

The OPERA algorithms for the reduction and analysis of ESPaDOnS spectro-polarimetric data

Eder Martioli^{1,2}, Doug Teeple², Nadine Manset², Andre Venne³, Daniel Devost², Kanoa
Withington², Megan Tannock⁴

Canada France Hawaii Telescope, 65-1238 Mamalahoa Hwy, Hawaii, USA

`emartioli@lna.br`, `eder@cfht.hawaii.edu`

ABSTRACT

This article describes the algorithms implemented in the OPERA pipeline for the reduction of cross-dispersed high-resolution spectro-polarimetric ESPaDOnS data. The algorithms presented here are particularly useful for fiber-fed echelle spectrographs that use an image slicer. We developed an additional calibration that uses an oversampled two-dimensional instrument profile. This allows an improved performance in the identification and characterization of spectral lines and in the determination of an optimal aperture for flux extraction. We also present an extended application of the Horne’s optimal algorithm for flux extraction that employs an oversampled profile calibration. Finally we show that this approach provides improved wavelength and flux calibration, better polarimetric precision, and unbiased measurements of quantities that depend on the morphology of line profiles.

Subject headings: facility: CFHT — instrument: ESPaDOnS — software: OPERA — techniques: spectropolarimetry, high resolution spectroscopy — general: data reduction

1. INTRODUCTION

The Open-source Pipeline for Espadons Reduction and Analysis (OPERA) is a Canada-France-Hawaii Telescope (CFHT) open-source software project to reduce the data produced

¹Laboratório Nacional de Astrofísica, Rua Estados Unidos, 154 Itajubá - MG, Brazil;

²Canada France Hawaii Telescope, 65-1238 Mamalahoa Hwy, Hawaii, USA;

³Université de Sherbrooke, Québec, Canada;

⁴University of Victoria, British Columbia, Canada.

by the echelle spectro-polarimeter ESPaDOnS (Donati *et al.* 2003; Manset *et al.* 2003). The preliminary design for the software architecture and a description of the overall software infrastructure of OPERA is described in Martioli *et al.* (2012). Other software documentation as well as the complete source software are available in the OPERA webpage <http://sourceforge.net/projects/opera-pipeline>.

1.1. Reduction of ESPaDOnS Data

The reduction of ESPaDOnS data consists of converting a set of raw 2k x 4k CCD images of cross-dispersed echelle spectra into calibrated physical quantities. There have been a number of packages and techniques developed in the past for the reduction of cross-dispersed echelle spectra (e.g., Piskunov *et al.* 2002; Moreno *et al.* 1982; Rossi *et al.* 1985; Ponz *et al.* 1986; Goodrich & Veilleux 1988; Marsh *et al.* 1989; Mukai *et al.* 1990; Hall *et al.* 1994; Valenti *et al.* 1994; Piskunov *et al.* 1995; Hinkle *et al.* 2000). Most of them, however, were designed for a particular instrument or data format, and therefore do not comply with all the requirements necessary to reduce ESPaDOnS data. For instance, the tilted and irregular shape of the pseudo-slit in ESPaDOnS, which in addition is under-sampled by the large pixel size, represents a complication for most of available packages. There is a working pipeline which is able to reduce ESPaDOnS data, the Libre-Esprit (LE) package, which is based on the Esprit package (Donati *et al.* 1997) initially developed to reduce the MuSiCoS spectropolarimeter instrument data (Donati *et al.* 1999). LE results have been taken as the baseline for comparison with OPERA results, which should perform similarly or better than LE. OPERA is not only intended to offer an alternative to LE for the reduction of ESPaDOnS data, it also improves the scientific capabilities of ESPaDOnS and provides better support for the community of users of this instrument.

ESPaDOnS is a bench-mounted cross-dispersed fiber-fed echelle spectrometer, which can obtain high resolution intensity and polarimetric spectra ranging from 370 nm to 1050 nm. It uses a Bowen-Walraven image slicer at the entrance pupil of the fiber(s) output, which produces a pseudo-slit as the dispersing element. The image of the pseudo-slit consists of a stack of slices of a circle, which is approximately the shape of illumination pattern of the fiber output. The pseudo-slit is intentionally tilted by an angle of about two degrees with respect to the direction perpendicular to the dispersion. The tilted pseudo-slit allows one to sample the spectrum with a spatial frequency smaller than one element per pixel.

ESPaDOnS has three modes of operation, star+sky (SP1), star-only (SP2), and polarimetry (POL). In SP1 mode two fibers are used to collect light, one for sky and one for the target, where each beam is split into three slices, giving a spectral resolution of

$R \approx 65,000$. In POL mode a similar configuration is used with two fibers and three slices and the same spectral resolution, but in this case the two fibers are used to collect the two polarization modes separately, one for the ordinary beam (iE) and the other for the extraordinary beam (iA). The SP2 mode uses a single fiber and the beam is divided into six slices, therefore the width of the projected pseudo-slit is thinner giving a higher spectral resolution of $R \approx 80,000$.

ESPaDOnS is currently an instrument used only by CFHT. However, there is an on going project, the Gemini Remote Access to CFHT ESPaDOnS Spectrograph - GRACES (Tollestrup *et al.* 2012), a collaboration between the Gemini Observatory and CFHT, which is developing a system with a new injector/slicer plus an optical fiber link that will allow the Gemini 8m telescope (near CFHT on Mauna Kea) to use ESPaDOnS remotely. The ESPaDOnS data format and methodology for data reduction is most likely to be unaffected for GRACES. Thereby, GRACES and the Gemini community may greatly benefit by making use of OPERA. OPERA is an open source software and should be able to reduce GRACES data with minor adaptation of existing routines.

The approach presented here for the reduction of ESPaDOnS data is divided into three major steps: (1) Calibration, (2) Reduction, and (3) Analysis. Each of these steps performs a number of operations, which will be explained in detail in the following sections. The main distinction between these steps is that Calibration makes use only of calibration images and produces the calibration products. Reduction makes use of the calibration products to extract the flux and polarimetric information from object images and Analysis uses both calibration and the extracted spectra to obtain physical information in various ways. This distinction will become more clear in the text.

1.2. ESPaDOnS Image Types

ESPaDOnS has basically five different types of image as shown in figure 1, where each type is defined as follows:

- Bias: exposure with minimum integration time and shutter closed.
- Flat: exposure of a halogen lamp illuminating the fiber inputs.
- Comparison: exposure of a Th-Ar comparison lamp for wavelength calibration.
- Align: exposure of a halogen lamp using a Fabry-Perot etalon, which produces a pattern of spectral lines with uniform illumination, which are distributed all over the

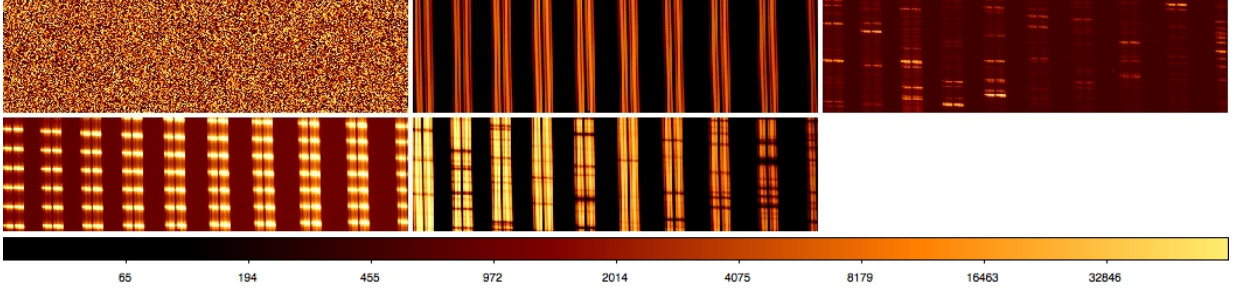


Fig. 1.— Samples for the 5 different image types of ESPaDOnS: bias (top-left), flat (top-center), comparison (top-right), align (bottom-left), and object (bottom-center).

echellogram. The align image is useful for instrument profile calibration and for measurements of the pseudo-slit tilt angle.

- Object: exposure of an object in the sky.

1.3. Image Coordinates

We find useful to define the reference system of coordinates to describe image quantities, which will be used throughout the text. Let us consider the image pixel value in Analogical-to-Digital Units (ADU), $I(x, y; \Delta t)$, where x and y are the column and row pixel coordinates, respectively, and Δt is the exposure time. Each image is also a function of time, t , which is omitted here for simplicity. The pixel coordinates (x, y) refer to the center of a squared pixel, which is given by its column and row zero-based indexes (i, j) plus half pixel size, i.e.,

$$x = i + 0.5, \quad (1)$$

$$y = j + 0.5. \quad (2)$$

The above definition allows one to identify a pixel by either its image indexes or coordinates,

$$I(x, y) = I_{ij} = I_{\text{pix}}, \quad (3)$$

where the indexes (i, j) must lie in the range $0 \leq i < \text{NAXIS1}$ and $0 \leq j < \text{NAXIS2}$, for NAXIS1 and NAXIS2 being the FITS header keywords that define the total number of columns

and rows in the image. The pixels considered for reduction may not cover the entire image (when a sub-image is used), then the total number of pixels will differ than the total size of the image. Thus the notation N_x and N_y may be used for the actual number of columns and rows in the sub image array. In this case, equations 1 and 2 become

$$x = i_0 + i + 0.5, \quad (4)$$

$$y = j_0 + j + 0.5, \quad (5)$$

where (i_0, j_0) are the image indexes for the first pixel considered in the sub-image array. In some cases the pixels may also be indexed by a single index “pix” as shown in equation 3, where it can be calculated from the image pixels by the equation

$$\text{pix} = i + jN_x, \quad (6)$$

for pix lying in the range $0 \leq \text{pix} < \text{NAXIS1} \times \text{NAXIS2}$, or equivalently for a sub-image, $0 \leq \text{pix} < N_p$.

2. CALIBRATION

The calibration of ESPaDOnS data consists of the processing steps for obtaining information from calibration images and reference data to produce the calibration products for a given data set. These products are used later for reduction and analysis of science data. Each calibration step is performed by a distinct OPERA module. The calibration modules are outlined below.

1. **operaReductionSet** - creates a list of file paths based on qualifiers being detector, amplifier, configuration mode and readout speed.
2. **operaMaster[Flat,Bias,Comparison,FabPerot]** - combines multiple images to produce master calibration images (masterbias, masterflat, mastercomparison, and masterfabryperot);
3. **operaGain** - measures CCD gain and electronic noise;
4. **operaOrderSpacingCalibration** - measures spacing between orders as a function of image coordinates;

5. `operaGeometryCalibration` - detects, traces, and enumerates spectral orders;
6. `operaInstrumentProfileCalibration` - measures a two-dimensional instrument profile as a function of image coordinates;
7. `operaExtractionApertureCalibration` - sets up and calibrates the aperture for extraction;
8. `operaWavelengthCalibration` - performs pixel-to-wavelength calibration using Th-Ar comparison spectrum;
9. `operaEchelleDispersionCalibration` - performs an overall pixel-to-wavelength calibration based on all cross-dispersed orders;

2.1. Reduction Set

Before data processing starts there is a preliminary step performed by the pipeline, which consists of recognizing and organizing the data files into separate groups, where each of these groups are associated to an specific instrument configuration. This step also considers whether an instrument mode has changed. If there is an instrument configuration change with movement of optical and/or mechanical parts in the spectrograph, then the pipeline will not associate the calibration data taken before the change, assuming that a new calibration will be done afterwards. In practice, calibration data may not always be available before or after an instrument mode change. Then, in this case, the pipeline will make use of either another set of calibration data taken with the same instrument mode and at the same night or a default calibration data, which allows a basic reduction with limited precision.

The grouping of the data is performed by the OPERA module `operaReductionSet` and the criteria used for grouping is based on a given set of qualifiers. Each qualifier is associated to a header FITS `KEYWORD`, where its `KEYVALUE` is matched against a given input value that is defined by an instrument mode. For ESPaDOnS, four header `KEYWORDS` are used to specify an instrument mode:

1. `DETECTOR`, which identifies the CCD detector used (EEV1 or Olapa);
2. `INSTMODE`, for spectroscopy/polarimetry mode (SP1, SP2, or POL);
3. `EREADSPD`, for detector readout speed (fast, normal, slow, or xslow);
4. `AMPLIST`, for the number of amplifiers used (a or ab);

The output of this module is lists of file paths in text format for each qualifier, which will be read later by other routines to perform calibration and reduction.

2.2. Master Calibration Images

The `operaMaster[type]` modules median-combine a set of exposures of the same type into a single master calibration image. These modules have the same functionality except for `operaMasterComparison`, which implements an additional method to combine comparison images. The method takes into account saturated pixel removal and the exposure time, which is explained below.

A Th-Ar lamp is used as the calibration source for comparison exposures. ESPaDOnS has a single detector to image the whole optical spectral range (360 nm to 1050 nm) in a single exposure, which presents a challenge for wavelength calibration. The red part of the Th-Ar spectrum has emission lines that are much brighter than the blue part. This makes it very difficult to obtain enough flux in the blue regions and at the same time avoid over-saturation in the red regions. This problem could be reduced by introducing a blue filter, however this would also dim fainter lines in the red that are lying between the few saturated ones. Without using a filter, we developed a way to obtain enough signal in the faint regions and at the same time not saturate the detector. This is done by taking several exposures with short exposure times (typically 8 s) and combining these images with a few exposures with long exposure time of 60 s. The module `operaMasterComparison` stacks a series of N_C Th-Ar exposures, where a given pixel for each exposure is represented by the symbol $C_{i,j}^k$, for k being the image index. Then the master comparison $C'_{i,j}$ is calculated as

$$C'_{i,j} = \frac{\sum_{k=0}^{k < N_C} [C_{i,j}^k - B'_{i,j}] M_{i,j}^k}{\sum_{k=0}^{k < N_C} \Delta t^k M_{i,j}^k} \times \Delta t_{out}, \quad (7)$$

where $B'_{i,j}$ is the master bias, Δt^k is the exposure time for a given comparison image, Δt_{out} is the output exposure time and the function $M_{i,j}^k$ is given by:

$$M_{i,j}^k = \begin{cases} 1 & \text{if } C_{i,j}^k < \text{SATURATION} \\ 0 & \text{if } C_{i,j}^k \geq \text{SATURATION.} \end{cases} \quad (8)$$

Figure 2 shows a sequence of three comparison images taken with exposure times of 5, 10, and 60 seconds and the resulting stacked image. Notice the improvement in the signal for faint lines in the stacked image when compared to the ones with short exposure times, and at the same time how the saturation has vanished. The efficiency of this method becomes clear when comparing the pixel-to-wavelength calibration obtained from a single 60 s exposure and from a master comparison using multiple exposure times.

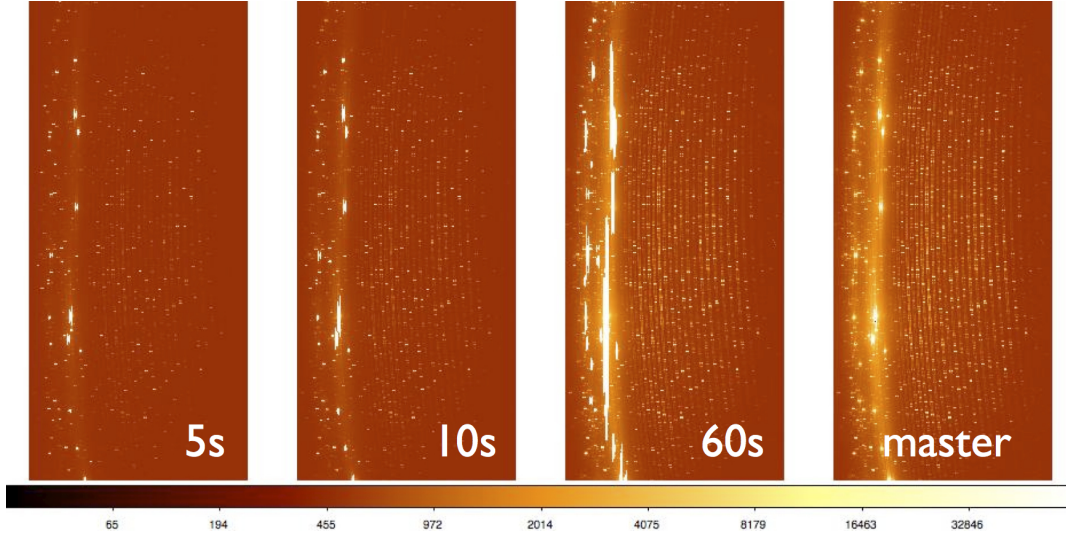


Fig. 2.— From left to right it shows a sequence of three Th-Ar comparison images using three different exposure times, 5, 10, and 60 seconds. The rightmost image is a stack of the three images in the sequence using the algorithm as described.

2.3. CCD Gain and Noise

The module `operaGain` performs measurements of the CCD gain (G) and electronic noise (σ_e), for each amplifier, obtained from a set of raw flat exposures ($F^{k=0,\dots,N_F}$) and a set of bias exposures ($B^{k=0,\dots,N_B}$), where $N_F \geq 2$ and $N_B \geq 1$. We apply the Janesick’s method (Janesick 2001), which is the same method implemented in the IRAF task `findgain` from `obsutil` package. The OPERA implementation of this method is explained below.

Let us first define the differential quantities:

$$\Delta F^P = F^k - F^{k+1} \quad (9)$$

$$\Delta B^P = B^k - B^{k+1}, \quad (10)$$

where the index P counts the number of pairs of images and therefore it ranges from $0 \rightarrow N_{F,B} - 2$.

In usual gain and noise calculations a set of pairs of flat images with variable exposure time or a variable source of light are used. Here, we implement a method using all flat images with the same exposure time. Note that an ESPaDOnS flat exposure contains variable levels of illumination, which allows one to sample different levels of flux within the same image. Thus, we select pixels lying within the same range of flux counts, and by using multiple bins

of flux we are able to construct a data set with measurements of signal-to-noise and variance for several flux count levels. These can be used to fit a linear model that provides a direct measurement of the gain and noise as follows.

From Janesick’s method the gain in units of electrons per ADU (e-/ADU) is given by

$$G = \frac{\langle F^k \rangle + \langle F^{k+1} \rangle - \langle B^k \rangle - \langle B^{k+1} \rangle}{\sigma_{\Delta F}^2 - \sigma_{\Delta B}^2}, \quad (11)$$

where the angle brackets represent the average flux count in units of ADU for a given image k in the sequence and its respective pair $k + 1$. $\sigma_{\Delta F}^2$ and $\sigma_{\Delta B}^2$ are the variances of the difference between the pairs of flats and bias respectively. The noise in units of electrons (e-) is given by

$$\sigma_e = G \frac{\sigma_{\Delta B}}{\sqrt{2}}. \quad (12)$$

By adding both terms of equations 11 and 12 one can obtain the following:

$$Y = GX + \sigma_e, \quad (13)$$

where Y and X are defined as

$$Y = \frac{\langle F^k \rangle + \langle F^{k+1} \rangle - \langle B^k \rangle - \langle B^{k+1} \rangle}{\sigma_{\Delta B} \sqrt{2}}, \quad (14)$$

$$X = \frac{\sigma_{\Delta F}^2}{\sigma_{\Delta B} \sqrt{2}}. \quad (15)$$

Therefore, by measuring the quantities Y (in units of e-) and X (in units of ADU) for several flux count ranges one can easily obtain the gain and noise from the slope and intercept of a linear fit to these data. The module **operaGain** performs a robust fit using the **MEDFIT** algorithm (Press et. al 2007), which fits a line by minimizing absolute deviation. Fig 3 shows the data and the linear fit for three examples where we used this method to measure the CCD gain and noise.

The two-amplifier mode of ESPaDOnS is a feature of the new CCD Olapa that is currently under study and that may be offered soon to the CFHT user’s community. The use of two-amplifiers reduces the readout time in a factor of about half, thus improving observing

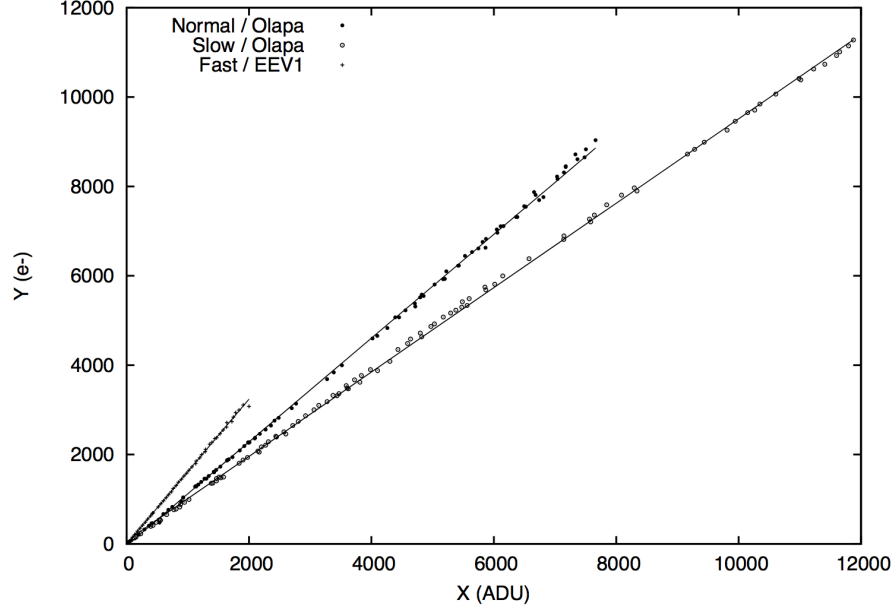


Fig. 3.— X,Y data and the respective linear robust fit obtained with the module `operaGain` for three ESPaDOnS modes of operation: Normal/Olapa (filled circles), Slow/Olapa (open circles), and Fast/EEV1 (crosses).

efficiency. The `operaGain` module supports multiple amplifiers, where it performs calculations of the gain and noise for each amplifier region independently. These measurements are used later in extraction to apply the adequate conversion between detector counts and photon-electrons for each amplifier.

2.4. Geometry Calibration

An echelle spectrograph such as ESPaDOnS produces images containing multiple spectral orders, which appear as multiple bands in the detector. For ESPaDOnS, the spectral orders run roughly parallel to detector columns, and perpendicular to rows, where orders with longer wavelengths (red) are in the lefthand side and shorter wavelengths (blue) in the righthand side of the image. The geometry calibration is done in two steps, first it measures the spacing between orders with the `operaOrderSpacingCalibration` module (see section 2.4.1) then the `operaGeometryCalibration` module uses an algorithm to detect, trace (fit a polynomial to the center of the order), and enumerate these orders automatically, explained in section 2.4.2. These calibrations require as input a well-exposed, unsaturated, master flat image, as illustrated in Figure 4.

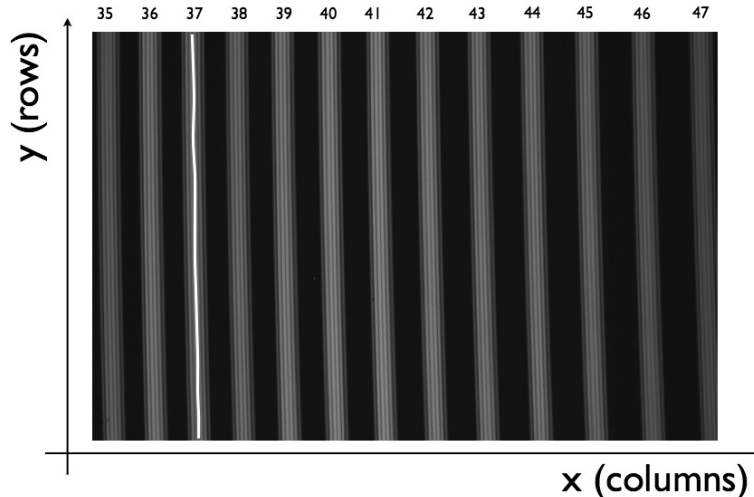


Fig. 4.— Segment of an ESPaDOnS flat-field image taken in SP2 mode. The orientation of the image is set such as columns are along x-axis and rows along y-axis. The white line illustrates the tracing function for order number 37.

The detection of orders is performed by the OPERA peak-detection function, which parses rows to detect well exposed orders. Figure 5 shows an example of a typical data set for which the peak-detection algorithm takes as input to search for orders. Each point in the data set shown in figure 5 consists of a median bin of 25 rows around row number 2300, in the middle of the detector. Notice that each order is a double peaked function due to the two fiber inputs (two beams) in POL mode, where each beam shows several variations due to the irregular shape of the slices produced by the pseudo-slit. These characteristics make it very difficult to apply conventional methods for order detection, and for this reason we

have developed a custom method, which is explained in section 2.4.3.

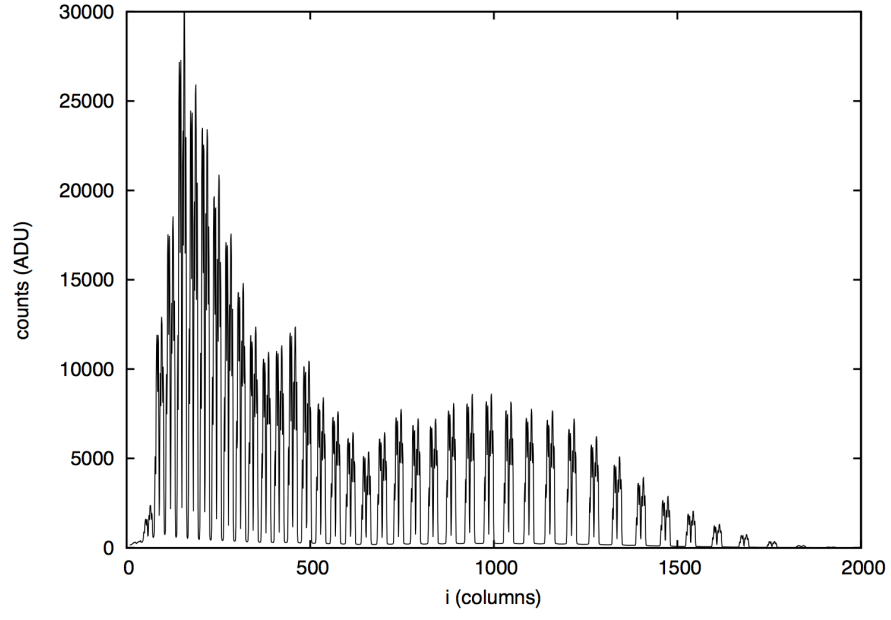


Fig. 5.— A typical data set for a median bin of 25 rows in the middle of a master flat-field ESPaDOnS image in POL mode.

2.4.1. Order Spacing Calibration

This calibration is performed by the `operaOrderSpacingCalibration` module. This module measures the distance between spectral order centers (“spacing”) along rows (x-axis) and performs a low order polynomial fit across the dispersion direction. The calibration is done in the central region of the detector, where most orders present maximum illumination in flat exposures. The calibration is performed in three steps:

1. Detect spectral orders from a master flat image using a peak-detection algorithm (see section 2.4.3);
2. Measure the order center in the x -direction (x_c^k), where the index k counts spectral orders from left to right. In this step it also calculates the spacing between adjacent order centers $\Delta x^P = |x_c^{k+1} - x_c^k|$;
3. Fit a low order polynomial to Δx^P versus $x_c^k + \Delta x^P/2$.

The order spacing is an intrinsic characteristic of the cross-dispersing element of the spectrograph. Therefore, this calibration can be used in geometry calibration, as explained in section 2.4.2, to allow absolute enumeration of orders and also to avoid hopping orders in the order-detection algorithm. Figure 6 shows an example of a calibration performed by this module.

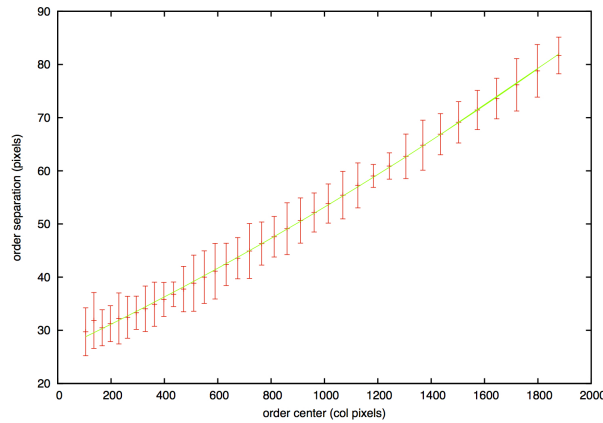


Fig. 6.— An example of measurements of order spacing and the fit polynomial model for calibration.

2.4.2. Geometry Calibration Algorithm

The algorithm for this module takes each bin of rows (or columns, depending on which orientation is set as the dispersion direction).

1. Measure instrument spatial profile (IP) (as will be detailed in section 2.4.3);
2. If (use center of symmetry = TRUE) then calculate the center of symmetry of the instrument profile and recenter the instrument profile coordinates. The center of symmetry is calculated by counting the number of peaks within the IP and setting the center as the minimum point between the two central peaks leaving the same number of peaks on both sides. Note that the instrument profile is usually centered using the photo center, however if the beams are not uniformly illuminated then the center would be biased towards the brighter beam.
3. If (FFT = TRUE) then it uses a Fast Fourier Transform (FFT) low-pass filter to remove noise and high-frequency variations from input data;
4. Detect orders using the peak-detection function `operaCCDDetectPeaks` (as will be detailed in section 2.4.3);
5. Use the order spacing calibration model to measure the center of orders that were missed by the peak-detection algorithm;
6. Enumerate orders given an input order number and spacing for the same order as the absolute reference;
7. Trace N orders, $k = k_0, \dots, k_{N_o-1}$, where k_0 is the absolute number of first order and k_{N_o-1} is the number of the last order. The word “trace” here means fitting a polynomial function up to the third degree ($n_p \leq 4$) to the vector $[x_c, y_c]_k$ of order center positions. Sample points of $[x_c]_k$ are obtained from peak-detection algorithm (see section 2.4.3) and $[y_c]_k$ is the y-coordinate of the center of binned rows. A practical detail here for ESPaDOnS is that due to the orientation of the curved shape of the order with respect to the detector, and in order to deal with a univocal function, we have to invert the independent variable and fit a set of polynomials of the form:

$$[x_c(y)]_k = \left[\sum_{i=0}^{n_p} \alpha_i y^i \right]_k, \quad (16)$$

where α_i are the coefficients of the polynomial. The fit is performed using the MP-FIT (Markwardt 2009) implementation of the Levenberg-Marquardt algorithm (Moré 1977). Hereafter the order index k will be omitted for simplicity.

Figure 7 shows a plot for all data points detected from the bins, the order absolute number on the right, and the tracing polynomial models for all orders detected from a master flat exposure.

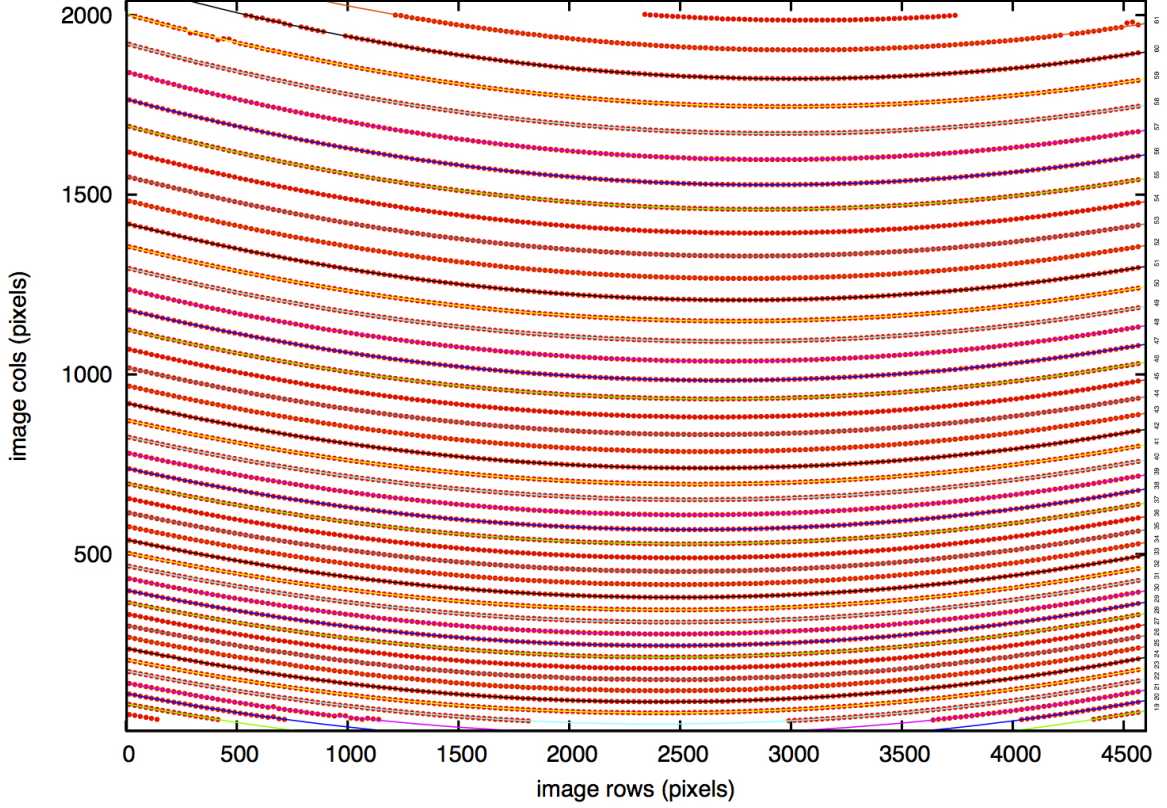


Fig. 7.— Geometry calibration plot showing the order center points and the trace polynomials. Notice that in this plot the independent variable has been inverted for reasons explained in the text.

2.4.3. OPERA Peak Detection Algorithm

The function `operaCCDDetectPeaks` is used to detect spectral orders in geometry calibration. The algorithm described here follows the fundamental ideas of the convolution method for detecting objects described in Starck & Murtagh (2006). This method requires a window function to be convolved with the data to improve the order detection capability. OPERA uses three window functions: top-hat, gaussian, or empirical instrument profile (IP). The latter in fact uses a gaussian function as first guess and then it measures a normalized spatial profile, which is used to refine order detections and to calculate the order center.

The basic input data for a peak-detection routine is a vector of x -positions, $x_{i=0,\dots,N_x}$, and respective flux count values, $F_{i=0,\dots,N_x}$, for a bin of rows (as illustrated in figure 5). The binning uses a median stack of several rows in order to eliminate bad pixels and to improve the data quality. The base algorithm for peak detection is given as follows.

For each column i at position x_i it calculates the photo-center $\hat{x}_i$ and the function $\hat{F}_i$ within the range $(x_i - A/2) < x < (x_i + A/2)$, where A is a given aperture in pixel units. The photo-center is calculated as the weighted mean position:

$$\hat{x}_i = \frac{\sum_{k=0}^{k < A} x_{i-A/2+k} F_{i-A/2+k}}{\sum_{k=0}^{k < A} F_{i-A/2+k}}, \quad (17)$$

and the function $\hat{F}_i$ is given by the convolution between the data and a window function Ψ , also truncated within the same window:

$$\hat{F}_i = (F * \Psi)(x_i) = \sum_{k=0}^{k < A} F_{i-A/2+k} \Psi_k. \quad (18)$$

The window functions available in OPERA are:

1. Gaussian:

$$\Psi_k = \frac{1}{\sigma\sqrt{2\pi}} \exp \left[\frac{-(k - A/2)^2}{2\sigma^2} \right], \quad (19)$$

where $\sigma = A/4$.

2. Instrument Profile (IP): this is a normalized strictly positive empirical function that gives the fraction of flux within a given window range. For instance, the IP for a given order centered at column $i = i_c$ can be calculated as:

$$\Psi_k = \frac{F_{i_c - A/2 + k}}{\sum_{k=0}^{k=A} F_{i_c - A/2 + k}}, \quad (20)$$

3. Top Hat: this function is given by a constant value $1/A$ for all points lying within the range $[i - A/2 : i + A/2]$ and zero otherwise.

Figure 8 shows a sample of (x_i, F_i) data around 3 orders. The quantity $\hat{F}_i$ is also shown for the three window functions described above. Note that the IP provides the highest peaks for $\hat{F}_i$, which reflects a better match with the actual shape of the pseudo-slit. However, the Gaussian provides a smoother function, which is less sensitive to noise and may be more reliable for peak-detection. For this reason we have also implemented the option of applying a FFT low-pass filter, which smoothes out the input data, giving more reliable results even when using the IP.

Next the orders can be detected by using a peak-detection algorithm, which makes the decision whether a given point $(\hat{x}_i, \hat{F}_i)$ is a peak or not by evaluating the peak probability, p_{peak} , and taking the maximum probability above a given threshold. p_{peak} for each point is calculated as

$$p_{\text{peak}} = p_{\text{localmax}} \times p_{\text{detection}} \times p_{\text{globalmax}}, \quad (21)$$

where the factors on the righthand side of equation 21 are given by:

- p_{localmax} : this is the probability of $\hat{F}_i$ being a maximum within the aperture (A) window range, i.e.,

$$p_{\text{localmax},i} = \begin{cases} 1 & \text{if } \hat{F}_i = \max\{\hat{F}_k : k = i - A/2, \dots, i + A/2\} \\ 0 & \text{otherwise.} \end{cases} \quad (22)$$

- $p_{\text{detection}}$: this is the probability of peak detection for peaks with signal-to-noise ratio greater than 1, i.e.,

$$p_{\text{detection},i} = \begin{cases} 1 & \text{if } \text{SNR}_i \geq 1 \\ 0 & \text{if } \text{SNR}_i < 1, \end{cases} \quad (23)$$

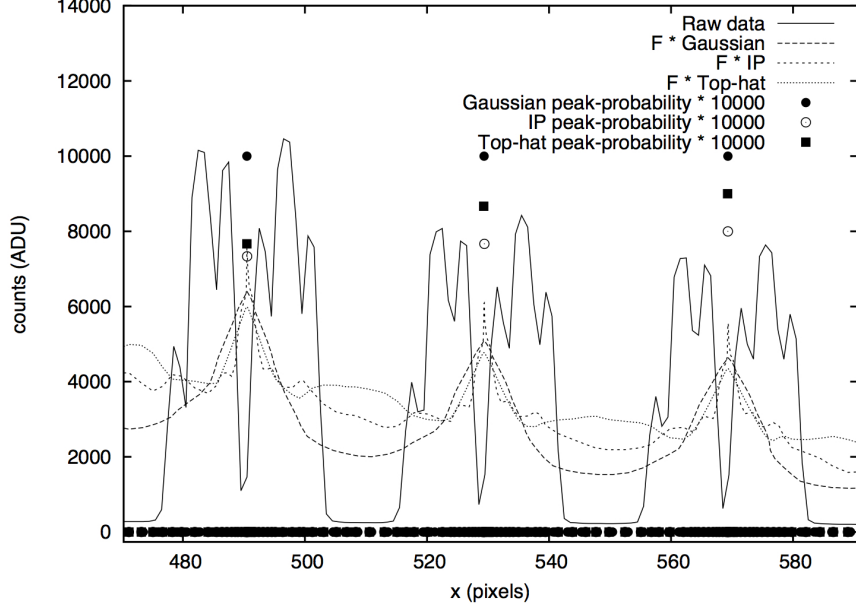


Fig. 8.— Raw data F_i (solid line), and the convolution $\hat{F}_i$ between raw data and the following window functions: Gaussian (dashed), IP (short-dashed), and top-hat (dotted). The filled circles, open circles, and filled squares show the peak-probabilities p_{peak} multiplied by 10,000 respective to each function mode, as indicated in the legend.

where the signal-to-noise ratio for a given point i is calculated as:

$$\text{SNR}_i = \frac{\hat{F}_i - (\hat{F}_{i-A/2} + \hat{F}_{i+A/2})/2}{\sigma_{\text{ADU}}}, \quad (24)$$

for σ_{ADU} being the noise in ADU.

- $p_{\text{globalmax}}$: this is the probability of $\hat{F}_i$ being a global maximum, which is calculated as the ratio:

$$p_{\text{globalmax},i} = \frac{n_{\uparrow}}{n_{\uparrow} + n_{\downarrow}}, \quad (25)$$

where $n_{\uparrow}$ is the number of points with slope growing towards point i and $n_{\downarrow}$ is the number of points with slope decreasing towards point i . Note that the calculation of

the slope depends on whether the point is on the left or righthand side of point i .

Although p_{localmax} and $p_{\text{detection}}$ are considered boolean values, these quantities could in fact be calculated as real probabilities ranging from 0 to 1. However, this simpler approach has shown to work well for ESPaDOnS data. The peak-probabilities (p_{peak}) are also plotted in figure 8.

2.5. Instrument Profile Calibration

This calibration is performed by the module `operaInstrumentProfileCalibration`. The module first measures a one-dimensional spatial profile across the dispersion direction (along rows for ESPaDOoS) using a master flat exposure, similarly to the IP calculated in section 2.4.3. Figure 9 shows spatial profile measurements for the three modes of ESPaDOoS (SP1, SP2, and POL) and also for an additional custom mode using 3 fibers and 2 slices.

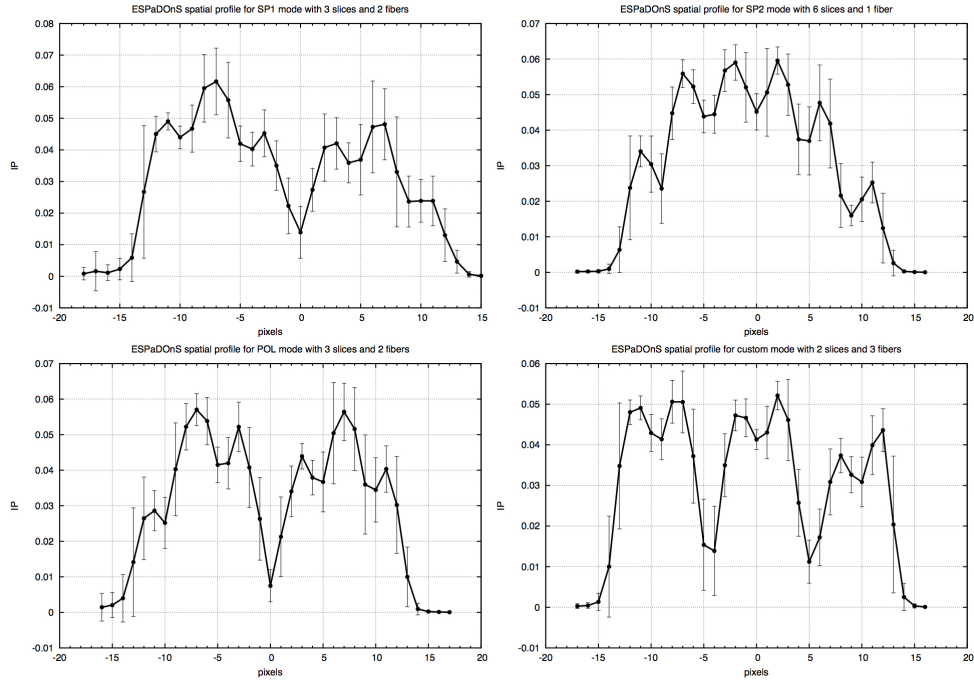


Fig. 9.— One-dimensional spatial profile measured along rows for four different configurations of ESPaDOoS (SP1, SP2, POL, and custom). Each instrument mode configuration is indicated on top of each panel.

The one-dimensional spatial profile is taken as an initial guess to create a two-dimensional profile (2D IP), assuming a Gaussian shape for the dispersion direction (y -direction, along columns for ESPaDOoS). This 2D IP is used to detect spectral lines from either a Th-Ar comparison lamp (comp) or a Fabry-Perot (align) exposure by means of cross-correlation. Once the lines are detected, then the 2D IP is measured empirically by combining the information obtained from several spectral lines. Below we explain the process of obtaining the 2D IP in more detail.

2.5.1. The 2-D Instrument Profile

The two-dimensional instrument profile (2D IP) is equivalent to a point spread function (PSF) used in imaging. The 2D IP is defined here as the distribution of the fraction of flux for a monochromatic image of the entrance slit projected onto the spectrograph focal plane. The fiducial set of coordinates for the IP is set with the ordinate oriented along the image columns (x), the abscissa along the rows (y), and the center at zero, which should coincide with either the photo-center or the center of symmetry between beams, according to the definition in geometry calibration (see section 2.4.2). The determination of an empirical 2D IP is useful for assessing several quantities that are frequently needed in spectroscopy, such as:

- spectrograph focus, which is useful for instrument calibration;
- spectral resolution in pixel units (requires wavelength calibration for $\lambda/\Delta\lambda$ units);
- pseudo-slit illumination pattern, which is useful for geometry calibration and determination of background region;
- pseudo-slit tilt angle, which is useful for extraction aperture given the maximum illumination for a given slit shape;
- inter-order contamination level, which is useful to evaluate the amount of flux contamination between orders and/or beams.

Note that the 2D IP is sometimes also called transfer function. The transfer function is an instrument characteristic that translates a given model spectrum into the measured spectrum. Therefore, it potentially allows one to produce a simulated echelle image for any given model spectrum. This characteristic can be useful for simulation of data, measurements of variable line profiles, high-precision radial velocity measurements, etc.

Let us first define an oversampled 2D IP (Φ), which is a matrix with elements $\phi_{i',j'}$, where i' is the sub-pixel index in the x -direction and j' the sub-pixel index in the y -direction. The oversampling factors are positive integer numbers given by X_{samp} and Y_{samp} . The IP is truncated at a given size $X_{\text{size}} \times Y_{\text{size}}$, which is given in pixel units. Therefore, the IP coordinates (x', y') , in image pixel units, can be calculated for a given sub-pixel (i', j') by:

$$x'_{i'} = \frac{(1 + 2i')}{X_{\text{samp}}} - \frac{X_{\text{size}}}{2}, \quad (26)$$

$$y'_{j'} = \frac{(1 + 2j')}{Y_{\text{samp}}} - \frac{Y_{\text{size}}}{2}, \quad (27)$$

where the sub-pixel indexes lie in the range $[i' = 0, \dots, N_{x'} - 1; j' = 0, \dots, N_{y'} - 1)$, where

$$N_{x'} = X_{\text{samp}} \times X_{\text{size}}, \quad N_{y'} = Y_{\text{samp}} \times Y_{\text{size}}. \quad (28)$$

Typically, for ESPaDOnS, we set an IP with size of 30 pixels (columns) by 6 pixels (rows), and oversampled by a factor of 5 in both directions.

The empirical measurements of a 2D IP depend on two preliminary calibrations. First the geometry that gives a polynomial function $x_c(y)$ for the center of an order, as explained in section 2.4. Then the center of spectral lines, given by $x_c(y_l)$, provided by the line-detection algorithm, which is explained below.

2.5.2. OPERA Line Detection Algorithm

The line-detection is similar to the peak-detection algorithm described in section 2.4.3. For line-detection we make use of a previously determined 2D IP to calculate the cross-correlation between the 2D IP and the image along the order trace function given by geometry calibration. An important detail for the calculation of the cross-correlation is that this function is sensitive to saturated pixels and cosmic rays. So it is important that a bad-pixel rejection method be included in this calculation. It becomes particularly important when the line detection algorithm is applied to Th-Ar comparison exposures, which tend to have highly saturated lines in the red part of the spectrum. The cross-correlation is calculated as follows:

$$(C' \star \Phi)(y) = \frac{\sum_{i',j'}^{N_{x'},N_{y'}} (C'_{i',j'} - \langle C' \rangle)(\phi_{i',j'} - \langle \phi \rangle)}{\sqrt{\left[\sum_{i',j'}^{N_{x'},N_{y'}} (C'_{i',j'} - \langle C' \rangle)^2 \right] \left[\sum_{i',j'}^{N_{x'},N_{y'}} (\phi_{i',j'} - \langle \phi \rangle)^2 \right]}}, \quad (29)$$

where quantities in the angle brackets are the average of useful points, given by:

$$\langle C' \rangle = \frac{\sum_{i',j'}^{N_{x'},N_{y'}} C'_{i',j'}}{n_{x'}n_{y'}}, \quad \langle \phi \rangle = \frac{\sum_{i',j'}^{N_{x'},N_{y'}} \phi_{i',j'}}{n_{x'}n_{y'}}, \quad (30)$$

for $n_{x'}$ and $n_{y'}$ being the number of points accounted in the sum, which may be different than $N_{x'}$ and $N_{y'}$, since pixels may be rejected. The same applies for equation 29, where all the sums must use or reject the same set of pixels.

Note that the pixel values ($C'_{i',j'}$) of the master comparison image are only known for image indexes (i, j) , therefore we have to use the following relationship to convert between the image and sub-pixel indexes:

$$i = \text{FLOOR}(x_c + x'_{i'}), \quad (31)$$

$$j = \text{FLOOR}(y_c + y'_{j'}), \quad (32)$$

where the function $\text{FLOOR}()$ rounds the number in the parenthesis downward to the closest integer, $x_c(y)$ is the trace polynomial and y_c is sampled in steps of 1 pixel throughout the extension of the image. Equations 26 and 27 give $x'_{i'}$ and $y'_{j'}$.

Analogously to the peak-probability defined in equation 21 let us define here the line-probability:

$$p_{\text{line}} = p_{\text{localmax}} \times p_{\text{globalmax}} \times (\mathbf{C}' \star \Phi), \quad (33)$$

where p_{localmax} is a boolean value with the same meaning as in equation 21. The probability $p_{\text{globalmax},i}$ of a given flux value $S(y_j)$ being the maximum within a given window range $(y_j - A/2 < y < y_j + A/2)$, for an aperture A , calculated as:

$$p_{\text{globalmax},j} = \frac{\sum_{k=0}^{k < A/2} (D_{j-A/2+k+1} - D_{j-A/2+k}) + \sum_{k=A/2+1}^{k < A} (D_{j-A/2+k-1} - D_{j-A/2+k})}{\sum_{k=0}^{k < A/2} |D_{j-A/2+k+1} - D_{j-A/2+k}| + \sum_{k=A/2+1}^{k < A} |D_{j-A/2+k-1} - D_{j-A/2+k}|}, \quad (34)$$

where $D_j = [S(y_j) - S_{\text{bkg}}]$, and S_{bkg} is the background flux within the window, which is given by a linear interpolation of the edge values, $S(y_{j-A/2})$ and $S(y_{j+A/2})$. Note that $p_{\text{globalmax}}$ here is conceptually equivalent to the quantity defined in equation 21, however in equation 34 we deal with flux measurements $S(y)$, not a convolved quantity. The extraction of this flux will be explained in detail in section 3.1. Another caveat here is that this approach works well even for blended lines, where the center of two peaks appear closer than the line

width. Also for this reason, the aperture considered for the calculation of p_{localmax} can be chosen as a fraction of A .

The cross-correlation term in equation 33 plays directly as a probability factor, since it is a quantity normalized between -1 and 1 . Negative values are excluded, since this algorithm is intended only for the detection of emission lines. OPERA also has an extended application of this algorithm for absorption lines, which will be presented later. Figures 10 and 11 show the same section of a Th-Ar and Fabry-Perot spectra and the respective probabilities for line detection as described in this section. An interesting aspect shown in these figures is that the cross-correlation spectrum presents a considerably higher resolution than the flux spectrum. This feature is used here to improve the identification of line positions. However one should note that this could potentially be used to characterize the morphology of spectral features and to improve any measurement that depend on this feature.

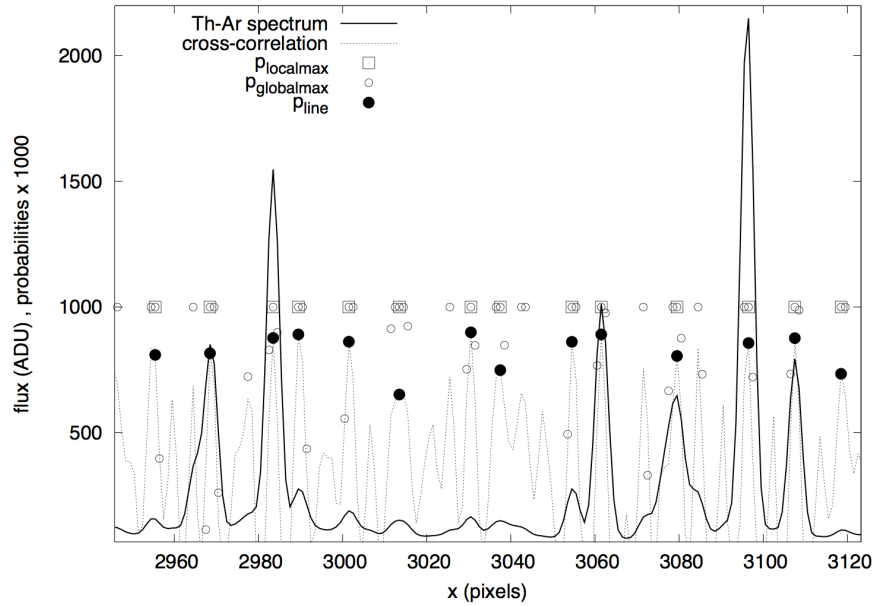


Fig. 10.— Section of a Th-Ar spectrum showing the flux (solid line), and the probability quantities from equation 33, which are multiplied by 1000 here for better visualization.

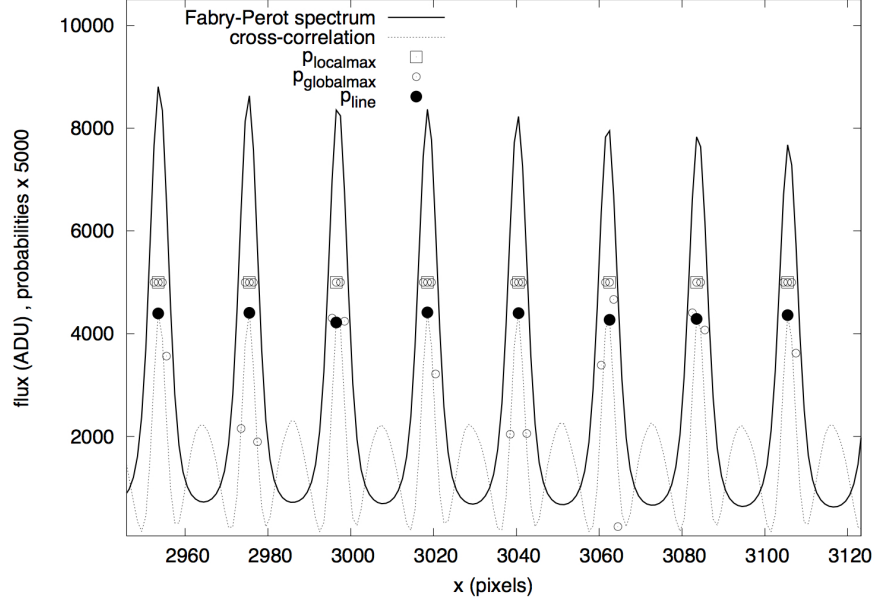


Fig. 11.— Section of a Fabry-Perot spectrum showing the flux (solid line), and the probability quantities from equation 33, which are multiplied by 5000 here for better visualization.

2.5.3. Empirical 2D IP

Once spectral lines have been detected the module performs empirical measurements of the 2D IP. In fact the measurements will lead to a calibration model of the IP. We choose a model which is a function of the distance $d(x, y)$ (in pixels) along the dispersion direction, which defines the dispersion axis and is given by the length of the trace polynomial, or the path integral:

$$d(y) = \int_{y_0}^y \sqrt{1 + \left(\frac{d[x_c(y')]}{dy'} \right)^2} dy' \quad (35)$$

The IP model $\Phi'(d)$ consists of a matrix of polynomials with elements given by $\phi'_{i,j'}(d)$, i.e. one polynomial for each sub-pixel. This allows our calibration model to account for possible optical field distortions or wavelength-dependent variations in the illumination profile.

The calibration is done by first reading IP values from the image pixels into an over-sampled 2D IP. Then we fit a 2D low-order polynomial to the outer frame to obtain the background. The outer frame consists of all sub-pixels in the edge of the IP window. Then we subtract the background model from the data and normalize the IP such as the sum of all sub-pixels is 1. Then we take the median of each sub-pixel for a given bin containing several lines, which must be greater than a given minimum number of lines (to avoid regions with insufficient number of lines). Finally, we fit a polynomial in the dispersion direction for each sub-pixel data, which results in the IP calibration model.

Figure 12 shows examples of measurements of the 2D IP for SP2 mode of ESPaDOnS using four different oversampling factors (1, 3, 5, and 8) in both directions X_{samp} and Y_{samp} . Note that even for a factor of 8 the measurements still show variations in the sub-pixel scale, which means that information can still be recovered at this level of precision. Figures 13 (SP2, Fabry-Perot), 14 (SP2, Th-Ar), 15 (POL, Fabry-Perot), and 16 (POL, Th-Ar) show samples of the 2D IP measurements for all detected orders of ESPaDOnS for SP2 and POL modes using Fabry-Perot and Th-Ar exposures, respectively. These samples were evaluated at the center of the image.

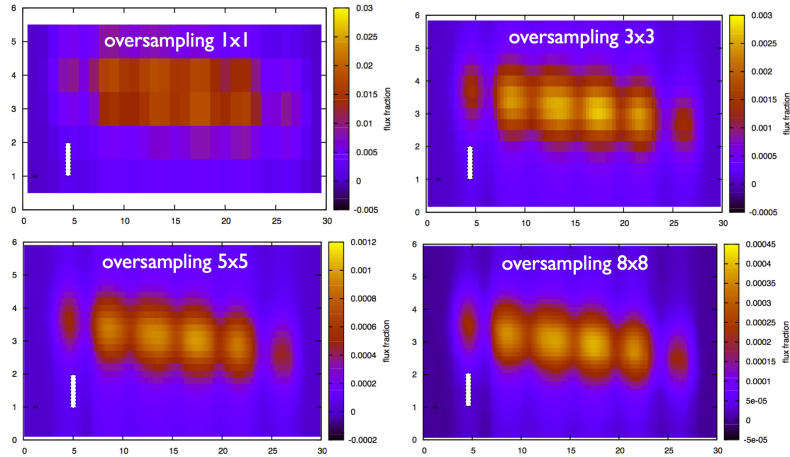


Fig. 12.— Example of measurements of a 2D IP for a single order in SP2 mode using four different oversampling factors, as indicated in the panels. The white rectangles represent the size of an image pixel.

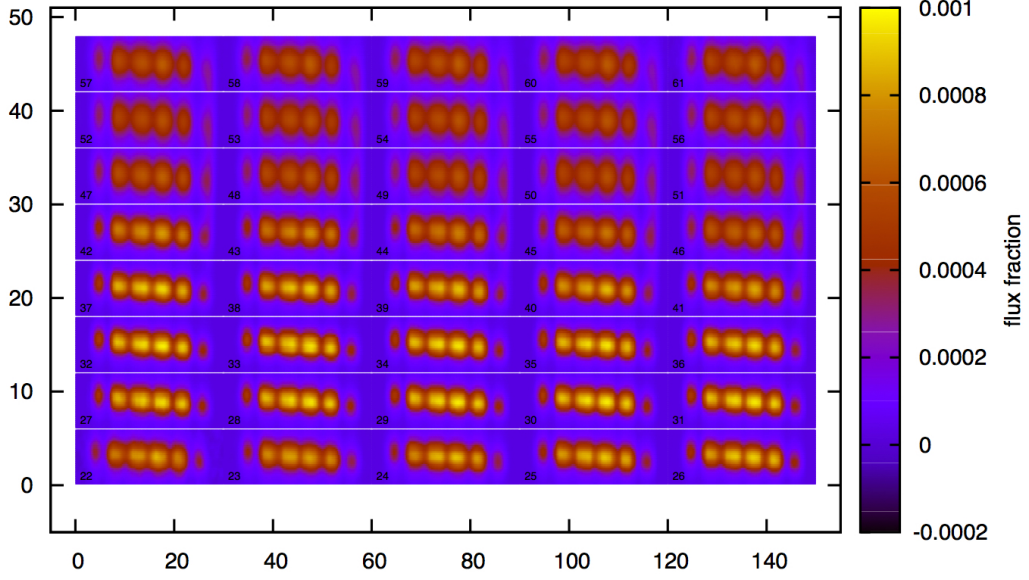


Fig. 13.— Empirical 2D IP for all spectral orders of ESPaDOnS in SP2 mode using a Fabry-Perot exposure.

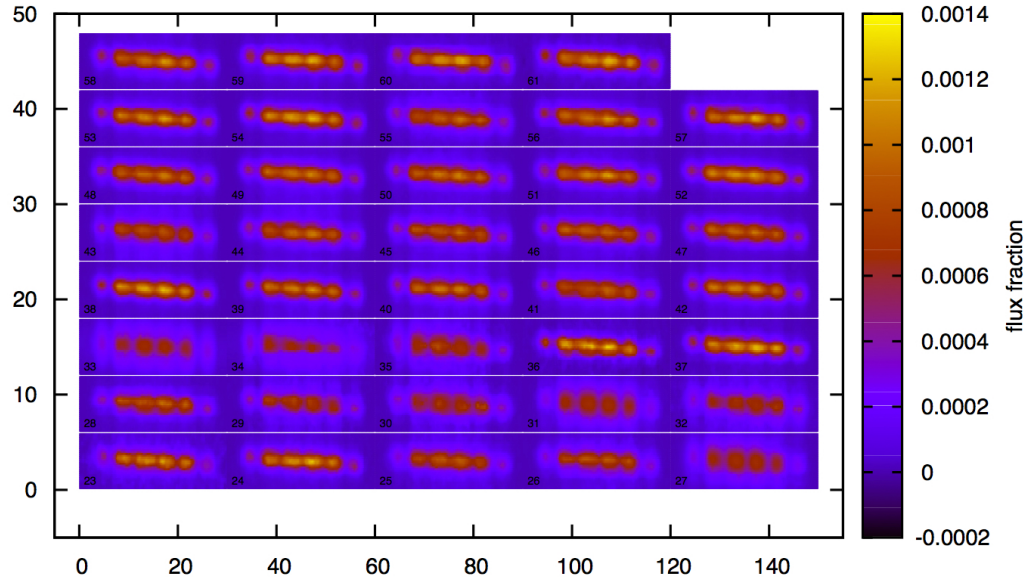


Fig. 14.— Empirical 2D IP for all spectral orders of ESPaDOnS in SP2 mode using a Th-Ar exposure.

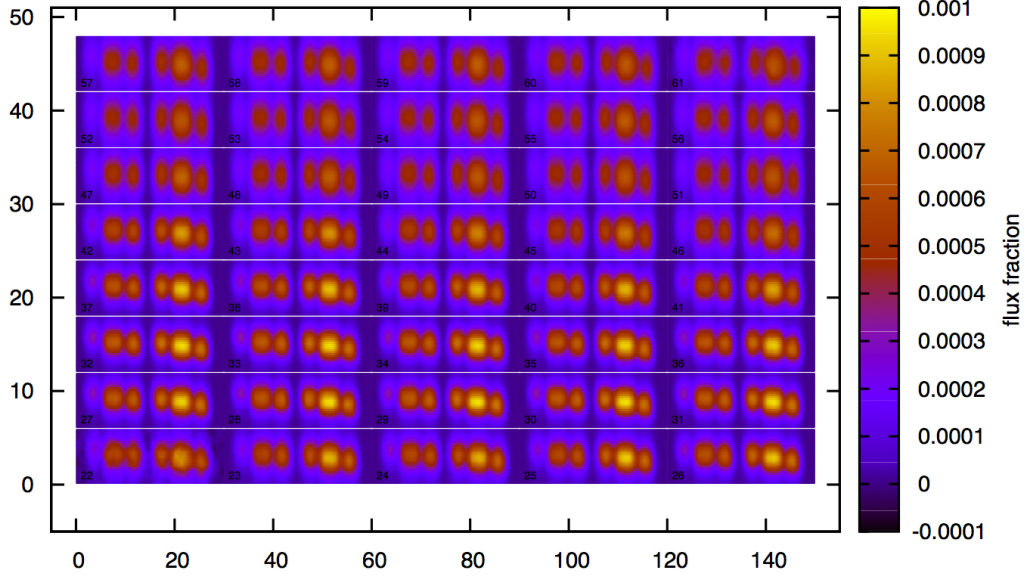


Fig. 15.— Empirical 2D IP for all spectral orders of ESPaDOnS in POL mode using a Fabry-Perot exposure.

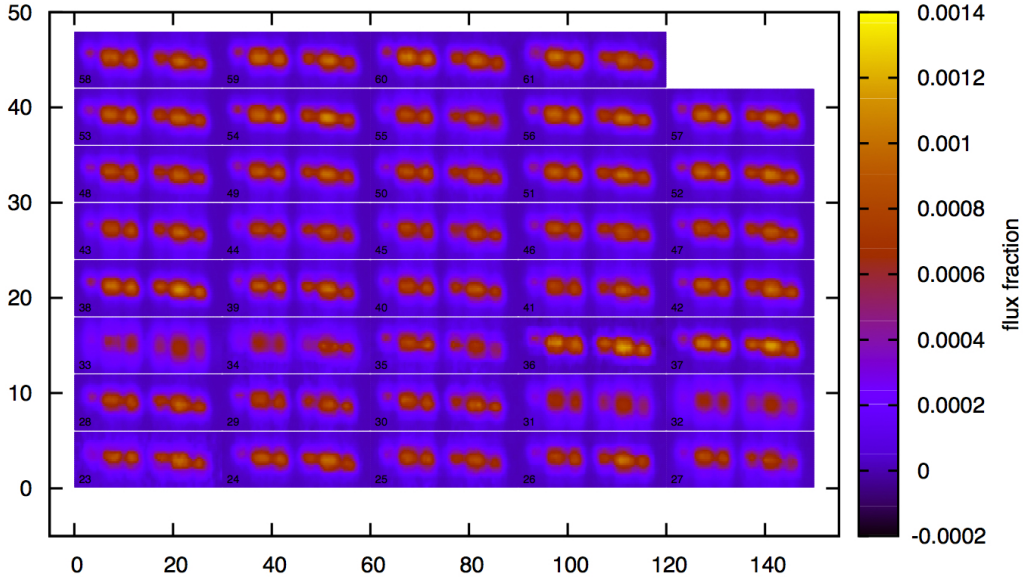


Fig. 16.— Empirical 2D IP for all spectral orders of ESPaDOnS in POL mode using a Th-Ar exposure.

2.6. Extraction Aperture Calibration

The module `operaExtractionApertureCalibration` performs measurements of the tilt angle of a rectangular aperture for extraction. The aperture shape is a tilted rectangle, allowing this to be divided into a number of smaller tilted rectangles for independent beam flux measurements as illustrated in figure 17. Two additional apertures can be added on both sides of the main aperture for background flux measurements. The tilt angle is calibrated by performing a robust linear fit to the photo center of an empirical 2D IP as illustrated in figure 18. This method obtains an aperture for extraction that is aligned with the monochromatic image of the pseudo-slit, even for irregular shaped profiles like in ESPaDOnS, thus allowing unbiased flux measurements of each spectral element. In particular, for polarimetric measurements it is common to find cross-talk contamination between polarization modes, which in some cases come from non-ideal extraction apertures. Figure 19 shows examples of the 2D IP for SP2 mode where the aperture sub-pixels are masked out. In these examples two different heights are used, 1.0 and 0.6 pixel.

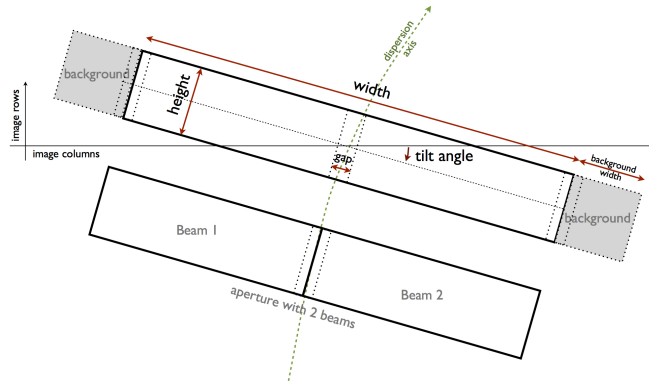


Fig. 17.— Configuration for the aperture for extraction.

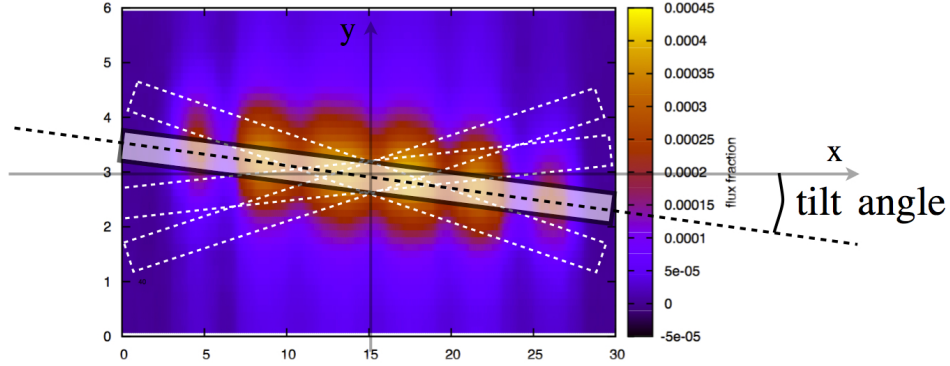


Fig. 18.— Illustration of how the tilt angle is measured with respect to the 2D IP.

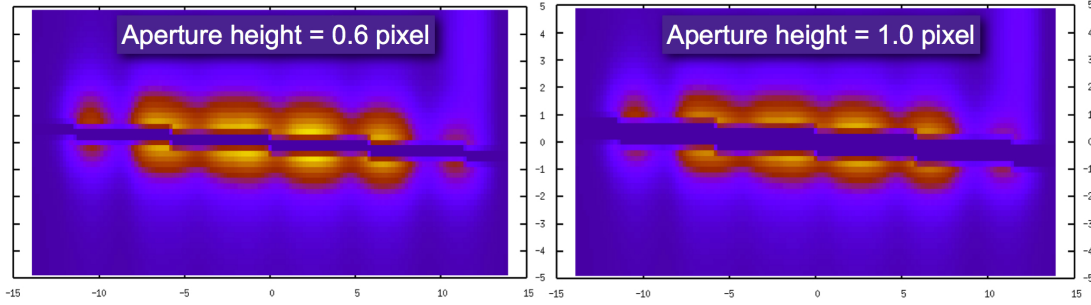


Fig. 19.— Example of two apertures with heights of 0.6 (left panel) and 1.0 pixel (right panel). The 2D IPs are plotted with the aperture sub-pixels masked out for better visualization.

2.7. Wavelength Calibration

The module `operaWavelengthCalibration` performs the pixel-to-wavelength calibration, where it detects spectral lines from a Th-Ar comparison exposure and combine these lines with known atlas data to create a calibration polynomial solution of the form:

$$\lambda(d) = a_0 + a_1d + a_2d^2 + a_3d^3 + \dots + a_{n_p}d^{n_p}, \quad (36)$$

where d is the distance vector given by equation 35, $a_0, \dots, a_{n_p}$ are the coefficients and n_p is the maximum order of the polynomial. For ESPaDOnS we found that it is sufficient to use a polynomial with $n_p = 3$.

The Th-Ar spectrum is extracted with the Raw Sum extraction method (see section

3.1). The lines in the Th-Ar spectrum are detected from the cross-correlation between the comparison image and the 2D IP using the line detection algorithm explained in section 2.5.2. Once the lines are detected it divides the lines into groups (also called features), where the grouping is defined by the separation between lines, which must be less than a given minimum distance to be in the same feature. Then a multiple gaussian model plus a slope function (for background) is used to fit each feature. This model is used to obtain the line positions, which should account well for blended lines.

The calibration starts from an initial guess (wavelength at the center of each order and wavelength scale) to select a set of spectral lines from the reference atlas. OPERA uses the atlas of Lovis & Pepe (2007). The spectral lines in the atlas are matched against the lines detected in the Th-Ar spectrum. The match is performed by searching the highest correlation between the line positions in the image and in the atlas. This gives a vector of wavelengths (in nm) and distances (equation 35; in pixel units) for a set of spectral lines. Then a sigma-clip filter is applied to these data in order obtain a cleaner data set, which is used to obtain a new pixel-to-wavelength solution by fitting a polynomial function (equation 36) to the data. An iterative process is applied to refine the number of matched lines and then refine the model. The process is run several times until it reaches convergence or until a given maximum number of iterations.

Figure 20 shows an example of the calibrated Th-Ar spectra for three orders (blue line), the Lovis & Pepe (2007) Th-Ar atlas (magenta line), and the detected lines that have been matched with the atlas (red circles), which are the points used to obtain the pixel-to-wavelength solution.

In figure 21 the top-left panel shows the wavelength precision obtained by the root mean square (RMS) of residuals, top-right panel shows the spectral resolution $R = \lambda/\Delta\lambda$, bottom-right panel shows the radial velocity precision in m/s for both a clean sample and the full set of matched lines, and finally, bottom-right panel shows statistics on the number of lines matched between the extracted spectrum and the atlas. These results have been obtained from a minimal number of images for calibration of ESPaDOnS data in SP2 mode.

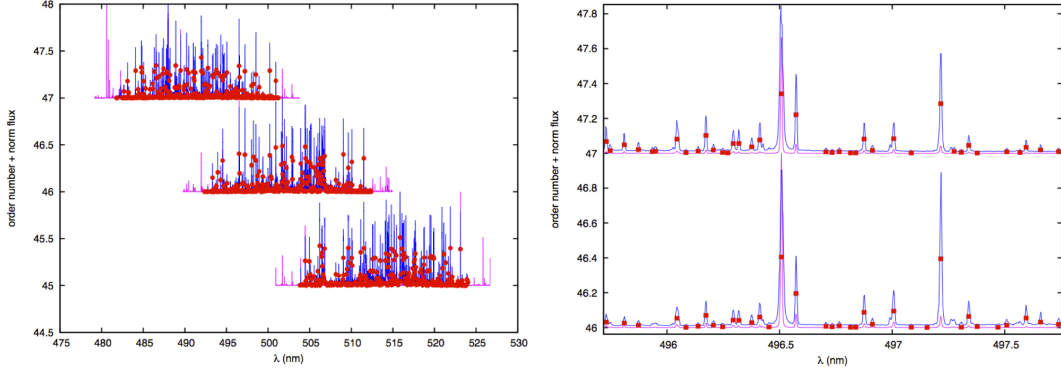


Fig. 20.— Th-Ar extracted spectra (blue), Th-Ar reference atlas (magenta), and detected spectral lines that have been matched (red circles). Left panel shows the wavelength calibrated Th-Ar spectra for three full orders and right panel shows a zoom of the spectra of two orders for a region where they overlap.

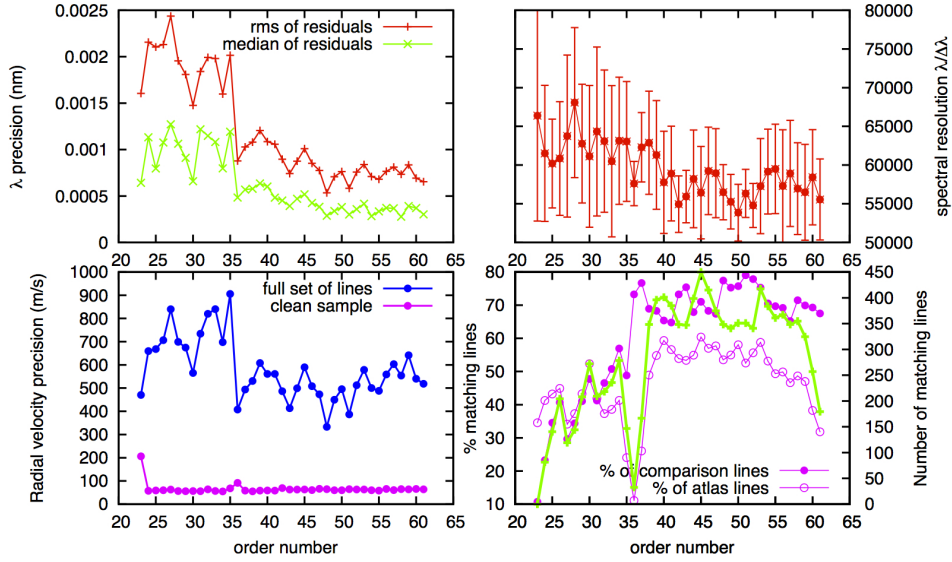


Fig. 21.— Statistical quantities for wavelength calibration.

2.8. Echelle Dispersion Calibration

The wavelength calibration described in section 2.7 is obtained for each spectral order individually and gives a different level of accuracy for each order. This is due to the fact that Th-Ar does not present a uniform density of spectral lines for all orders and the lines are not homogeneous. This results in a variable wavelength accuracy over the spectrum. In order to make the solution uniform OPERA implements an additional step in the wavelength calibration, which combines the solution from all orders to find a global solution. This is done by the module `operaEchelleDispersionCalibration` and the procedure for calibration is explained as follows.

Let us first redefine equation 36 using the index k to represent each spectral order:

$$\lambda_k(d) = \left[\sum_{n=0}^{n \leq 4} a_n d^n \right]_k. \quad (37)$$

The wavelength calibration described in section 2.7 provides a set of N_o (number of orders) solutions, each given by a polynomial as in equation 37. The relationship between order number and wavelength is given by the echelle grating dispersion (e.g., Ballester & Rosa 1997) where

$$\lambda \propto k^{-1}. \quad (38)$$

A function like equation 38 can be expanded into a Laurent polynomial, which differs from ordinary polynomials that it includes the negative degrees. Therefore, OPERA fits a Laurent polynomial to each coefficient n of equation 37 to data obtained from all spectral orders. This will give a global solution that can be obtained for any order at any distance. Figure 22 shows a separate plot for each coefficient a_n of equation 37 obtained for all orders and also the Laurent polynomial fit model obtained from the calibration. In order to improve the quality of our fit and also to deal with outliers we have implemented a piecewise median filter, which excludes points with absolute deviation greater than three times the median absolute deviation of data around a local robust linear fit. Then it applies a Levenberg-Marquardt method to fit the Laurent polynomials to the filtered data. In figure 22 the hollow circles represent outliers that have been excluded using this method.

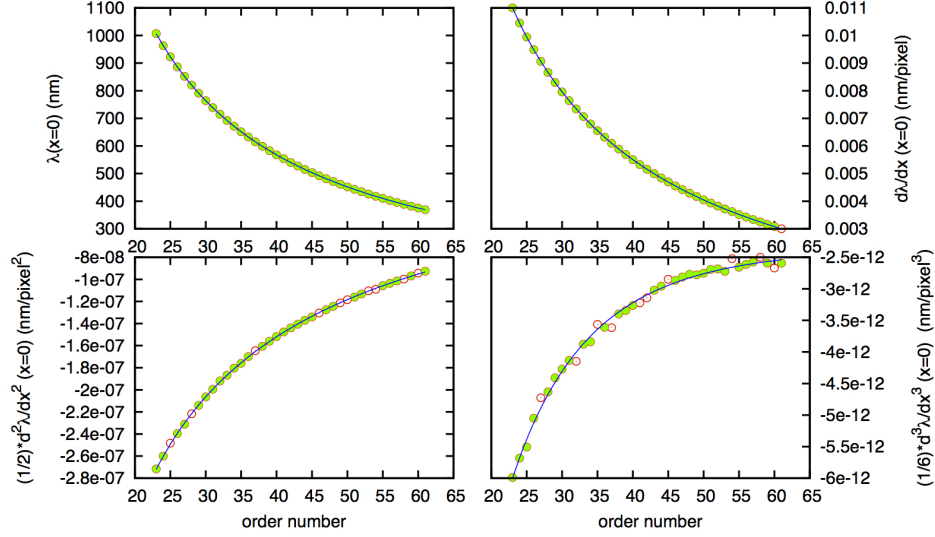


Fig. 22.— The data points (red circles) are the coefficients of the pixel-to-wavelength polynomial, where each panel shows one of the coefficients for all spectral orders. Hollow circles are data points excluded by the median filter, as explained in the text. The lines are the fit Laurent polynomials for the echelle dispersion calibration.

3. Reduction

Reduction is defined here as the steps to measure the energy flux and polarimetric information from the two-dimensional object images and also to perform calibrations and other measurements that make use of object exposures. Below we list the OPERA reduction modules followed by a short description of their functionalities.

1. `operaExtraction` - extracts the energy flux spectrum;
2. `operaNormalize` - normalizes spectrum by the continuum;
3. `operaFluxCalibration` - applies an instrument response function and a flux conversion factor to calibrate the flux;
4. `operaPolar` (only for POL mode) - calculates polarimetry using a sequence of 2 or 4 polarimetric images;
5. `operaPolarIntensity` (only for POL mode) - calculates the total flux measured from the two input fibers;
6. `operaStarPlusSky` (only for SP1 mode) - subtracts the flux measured in the sky fiber from the flux measured in the object+sky fiber;
7. `operaStarOnly` (only for SP2 mode) - calculates the flux measured from the single fiber;
8. `operaTelluricWavelengthCorrection` - performs a correction in the wavelength calibration based on measurements of telluric lines in the object spectrum;
9. `operaBarycentricWavelengthCorrection` - applies a radial velocity shift correction in the wavelength calibration to switch between topocentric to the Solar System barycentric system of coordinates.

3.1. Extraction of Spectra

The extraction of spectra is performed by the module `operaExtraction`. It consists of steps for obtaining the energy flux information for each wavelength element from the two-dimensional echellogram spectral image. OPERA adopts the fundamental ideas of the optimal extraction algorithm (Horne *et al.* 1986; Marsh *et al.* 1989). The optimal extraction algorithm is applied for an oversampled tilted aperture, in which the tilt angle is measured from a two-dimensional instrument illumination profile as explained in section 2.6. The use of a 2D IP for flux extraction seems to be a necessary calibration for irregular under sampled tilted profiles, typically found in fiber-fed spectrographs that use a slicer to produce the pseudo-slit and with limited CCD pixel size, such as in ESPaDOnS.

The three methods for extraction implemented in `operaExtraction` are:

1. RAW: Raw Sum;
2. STD: Standard Extraction (with background subtraction);
3. OPT: Optimal Extraction.

The algorithms for each of these methods are described in more detail as follows.

3.1.1. Raw Sum

This method obtains the energy flux density spectrum by counting the total number of photo-electron events in each spectral element. The flux is given by the sum of sub-pixel values over an extraction area defined by the extraction aperture calibration (see section 2.6) and the variance includes contributions of both the detector readout and photon shot noise. The raw flux $f_{i'j'}$ for each individual sub-pixel is given by:

$$f_{i'j'} = M_{i'j'} \frac{(I_{i'j'} - B'_{i'j'})GA_s}{\mathfrak{F}_{i'j'}}, \quad (39)$$

where $I_{i'j'}$ is the raw value of an image pixel, $B'_{i'j'}$ is the raw value of a master bias image, $\mathfrak{F}_{i'j'}$ is the normalized pixel sensitivity function (flat-field), G is the detector gain, A_s is the fractional area of a sub-pixel, i.e.,

$$A_s = \frac{1}{X_{\text{samp}}Y_{\text{samp}}}, \quad (40)$$

and $M_{i'j'}$ is a bad pixel mask given by:

$$M_{i'j'} = \begin{cases} 1 & \text{if } I_{i'j'} < \text{SATURATION} \ \& \ m_{i'j'} = 1 \\ 0 & \text{otherwise,} \end{cases} \quad (41)$$

where the quantity $m_{i'j'}$ is a boolean for a pre-defined bad pixel mask. Note that one can easily obtain the image pixel indexes (i, j) from the sub-pixel indexes (i', j') using equations 31 and 32.

The output spectrum is given by an array of spectral elements, where each element flux $S_{\text{raw}}(d)$ and the variance $\sigma_{\text{raw}}^2(d)$ are calculated as the sum of sub-pixels within an aperture placed at distance d , i.e.,

$$S_{\text{raw}}(d) = \gamma \left(\sum_{i'}^{N'_x} \sum_{j'}^{N'_y} f_{i'j'} \right) \quad (42)$$

$$\sigma_{\text{raw}}^2(d) = \gamma \sum_{i'}^{N'_x} \sum_{j'}^{N'_y} (2\sigma_e^2 \sqrt{A_s} + f_{i'j'}), \quad (43)$$

where N'_x and N'_y are the total number of sub-pixels within the aperture in each respective direction and γ is a weight function to compensate missing bad pixels, which is given by the fraction of useful sub-pixels in the array,

$$\gamma = \frac{N'_x N'_y}{n'}, \quad (44)$$

for n' being the total number of good sub-pixels, i.e.,

$$n' = \sum_{i'}^{N'_x} \sum_{j'}^{N'_y} M_{i'j'}. \quad (45)$$

In equation 43 the variance has two terms in the sum. The first is to account for the detector noise and the second for the photon “shot” noise, assuming a Poisson distribution for the probability of detecting a given photo-electron event. Note that in the first term the factor 2 is due to the operation of bias subtraction. The factor $\sqrt{A_s}$ is due to the division of a pixel into sub-pixels, where the sum of variances $\sigma_{i'j'}^2$ of sub-pixels within a single pixel must be equal to the pixel variance σ_{ij}^2 , i.e.,

$$\sigma_{ij}^2 = \sum_{i'}^{X_{\text{samp}}} \sum_{j'}^{Y_{\text{samp}}} \sigma_{i'j'}^2, \quad (46)$$

therefore, by assuming equal variances for all sub-pixels, equation 46 can be rearranged to calculate the error of a given sub-pixel, i.e.,

$$\sigma_{i'j'} = \frac{1}{\sqrt{X_{\text{samp}} Y_{\text{samp}}}} \sigma_{ij}, \quad (47)$$

where the factor in the righthand side is given by $\sqrt{A_s}$, from equation 40.

The spectrum S_{raw} in equation 42 is given in units of photo-electron events per spectral bin (e-/bin), where the bin size is given by the choice of the aperture height (in pixels), which can be converted to wavelength ($\Delta\lambda$) by using the pixel-to-wavelength calibration obtained in sections 2.7 and 2.8. Notice that each spectral element defined in equations 42 and 43 can be obtained for any given distance d . Therefore, in order to obtain the full spectrum one needs to sample the function S_{raw} over the entire range of a spectral order. Because the extraction aperture is defined as a tilted rectangle, the steps to sample distance d for the construction of the spectrum is calculated such as the top line of the rectangle for the aperture at a given position d must coincide with the bottom line of the aperture rectangle of an adjacent spectral element at position $d + \Delta d$.

One may be interested in the signal-to-noise ratio per spectral bin, which can be calculated using equations 42 and 43, as follows:

$$\text{SNR} = \frac{S_{\text{raw}}}{\sqrt{\sigma_{\text{raw}}^2}}. \quad (48)$$

3.1.2. Standard Extraction

The Standard extraction method is similar to the Raw Sum method, where the Standard method evaluates and subtracts the background scattered light from the raw flux. Let us consider the background flux b_k for a given bin of fluxes indexed by k , which is centered at a given distance d_k . The background flux $b_k(d)$ is calculated by taking the median of flux values (S_{raw}^b) over a range of spectral elements in the bin, where each element is calculated using equations 42 and eq:rawsumspectralelementvariance, but considering only sub-pixels in the background apertures, as defined in section 2.6. Thus, the background flux per bin k

is given by:

$$b_k(\bar{d}_k) = \text{MEDIAN} [S_{\text{raw}}^b(d = d_i, \dots, d_f)] , \quad (49)$$

where d_i and d_f are the first and last distance in the bin range. The distance for the center of each bin is given by $\bar{d}_k = d_i + (d_f - d_i)/2$. All bins over the extension of an order are combined using a cubic spline interpolation along the dispersion direction, which gives the background flux $b(d)$ at any given distance d or the background flux $b_{i'j'}$ at any given sub-pixel (i', j') . The background error $\sigma_{b,k}$ is given by the absolute deviation of flux measurements (S_{raw}^b) about the median b_k .

Therefore, the standard flux $f_{i'j'}$ for each individual sub-pixel is given by:

$$f_{i'j'} = \left[\frac{M_{i'j'}(I_{i'j'} - B'_{i'j'})G}{\mathfrak{F}_{i'j'}} - b_{i'j'} \right] A_s, \quad (50)$$

then the Standard spectrum $S_{\text{std}}(d)$ can be obtained using equation 42 in exactly the same way as for the Raw Sum spectrum, and the standard variance, which includes the background term σ_b^2 , is given by

$$\sigma_{\text{std}}^2(d) = \gamma \sum_{i'}^{N'_x} \sum_{j'}^{N'_y} \left[(2\sigma_e^2 + \sigma_b^2) \sqrt{A_s} + f_{i'j'} \right]. \quad (51)$$

3.1.3. Optimal Extraction

OPERA implements the optimal extraction algorithm by Horne *et al.* (1986) and Marsh *et al.* (1989). Although OPERA calculates the spatial profile (weight function) in a different way. The profile is constrained to sub-pixels lying within the extraction aperture, where each sub-pixel is fit by a polynomial function, similar to the way the 2D IP is measured in section 2.5. In principle, fiber fed spectrographs could use flat-field images to measure the spatial profile, however it seems that profiles obtained directly from the object image provide better results. The latter seems to work well even for very faint objects as it will be shown in the results section. Below we present a summary of the optimal extraction algorithm using a notation that is consistent with the rest of this paper. The optimal extraction method performs the following steps:

1. Extract Standard or Raw spectrum ($S_{\text{std/raw}}$) and respective variances ($\sigma_{\text{std/raw}}^2$), as described in sections 3.1.1 and 3.1.2.
2. Construct spatial profile (Φ), where the fit profile data $\hat{\phi}_{i'j'}$ for each sub-pixel (i', j') is given by:

$$\hat{\phi}_{i'j'}(d) = \text{FIT}_d \left(\frac{f_{i'j'}}{\sum_{i'}^{N'_x} \sum_{j'}^{N'_y} f_{i'j'}} \right), \quad (52)$$

where $f_{i'j'}$ is given by equation 50 and the sum is calculated for sub-pixels lying within the extraction aperture. The function FIT_d represents a fit along dispersion direction analogously to the fit used for the elements of the 2D IP, as described in section 2.5.

3. Revise variance estimates:

$$\sigma_{\text{new}}^2 = \sum_{i'}^{N'_x} \sum_{j'}^{N'_y} \left[(2\sigma_e^2 + b_{i'j'}) \sqrt{A_s} + \hat{\phi}_{i'j'} S_{\text{prev}} \right], \quad (53)$$

where S_{prev} is the flux previously calculated using either Standard/Raw (first iteration) or Optimal (in further iterations) method.

4. Mask optimal outliers. In this step the highly deviant sub-pixel values are identified and ignored in the flux calculation (step 5) and in the refinement of the spatial profile (step 2 - above second iteration). So, the mask function $M_{i'j'}$ is updated as follows:

$$M_{i'j'} = \begin{cases} 1 & \text{if } I_{i'j'} < \text{SATURATION} \ \& \ m_{i'j'} = 1 \ \& \ (f_{i'j'} - \hat{\phi}_{i'j'} S_{\text{prev}})^2 < \eta \sigma_{\text{new}}^2 \\ 0 & \text{otherwise,} \end{cases} \quad (54)$$

where η is an input threshold which defines the cutoff in units of σ^2 . For ESPaDOnS we use as default the value $\eta \approx 7$, which means a 2.5σ cut.

5. Extract optimal spectrum S_{opt} and variances σ_{opt}^2 ,

$$S_{\text{opt}} = \frac{\sum_{i'}^{N'_x} \sum_{j'}^{N'_y} \left(\hat{\phi}_{i'j'} f_{i'j'} / \sigma_{\text{new}}^2 \right)}{\sum_{i'}^{N'_x} \sum_{j'}^{N'_y} \left(\hat{\phi}_{i'j'}^2 / \sigma_{\text{new}}^2 \right)} \quad (55)$$

$$\sigma_{\text{opt}}^2 = \frac{\sum_{i'}^{N'_x} \sum_{j'}^{N'_y} \hat{\phi}_{i'j'}}{\sum_{i'}^{N'_x} \sum_{j'}^{N'_y} \left(\hat{\phi}_{i'j'}^2 / \sigma_{\text{new}}^2 \right)} \quad (56)$$

6. Iterate steps 2 through 5

3.1.4. Tests for Extraction

This section presents some test cases to demonstrate the efficacy of the extraction algorithms discussed in the previous sections. We selected a sample data set of ESPaDOnS images using different configurations to explore as much as possible the capabilities and limitations of algorithms presented here.

Extraction of Calibration Data

As a first test case we present the extracted spectra of calibration data in POL mode. Figure 23 shows the extracted spectra of a single order (order number 35) from each of the following exposures: bias, flat, Th-Ar lamp, and Fabry-Perot. All shows the combined spectrum from the two beams of POL mode, where they have been reduced using both Raw Sum and Optimal methods for extraction as indicated in the figure.

Notice that even the extremely low levels of flux in the bias exposure does not degrade the performance of extraction. Also note that it subtracts a master bias, which explains the negative values. In exposures with a relatively stable amount of flux as in the flat and Fabry-Perot exposures, one can observe very small discrepancy between Raw and Optimal spectra, which means that there are very few optimal outliers and equation 54 rarely returns zero value. The Th-Ar lamp spectrum shows an example of how saturated lines are handled by both Raw and Optimal algorithms, where for the Optimal extraction the results seem to be more robust.

Performance of Extraction at Different Flux Levels

The robustness of extraction algorithms implemented in OPERA and their ability to identify and ignore cosmic rays, bad pixels, and other spurious features at a wide range of flux levels is demonstrated here in the following two test cases.

First a highly saturated spectrum of Vega shown in figure 24, where it is evident that the Optimal spectra (in green) are much less affected by the presence of saturated pixels than the Raw Sum spectra (in red), even though the Raw Sum algorithm also identifies and excludes saturated pixels. This confirms the better performance of Optimal algorithm that was observed in the Th-Ar saturated lines shown in figure 23.

Second, figure 25 presents the extracted spectra for several flux ranges. The top panels show the spectra of two adjacent orders from two detector regions for a relatively faint target with $V = 13.2$ and exposure time of about 1000s and the bottom panels show the spectra

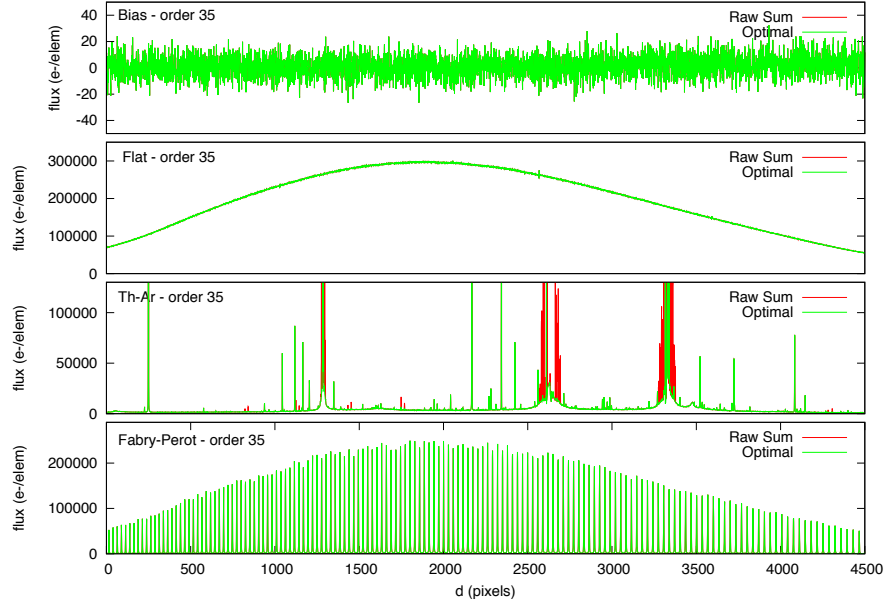


Fig. 23.— From top to bottom it shows the extracted spectra for order 35 from the following calibration exposures: bias, flat, Th-Ar lamp, and Fabry-Perot. The exposures were obtained in POL mode and have been reduced using both Raw Sum (red line) and Optimal (green line) algorithms.

from the same orders for a bright target $V = 3.4$ with exposure time of 10s. The order numbers and the extracted regions are indicated in the figure. The signal-to-noise (SNR) range covered by each of these regions is also shown in the rightmost side of the figure. Notice in the top left panel the two emission lines, which are intrinsic from the source, and have not been mistaken by cosmic rays in the Optimal spectra. Even though cosmic rays and emission lines appear with similar shapes and intensities in the Raw Sum spectra. This demonstrates that cosmic rays, bad pixels, and other spurious events are correctly identified and filtered out by the Optimal algorithm, even considering a wide range of SNR.

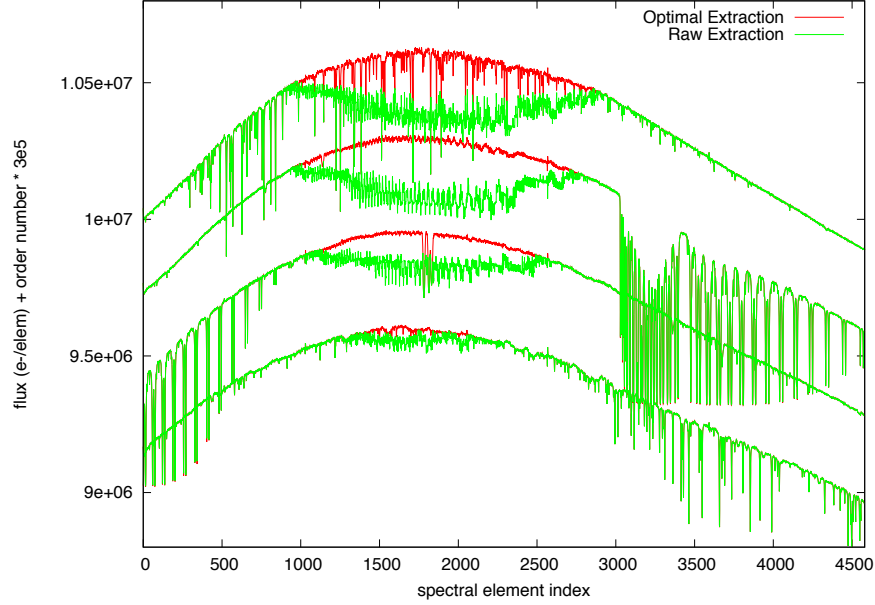


Fig. 24.— Raw Sum (red line) and Optimal (green line) extracted spectra of orders 29, 30, 31, and 32 from a 6 s highly saturated exposure of Vega in POL mode.

High-Resolution Test

An interesting case to test the efficiency of OPERA in extracting the high resolution spectra of ESPaDOnS is shown in figure 26. This presents the extracted spectra in the region around the Sodium (Na) doublet ($D_1 = 589.592$ nm and $D_2 = 588.995$ nm). These observations were carried out in two modes, POL (left panels) and SP2 (right panels), from a 2 s exposure of Vega (HR 7001; α -Lyrae). The doublet can be easily recognized with a depth of $SNR \approx 50$. It is noticeable that the Na features are broaden with irregular shapes. The same spectrum extracted using Libre-Esprit pipeline is shown for comparison, and it presents basically the same shape with similar levels of noise and same spectral resolution. This shows that OPERA extraction performs to a comparable degree as Libre-Esprit.

It should be noted that the nominal resolution of ESPaDOnS from its optical design is about $R=80$ k for POL mode, which is obviously not attained in any of the extracted spectra shown in figure 26. One may look at the sodium doublet model with $R=80$ k (in red) for resolution comparison. This issue is known, but the causes are not well understood. In (ref

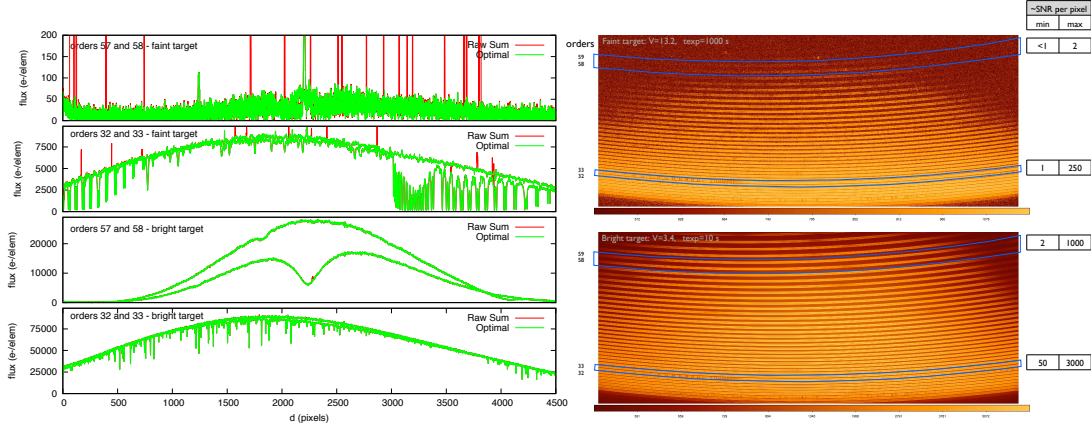


Fig. 25.— Right panels show two echellogram images, where the top image is a 1000 s exposure of a relatively faint $V = 13.2$ star and the bottom image is a 10 s exposure of a bright $V = 3.4$ star. The left panel shows the extracted spectra of orders indicated in the figure, where red lines are the Raw Sum and green lines are Optimal spectra. The rightmost column shows the range of SNR per pixel measured in each section of the images where orders have been extracted.

- Greg memorandum) he used a detector with smaller pixel size to measure the resolution of ESPaDOnS. He measured a higher resolution closer to the nominal value, which makes us believe that this issue is caused by an under sampled spectrum due to the large pixel size of ESPaDOnS detector.

Therefore it indicates that the extracted spectra cannot recover the full resolution of the instrument, even though it has been used an aperture width smaller than the pixel size (≈ 0.7 pixel). However, one may notice in figure 26 the cross-correlation between the 2D IP and the image (black lines), which provides a better resolving power than the extracted spectra. This can be observed in each individual line of the Sodium doublet. Each line is composed by two components, the atmospheric (without significant wavelength shift) and the stellar (shifted to the right). The wavelength shift of Na lines observed in Vega is due to its systemic radial velocity, $v \approx -13.9$ km/s (ref), plus the barycentric radial velocity, $v \approx -13.7$ km/s (see section 3.6), which is roughly what was measured from the distance between the two minimum correlations around Na lines observed in the cross-correlation curves, as indicated in the figure.

In section 2.5 we showed that the 2D IP can be measured with much higher spatial resolution than the pixel sampling. Also, the intrinsic flux fraction distribution of a spectral

element that is given by the shape of the pseudo-slit (piled slices) is more complex than a tilted rectangle, as the one used for extraction. Therefore, the empirical 2D IP represents a much better match to this complex shape, which allows the information obtained from the cross-correlation to be recovered in a finer grid than when using a rectangle. This is basically what limits the resolution of the extracted spectra for an under sampled spectrum like in ESPaDOnS.

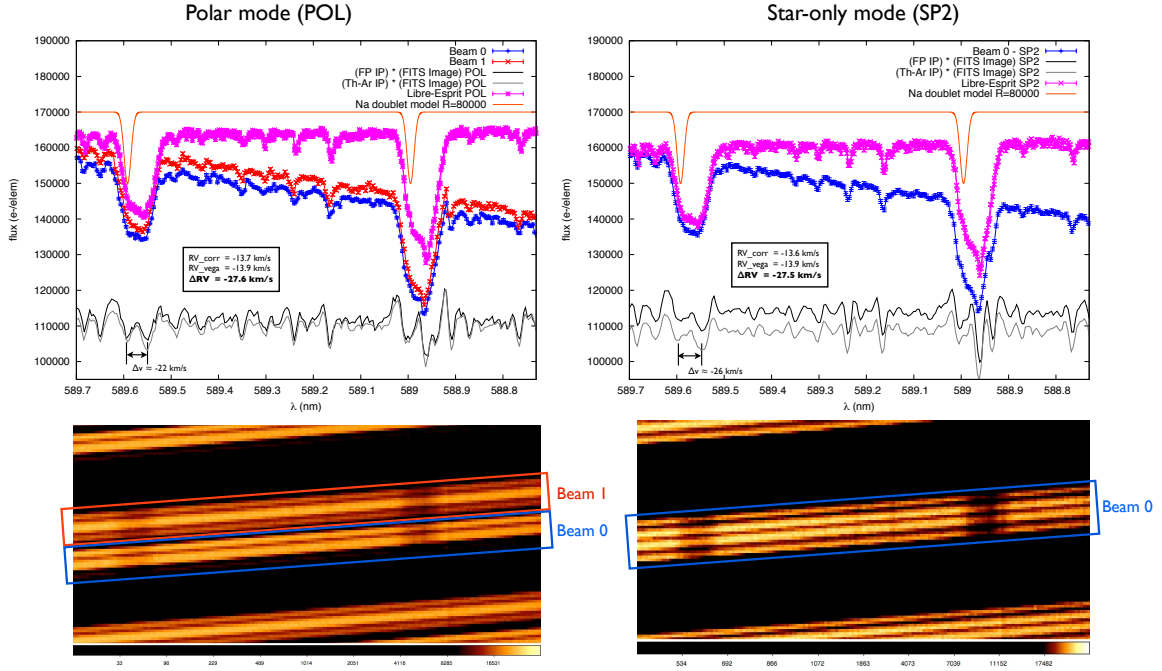


Fig. 26.— Sodium doublet from a 2s exposure of Vega (HR 7001; α -Lyrae). The bottom panels show the section of the FITS images, where the extracted regions are indicated with rectangles in the respective colors for each beam. The top panels show the extracted spectra in POL (left panels) and SP2 (right panels) modes, using both OPERA (blue and red points) and Libre-Esprit (magenta points), where the latter has been rescaled by a factor of 220000 for better visualization. Orange lines represent the sodium doublet model with spectral resolution of $R = 80\text{ k}$, assuming gaussian profiles. Black lines show the cross-correlation between the 2D IP and the FITS image using the OPERA instrument profile calibration obtained from both Th-Ar and Fabry-Perot images, as indicated in the legend.

3.2. Normalization of Spectra

This module detects the continuum emission in an object spectrum and normalizes the flux to the continuum. The continuum is not necessarily the intrinsic emission of the source but a combination of any low frequency signal imprinted on the spectra. This will generate a relative flux which is normalized to 1. The normalization is performed for each spectral order independently, therefore most of the flux within an order is required to contain information of the continuum flux. Broad absorption or emission lines may cause the algorithm to fail. The normalization of a given spectrum $S(d)$ for each spectral order is done in two steps:

1. Detect the continuum flux, $S_c(d)$, using the `operaDetectContinuum` routine, explained in section 3.2.1;
2. Divide the flux of each spectral element by the continuum to obtain the normalized spectrum, i.e., $S_N(d) = S/S_c$.

3.2.1. OPERA Detect Continuum Algorithm

The algorithm to detect continuum is used in the normalization of spectra and also in the flux calibration. OPERA uses the `operaDetectContinuum` routine, which implements the algorithm described as follows.

Let us first consider an extracted spectrum $S(d)$ with N_p spectral elements, $\{S_j; j = 0, \dots, N_p - 1\}$. Then the spectrum is divided into N_s samples, where N_s is given by the total number of points divided by the bin size, i.e., $N_s = N_p/N_b$. Therefore, each sample $k = 0, \dots, N_s - 1$ contains the elements in the range $kN_b \leq j < (k+1)N_b$. Then for each sample k , for $k = 1, \dots, N_s - 2$, do the following:

1. Obtain a robust linear fit (with LADFIT - Least Average Deviation) to points in samples $k - 1$, k , and $k + 1$. This will provide a function $S'(d)$. For the first sample ($k = 0$) the fit is obtained for points in samples k , $k + 1$, and $k + 2$, and the last sample ($k = N_s - 1$) uses points in samples k , $k - 1$, and $k - 2$.
2. Calculate residuals from the linear fit, i.e., $\Delta S_j = S_j - S'(d_j)$;
3. Eliminate residuals greater than the absolute median deviation, i.e., points where $\Delta S_j > \sigma_{\text{abs}}$;
4. Perform a robust linear fit again using only the remaining selected points;

5. Sort residuals in descending order;
6. Go over the 50% highest ranked residuals in the latter step and select the highest positive value lower than a given threshold, which is defined in units of σ_{abs} , i.e., $\Delta S_{\text{max}} = \text{MAX}\{\Delta S_{j'=j_{\text{sel}}}\}$, for j' being points where $(0 < \Delta S_j < n_{\text{cut}}\sigma_{\text{abs}})$, σ_{abs} being the median absolute deviation of the second fit and n_{cut} an input threshold.
7. Then the continuum S_c^k within the sample k is set as the robust fit evaluated in the middle of the sample plus a shift given by the maximum residual selected above, i.e.,

$$S_c^k = S'([d_{(k+1)N_b-1} - d_{kN_b}]/2) + \Delta S_{\text{max}}. \quad (57)$$

The steps above result in a vector of sample data points for the continuum, $\{S_c^k; k = 0, \dots, N_s - 1\}$. Then the continuum $S_c(d)$ can be evaluated at any point of the spectrum by using a cubic spline interpolation. Note that the bin size is a key parameter for normalization. Each object spectrum may contain different characteristics, such as broad band absorption features or emission lines, therefore the most appropriate bin size depends on the nature of the source. A typical value used by OPERA is $N_b = 110$.

3.2.2. Normalization Results

Figure 27 shows an example of extracted spectra for three orders where the normalization algorithm has been applied. The spectrum used was obtained from an object exposure in POL mode. Left panel in figure 27 shows the continuum sample data points S_c^k and the blue line shows the continuum $S_c(d)$ obtained for each spectral elements from interpolations. Right panel in 27 shows the normalized spectra $S_N(d)$ for the same three orders. Figure 28 also shows the normalized spectra $S_N(d)$ of the same object exposure, but showing all 40 orders of ESPaDOnS together. This represents the robustness of our method, where all orders have been adequately normalized independently.

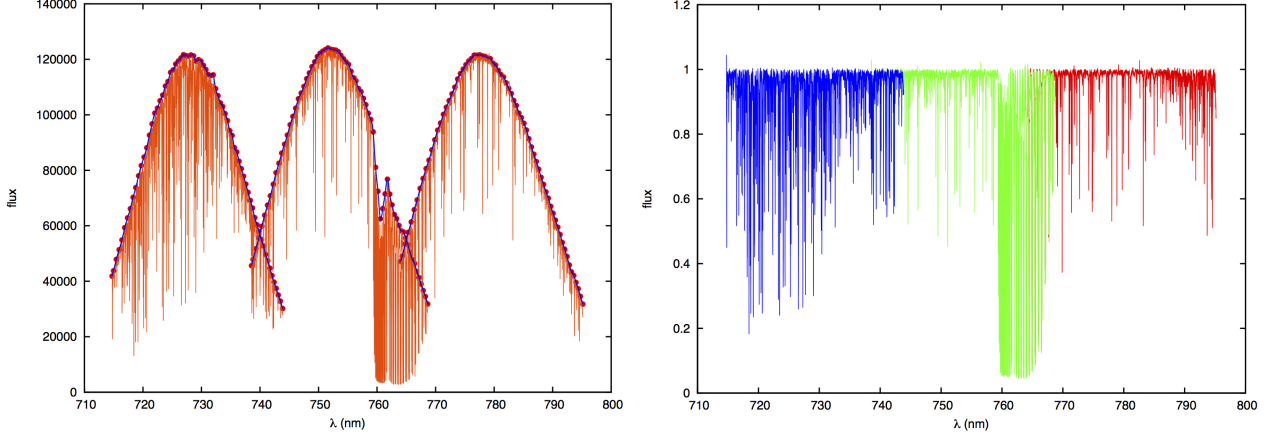


Fig. 27.— Object spectrum for three orders of ESPaDOnS in POL mode. Left panel shows the extracted spectra $S(d)$ for three orders (orange line), the sample data points S_c^k for the continuum (red circles), and the continuum flux $S_c(d)$, evaluated from interpolations (blue line). Right panel shows the normalized flux $S_N(d)$ for the same three orders.

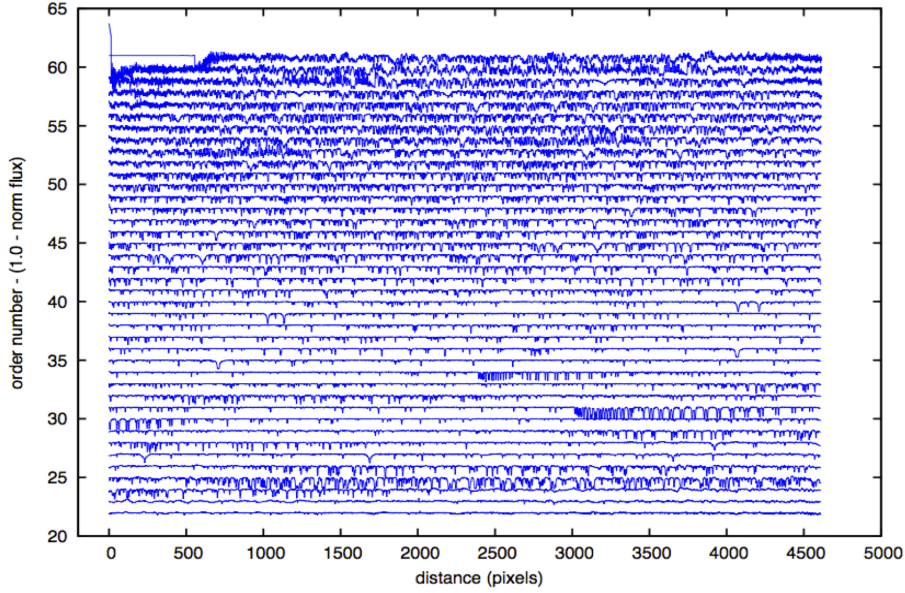


Fig. 28.— Normalized flux of an object spectrum for 40 spectral orders of ESPaDOnS in POL mode.

3.3. Flux Calibration

OPERA performs flux calibration in three steps:

1. **operaCreateFluxCalibration** - creates a flux calibration data file (**.fcal**) out of a single observation of a spectro-photometric calibrator, typically A-type standard stars.
2. **operaMasterFluxCalibration** - combines multiple flux calibration data files into a single master calibration. It also resamples the result to a given spectrum, so the calibration can be directly applied to this spectrum;
3. **operaApplyFluxCalibration** - applies the flux calibration to an uncalibrated extracted spectrum.

The algorithms for these modules are explained as follows. Let us first consider a given uncalibrated continuum spectrum of a standard star, $F_c(\lambda)$, in units of electrons per spectral element (e^-/elem), for spectral elements with size $\Delta\lambda$. Notice that the element size in units of wavelength varies with λ , since the spectral elements are defined by the extraction aperture and it has a fixed height in pixels, where the pixel-to-wavelength scale varies with detector position. Also notice that the uncalibrated continuum spectrum can be obtained directly from the observed spectrum by making use of the detect continuum algorithm described in section 3.2.1. Let us consider now the flux calibration conversion factor $\kappa(\lambda)$ given by:

$$\kappa(\lambda) = \Delta t \frac{S_s}{F_c}, \quad (58)$$

where Δt is the exposure time and S_s is the calibrated flux density spectrum of a given standard star. Therefore κ can be measured for any given spectral element from observations of known standards. Once κ is known one can obtain the calibrated flux S_o of a given science target by applying the calibration,

$$S_o = \kappa(\lambda) \frac{F_o}{\Delta t_o}, \quad (59)$$

where Δt_o and F_o are the exposure time and uncalibrated continuum flux of the science target, respectively.

This approach may work well for observations of standards performed under conditions very similar to the target. However, there are several factors that play against it, such as sky transparency variability, atmospheric seeing variations, fiber transmission, atmospheric absorption, etc. These factors can be minimized by observing a standard star as close as possible in time and sky position of the target, but the low efficiency of echelle spectrographs, at cost of the high-resolution, makes it very difficult to obtain reasonable levels of accuracy for absolute flux calibration. In particular, for ESPaDOnS, the fiber transmission is the

major contributor due to its unpredictable behavior in transmission (see ref). Note however, that most of these factors affect only the overall transmission having a weak dependency with wavelength. Therefore, one can define a quantity $\tau(\lambda)$ that gives the relative spectral response of the instrument rather than the absolute,

$$\tau(\lambda) = \left[\frac{F_c}{F_c(\lambda_m)} \right] \left[\frac{S_s(\lambda_m)}{S_s} \right], \quad (60)$$

where $S_s(\lambda_m)$ is the flux density of the standard star at a given reference wavelength, λ_m , which can be chosen, for example, at the maximum flux or at any reference position. In fact, for better calibration, the reference wavelength should be chosen in a region of the spectrum where the continuum is well exposed and as much as possible free of absorption or emission lines. Notice that the exposure time has been canceled out together with other hidden factors that affect transmission. Then, analogously to equation 59 one can obtain the calibrated flux S_o of a given science target by:

$$S_o = \tau(\lambda) \left[\frac{F_o(\lambda_m)}{F_o} \right], \quad (61)$$

for λ_m being the same reference wavelength as in equation 60. The resulting calibrated spectrum of the target is normalized to 1 at λ_m . Hence one could easily convert S_o to any flux units by multiplying the spectrum by a constant factor, which is given by the calibrated flux value at reference wavelength. For example, Vega has a flux of 9.876×10^7 photons/(s m² nm) at wavelength $\lambda = 548$ nm. Equation 61 may not provide as good accuracy as with equation 58, since it will be limited to the accuracy of a previously calibrated flux value at reference wavelength. However, since equation 61 is insensitive to transmission losses, it may provide a much better precision for the long stability calibration of the instrument. For this reason we have also implemented the `operaMasterFluxCalibration` module to combine multiple flux calibrations, i.e., multiple measurements of κ and τ , into a single master calibration, which can be applied to any data. This is particularly interesting for calibrating data obtained on nights without observations of standards or non-photometric nights.

3.3.1. Flux Calibration Results

3.4. Polarimetry

The module `operaPolar` performs measurements of the degree of polarization for a given Stokes parameter. For spectro-polarimetry, ESPaDOnS is operated in POL mode, which requires a minimum of four exposures in order to create a single polarimetric product for each Stokes parameter (Q, U or V). Each of these exposures is obtained with the retarding plates in specific rotations with interleaving positions, which allow a differential measurement of the degree of polarization. This module uses the flux information obtained from extraction. It also provides the usual intensity spectrum (Stokes I) for the sum of exposures.

The polarimetric unit installed at the cassegrain focus of the telescope allows ESPaDOnS to perform polarimetric measurements of the spectra. OPERA also reduces spectro-polarimetric data. The spectro-polarimetric products consist of the measurements of the degree of polarization of a given Stokes parameter for each spectral element. For spectro-polarimetry, ESPaDOnS is operated in polar mode, which requires a minimum of four sub-exposures per Stokes parameter (Q, U or V), where each of these sub-exposures is obtained with the retarding plates in specific rotations with interleaving positions, which allow a differential measurement of the degree of polarization. Each polarimetric measurement also provides the intensity spectrum (Stokes I). The sections below describe how OPERA performs the polarimetric measurements.

3.4.1. Polarimetric Optical Train of ESPaDOnS

The optical train for the polarimetric unit of ESPaDOnS is illustrated in Figure 29. The incident beam goes through two rotatable half-wave Fresnel rhombs and one fixed quarter-wave Fresnel rhomb. The two half-wave rhombs can be rotated in order to generate the four sub-exposures, which are appropriate for the measurement of each Stokes parameter. Then the beam goes into a Wollaston prism, which splits the light into two orthogonally polarized components. The two output beams are fed into two optical fibers that direct the light to the spectrograph entrance slit. Since the Wollaston prism can only affect linearly polarized light, the quarter-wave rhomb is a necessary component for measurements of circular polarization (Stokes V). The principal plane of the prism is aligned with the reference axis designed by $\theta = 0^\circ$ in the following.

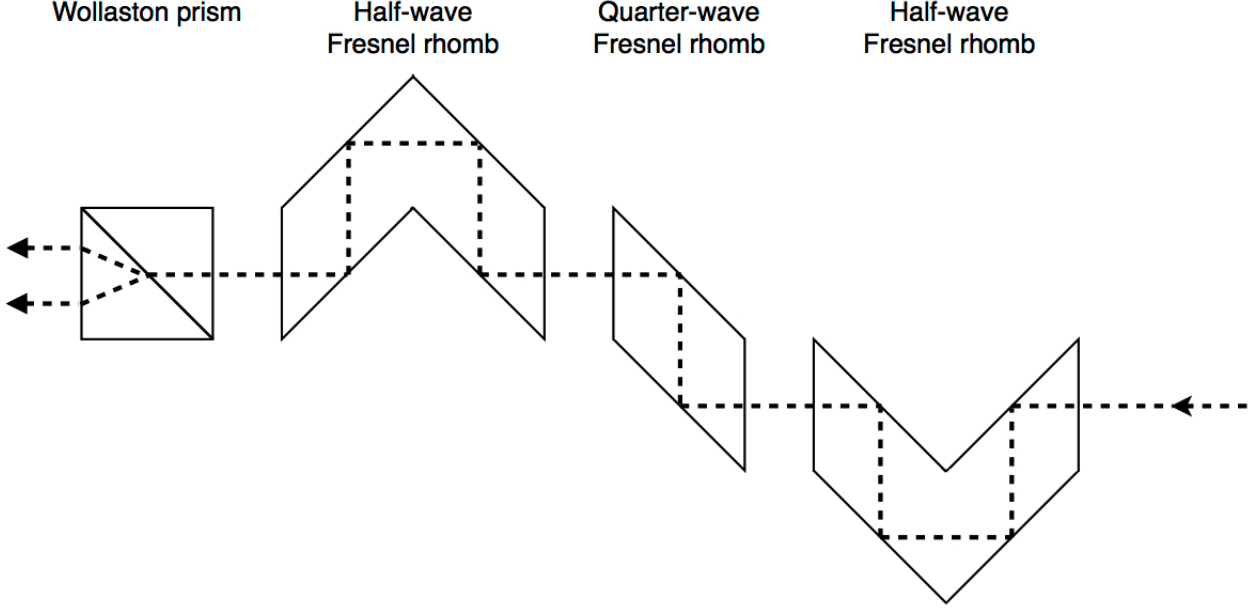


Fig. 29.— Optical train for ESPaDOnS polarimetric unit.

3.4.2. Measurements of the Stokes Parameters

In order to measure the Stokes parameters and consequently the degree of polarization for each Stokes component, ESPaDOnS makes use of four exposures. The rotation position for each rhomb and for each exposure in the sequence are summarized in Table 1.

When a beam interacts with an optical component, it changes its Stokes parameters. Assuming the new set of Stokes parameters can be expressed as a linear combination of the four incident parameters, a transformation matrix known as the Mueller matrix is applied. Each optical component has its unique Mueller matrix.

$$\begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix}_{\text{observed}} = \begin{bmatrix} m_{00} & m_{01} & m_{02} & m_{03} \\ m_{10} & m_{11} & m_{12} & m_{13} \\ m_{20} & m_{21} & m_{22} & m_{23} \\ m_{30} & m_{31} & m_{32} & m_{33} \end{bmatrix} \begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix}_{\text{incident}} \quad (62)$$

- Solution for each Stokes parameter

The Stokes vector for the incident beam appears after calculating the inverse of the Mueller matrix and applying it to the Stokes vector of the observed beam.

Table 1: Fresnel rhomb rotation positions

Stokes	Exposure number	1st rhomb $\phi = 180^\circ$		2nd rhomb $\phi = 90^\circ$	3rd rhomb $\phi = 180^\circ$	
		pos	angle θ	$\theta = 0^\circ$	pos	angle θ
Q	1	P1	0°	fixed	P1	0°
	2	P5	90°	fixed	P3	45°
	3	P3	45°	fixed	P5	90°
	4	P7	135°	fixed	P7	135°
U	1	P2	22.5°	fixed	P1	0°
	2	P6	112.5°	fixed	P3	45°
	3	P4	67.5°	fixed	P5	90°
	4	P8	157.5°	fixed	P7	135°
V	1	P1	0°	fixed	P4	67.5°
	2	P5	90°	fixed	P2	22.5°
	3	P3	45°	fixed	P2	22.5°
	4	P7	135°	fixed	P4	67.5°

- Differential and Ratio methods

Other ways to calculate the Stokes parameters are the differential and ratio methods. It is assumed that they take into account all optical effects from the optical train and acquisition errors.

Differential method :

$$P_X = \frac{1}{4} \sum_{k=1}^2 \left(\left[\frac{i_{\parallel} - i_{\perp}}{i_{\parallel} + i_{\perp}} \right]_{2k-1} - \left[\frac{i_{\parallel} - i_{\perp}}{i_{\parallel} + i_{\perp}} \right]_{2k} \right) \quad (63)$$

Ratio method :

$$P_X = \frac{\left(\prod_{k=1}^2 \frac{[i_{\parallel}/i_{\perp}]_{2k-1}}{[i_{\parallel}/i_{\perp}]_{2k}} \right)^{\frac{1}{4}} - 1}{\left(\prod_{k=1}^2 \frac{[i_{\parallel}/i_{\perp}]_{2k-1}}{[i_{\parallel}/i_{\perp}]_{2k}} \right)^{\frac{1}{4}} + 1} \quad (64)$$

where X represents the parameters Q, U and V, k is the number of pair of exposures, which are listed in Table 1, and i is the observed flux. The beam associated with $i_{\parallel}$ is the

beam with a polarization parallel to the principal plane of the Wollaston prism. Therefore, the beam associated with $i_{\perp}$ is the beam with a polarization perpendicular to the principal plane.

Both methods give the same result.

3.4.3. Errors

The propagation of uncertainty assumes that the fluxes are uncorrelated, so covariance is not taken into account.

3.4.4. Null Polarization Spectra

A way to identify problems with spurious polarizations introduced by the system or in the reduction is to inspect the null polarization spectra. The null polarization spectra can be obtained by two methods, the differential method and ratio method, both of which are provided as part of an OPERA polar product. The null spectra is calculated as follows:

Differential method :

$$N_X = \frac{1}{4} \sum_{k=1}^2 (-1)^{k-1} \left(\left[\frac{i_{\parallel} - i_{\perp}}{i_{\parallel} + i_{\perp}} \right]_{2k-1} - \left[\frac{i_{\parallel} - i_{\perp}}{i_{\parallel} + i_{\perp}} \right]_{2k} \right) \quad (65)$$

Ratio method :

$$N_X = \frac{\left(\prod_{k=1}^2 \left(\frac{[i_{\parallel}/i_{\perp}]_{2k-1}}{[i_{\parallel}/i_{\perp}]_{2k}} \right)^{(-1)^{k-1}} \right)^{\frac{1}{4}} - 1}{\left(\prod_{k=1}^2 \left(\frac{[i_{\parallel}/i_{\perp}]_{2k-1}}{[i_{\parallel}/i_{\perp}]_{2k}} \right)^{(-1)^{k-1}} \right)^{\frac{1}{4}} + 1} \quad (66)$$

3.4.5. Simulations

... Here we present the simulations and measurements of the degree of polarization performed on the simulated data. Present the dependence of uncertainty on the degree of polarization and the input noise. Show three cases: input photon noise (Poisson), noise with normal distribution (Gaussian), and systematic errors.

3.4.6. Polarimetry of Polarized Data

... Here we present the results obtained with the polarizers. Dependence of uncertainty with wavelength, detector position, etc. Calculate level of contamination between beams. Also show cross-talk between polarization modes.

3.4.7. Polarimetry of Standard Stars

... Here we present the results obtained for stars with known polarization. Present measurements of the degree of polarization on spectral lines (H-alpha, calcium lines, sodium doublet, etc). Compare OPERA with Libre-Esprit results. Analyze null spectra for both results. Plot CDF (cumulative distribution function) to determine which kind of statistics is present on each data set. What is the dispersion per wavelength. What is the uncertainty versus S/N.

3.4.8. Continuum Polarization

This section presents results on measurements of the continuum degree of polarization measured for polarimetric standards. Compare with expected results.

3.5. Wavelength Telluric Correction

This module identifies atmospheric emission/absorption spectral lines on science images to improve the wavelength calibration. The signal-to-noise for these lines depends on the exposure time and on the target brightness, therefore the quality of this correction is not consistent for all objects observed. For this reason, this module produces an additional vector of corrected wavelength values.

3.6. Barycentric Wavelength Correction

The module `operaBarycentricWavelengthCorrection` calculates the barycentric radial velocity correction for the target observed. This is done by calculating the velocity of the target observed with respect to the barycenter of the Solar System. OPERA uses software routines from the IAU SOFA Collection (ref) to perform these calculations. The radial velocity correction Δv is then used to apply wavelength corrections $\Delta \lambda$, where,

$$\Delta \lambda = \Delta v \frac{\lambda}{c}, \quad (67)$$

for c being the speed of light in vacuum ($c = 299,792,458$ m/s) and λ the wavelength observed.

4. CONCLUSIONS

We would like to acknowledge the many reviewers who participated in the OPERA reviews and provided us with invaluable insights and contributions. The reviewers are mainly CFHT staff, scientists of the Gemini Observatory, and astronomers from France, Canada, Taiwan, Brazil, and University of Hawaii. We would also like to note that this work would not have been possible without the support and incentive of our former director Dr. Christian Veillet, who also gave important contributions in the reviews and is the inventor of the OPERA acronym. In addition, we would like to thank Dr. J.-F. Donati, who developed the current Libre-Esprit ESPaDOnS pipeline running at CFHT and who has provided us with valid inputs for OPERA. Finally, we would like to acknowledge the members of the CFHT Scientific Advisory Committee, for their continued support in the development of OPERA.

Facilities: CFHT.

REFERENCES

- Baraffe, I. *et al.* , 2001, A&A, 382, 563
- Donati, J.-F. *et al.* , 1997, MNRAS, 291, 658-682
- Donati, J.-F. *et al.* , 1999, A&AS, 134, 149, 291, 658-682.
- Donati, J.-F. *et al.* , 2003, ??, ?, ???-???
- Manset, N. *et al.* , 2003, ??, ?, ???-???
- Martiotoli, E. *et al.* , 2012, ??, ?, ???-???
- Piskunov, ?. *et al.* , 2002, ??, ?, ???-???
- Moreno, ?. *et al.* , 1982, ??, ?, ???-???
- Rossi, ?. *et al.* , 1985, ??, ?, ???-???
- Ponz, ?. *et al.* , 1986, ??, ?, ???-???
- Goodrich, E. *et al.* , 1988, ??, ?, ???-???
- Marsh, ?. *et al.* , 1989, ??, ?, ???-???
- Mukai, ?. *et al.* , 1990, ??, ?, ???-???
- Hall, ?. *et al.* , 1994, ??, ?, ???-???
- Valenti, ?. *et al.* , 1994, ??, ?, ???-???
- Piskunov, ?. *et al.* , 1995, ??, ?, ???-???
- Hinkle, ?. *et al.* , 2000, ??, ?, ???-???
- Horne, K., 1986, ??, ?, ???-???
- Tollestrup, E. *et al.* , 2012, SPIE, ?, ???-???
- Janesick, J. R., 2001, SPIE, Bellingham, WA.
- Alard, C., & Lupton, R.H., 1998, ApJ, v. 503, p. 325
- Markwardt, C., 2009, Astronomical Data Analysis Software and Systems XVIII, v. 411, p.

- Moré, J., 1977, “The Levenberg-Marquardt Algorithm: Implementation and Theory,” in Numerical Analysis, v. 630, ed. G. A. Watson (Springer-Verlag: Berlin), 105
- Starck, J-L., Murtagh, F., 2006, Astronomical Image and Data Analysis: Astronomy and Astrophysics Library. ISBN 978-3-540-33024-0. Springer-Verlag
- Lovis, C., & Pepe, F., 2007, A&A, v.468, p. 1115
- Ballester, P., & Rosa, M.R., 1997, A&AS, Vol. 126, December II 1997, 563-571.