                     spec[ext, row]
478                 )
479                 # f_2d = interpolate.interp2d(
480                 #     wav_sol[ext, row],
481                 #     np.arange(rows),
482                 #     spec[ext],
483                 # )
484                 # cs[ext] = f_2d(cw[ext, row], np.arange(rows))
485
486         # Plot results
487         if res_plot:
488             fig, axs = plt.subplots(2, 1, figsize=[20, 4])
489             for ext in range(len(self.beams)):
490                 axs[ext].imshow(
491                     cs[ext],
492                     vmax=cs[ext].mean() + 2 * cs[ext].std(),
493                     vmin=cs[ext].mean() - 2 * cs[ext].std()
494                 )
495
496                 logging.debug(f"{'E' if ext else 'O'} Average continuum
                    ↪ = {np.median(np.median(cs[ext], axis=0)):4.3f}")
497
498                 axx = axs[ext].twinx()
499                 axx.hlines(
500                     np.median(np.median(cs[ext], axis=0)),
501                     0,
502                     cs[ext].shape[-1],
503                     colors='black'
504                 )
505                 axx.plot(
506                     cs[ext].mean(axis=0),
507                     "k",
508                     label=f"mean {'E' if ext else 'O'}"
```

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

```
563             color = next(axs[0, 0]._get_lines.prop_cycler)['color']
564
565             for ext in range(len(self.beams)):
566
567                 ccdrange = spectra[1][fl][ext].shape[-1] // self.ccds
568                 for ccd in range(self.ccds):
569                     # MARK: plot spectrum
570                     # (transformed)
571                     axs[0, ccd].plot(
572                         wavelengths[1][fl][ext][
573                             ccdrange * ccd:ccdrange * (ccd + 1)
574                         ],
575                         norm(spectra[1][fl][ext][
576                             ccdrange * ccd:ccdrange * (ccd + 1)
577                         ]) * 100 + 10 * ext + 30 * fl,
578                         color=color,
579                         linestyle='dashed' if ext else 'solid',
580                         label=f"${{{{self.beams[ext]}}}_{{{fl + 1}}}^{{+
                            ↪ {10 * ext + 30 * fl}}}$" if ccd == 0 else
                            ↪ None,
581                     )
582
583                     # MARK: plot dev
584                     # noinspection PyTypeChecker
585                     sky_wavs, dev, peak_idx = self.min_diff_matrix(
586                         lines['wav'],
587                         wavelengths[1][fl][ext][peaks[1][fl][ext]],
588                         max_diff=self.max_difference,
589                     )
590
591                     # # MARK: width/width_init
592                     # width = properties[1][fl][ext]['widths'][peak_idx]
593                     # width_i = np.zeros_like(width)
594
595                     # sky_i, i_dev, i_idx = self.min_diff_matrix(
596                     #     lines['wav'],
597                     #     wavelengths[0][fl][ext][peaks[0][fl][ext]],
598                     #     max_diff=self.max_difference,
599                     # )
600
601                     # width_i = np.array([
602                     #     properties[0][fl][ext]['widths'][
603                     #         np.where(wav == sky_i)[0][0]
604                     #     ]
605                     #     if wav in sky_i else 1000
606                     #     for wav in sky_wavs
607                     # ])
608                     # width_ratio = (width / width_i) - 1
609                     # width_ratio[width_ratio < 0] = 0
610
611                     # ylolims = width_ratio > self.max_difference
612                     # width_ratio[
613                     #     width_ratio > self.max_difference
614                     # ] = self.max_difference // 2
615
616                     ok = np.where(
617                         (sky_wavs >=
                            ↪ wavelengths[1][fl][ext].data[ccdrange *
```

```
                        ↪ ccd]) &
618                     (sky_wavs <=
                        ↪ wavelengths[1][fl][ext].data[ccdrange * (ccd
                        ↪ + 1)])
619                 )
620                 axs[1, ccd].plot(
621                     sky_wavs[ok],
622                     dev[ok],
623                     # yerr=(width_ratio[ok] * 0, width_ratio[ok]),
624                     # lolims=ylolims[ok],
625                     "." if ext else "x",
626                     # fmt="." 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)):2.3f}")
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]:
655                 axs[0, ccd].axvline(x, ls='dashed', c='0.7')
656
657         axs[0, 0].set_ylabel("Rel. Intensity ($\%$)")
658         axs[1, 0].set_ylabel(
659             "Closest Peak ($\Delta\lambda$)"
660         )
661         # for ax in axs[:, 0]:
662         #     ax.legend(loc='upper left', ncols=(fl + 1) * (ext + 1) +
        ↪ 1)
663         leg = fig.legend(
664             loc='center',
665             ncol=min(8, len(spectra[0]) + 1),
666             columnspacing=0.5,
667             bbox_to_anchor=(
668                 np.mean((
```

```
                    plt.rcParams['figure.subplot.left'],
                    plt.rcParams['figure.subplot.right']
                )),
                np.mean((
                    plt.rcParams['figure.subplot.bottom'],
                    plt.rcParams['figure.subplot.top']
                ))
            ),
        )
        leg.set_draggable(True)
        for ax in axs[1, :]:
            ax.grid(axis='y')

        # fig.add_subplot(111, frameon=False)
        # # hide tick and tick label of the big axis
        # plt.tick_params(
        # labelcolor='none',
        #    which='both',
        #    top=False,
        #    bottom=False,
        #    left=False,
        #    right=False
        # )
        axs[-1, 0 if self.ccds == 1 else 1].set_xlabel(
            f"Wavelength ({self.wav_unit})"
        )

        # plt.tight_layout()

        plt.show()

        # Save results
        if self.save_prefix:
            fig.savefig(fname=self.save_prefix)

        return

        # MARK: Process all listed images

    def process(self, arc: bool = False) -> None:
        files = self.fits_list
        if arc:
            files = self.arc_list

        logging.info(f"Processing '{self.beams}' lines.")

        spectra = [[], []]
        wavs = [[], []]
        peaks = [[], []]
        peak_props = [[], []]

        for fl in files:
            # Load data
            spec2d, wav2d, bpm2d = self.load_file_data(fl)

            # Mask traces in BPM
            bpm2d = self.mask_traces(
                spec2d,
```

```
                bpm2d,
                max_traces=0,
                bg_margin=15,
                h_min=0.05
            )
            m_spec2d = np.ma.masked_array(spec2d, mask=bpm2d)  # spec2d
            m_wav2d = np.ma.masked_array(wav2d, mask=bpm2d)  # wav2d

            # Initial spectra
            spec_i = np.mean(m_spec2d, axis=-2)
            wav_i = np.mean(m_wav2d, axis=-2)

            # Transform data
            t_spec2d, t_wav = self.transform(
                m_spec2d,
                m_wav2d,
                res_plot=self.can_plot
            )

            # Final spectra
            spec_f = np.mean(t_spec2d, axis=-2)
            wav_f = t_wav

            # Find peaks
            peaks_i, props_i = self.find_peaks(
                spec_i,
                **FIND_PEAK_PARAMS
            )
            peaks_f, props_f = self.find_peaks(
                spec_f,
                **FIND_PEAK_PARAMS
            )

            spectra[0].append([*spec_i])
            spectra[1].append([*spec_f])
            wavs[0].append([*wav_i])
            wavs[1].append([*wav_f])
            peaks[0].append([*peaks_i])
            peaks[1].append([*peaks_f])
            peak_props[0].append([*props_i])
            peak_props[1].append([*props_f])

        # Plot results
        self.plot(spectra, wavs, peaks, peak_props, arc=arc)

        if arc:
            return
        elif self.arc_list:
            self.process(arc=True)

        return


# MARK: Main function
def main(argv) -> None:
    return


```

```
785 if __name__ == "__main__":
786     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.