Chapter 7

Echelle Spectra

This Chapter provides the basic information necessary to understand the echelle package implemented in MIDAS. It includes the description of the reduction method and the system implementation, without reference to a particular instrument. A detailed description of the operation and relevant parameters for the different instruments supported are described in the corresponding Appendix D. Tutorial examples are available in the system (command TUTORIAL/ECHELLE) and are also included in the Appendix D so that users without previous experience in MIDAS could become familiar with the calibration procedures.

The package follows a very flexible scheme, where most of the reduction steps include several algorithms which can be dynamically chosen and some of the steps can be executed optionally. Experienced users could modify the scheme to adapt it to their data configuration. The methods described here are generally sufficient to cover a wide range of echelle formats. The ESO instruments supported by the package are CASPEC (Cassegrain Echelle Spectrograph), EFOSC(1+2), ECHELLEC, and EMMI.

The package provides a set of about 30 first-level basic commands to perform the reduction, most of them having the qualifier ECHELLE. These commands are structured in five main MIDAS procedures to perform complete steps of reduction. In Section 7.1 we describe the algorithms used in the echelle reduction, i.e. the algorithms to find the position of the echelle orders, order extraction procedures, wavelength calibration and instrument response correction. In Section 7.10 we include a brief outline of the different data formats involved in the reduction and a summary of the commands. Finally, the session parameters are detailed in Section 7.11

Note

This chapter only provides a synopsis of the commands needed for the reduction of echelle. It is important to realise that it can neither substitute the HELP *information available for each command nor be exhaustive, especially not with regard to the usage of general utilities such as the* MIDAS *Table System, the* AGL *Graphics package, etc. Reduction steps which are not specific to echelle spectra are described in more detail in Chapter L. The Appendix D provides a practical approach to echelle reduction.*

7.1 Echelle Reduction Method

7.1.1 Input Data and Preprocessing

The information involved in a reduction session consists of user data and system tables. User data is a set of echelle images, observed with the same instrument configuration, including a wavelength calibration image (WLC), a flat field image (FLAT) and astronomical objects OBJ. Optionally, this set will include standard stars (STD) to be used in the absolute or relative flux calibration, and dark images (DARK). Catalogues with comparison lines and absolute fluxes for standard stars are available in the system as MIDAS tables.

Before starting the actual reduction some preprocessing of the data is required to correct for standard detector effects as follows:

- Rotation of input frames.
  After this rotation, the dispersion direction of the echelle orders will be horizontal, with wavelengths increasing from left to right and spectral order numbers decreasing from bottom to top of the image. As always in MIDAS, the origin is the pixel $(1,1)$, located in the lower left corner of the image.
- Updating START and STEP descriptors.
  Descriptors START and STEP must be set to 1.,1. for all images processed. Session keyword CCDBIN must be set to the original binning factor along x- and y-axis. Image rotation and descriptors update are performed by the command ROTATE/ECHELLE.
- Cleaning of bad columns.
  First, bad columns – bad rows after the rotation – can be removed with the command COMPUTE/ROW. The cleaning of bad columns is required for FLAT images where the variation of the intensity due to these columns can affect the automatic detection of the orders.
- Cleaning of hot pixels.
  Hot pixels can be eliminated by filtering the images. In case the observation has been splitted in several exposures and more than one image is available with the same information, the images can be averaged with the command AVERAGE/WINDOW; this command can, optionally, interpolate pixel values with large deviations from the average value. Removal of hot pixels is required for DARK images and is recommended for OBJ exposures. General methods to clean bidimensional spectra are described in Chapter L (Removing Cosmic Ray Hits). The command FILTER/ECHELLE, adapted to echelle spectra is described in Section 7.3
- Subtraction of dark current from FLAT, OBJ and STD frames. The dark level is estimated from a series of DARK exposures of short duration which are averaged to reduce the effect of the read–out noise of the CCD and to eliminate hot pixels as described before. If preflashing is necessary, a set of preflashed DARK exposures should be obtained in a similar manner. It is advisable to obtain a set of DARK images with similar exposure times as the object and standard star frames, or to scale the dark level to the observed exposure.

- Checking exposure times in `OBJ` and `STD` frames. For images generated by ESO instruments, the exposure time (in seconds) is stored in the descriptor `O_TIME(7)`. If necessary this descriptor can be created as `O_TIME/D/1/7` with the command `WRITE/DESCRIPTOR`.

7.1.2 Retrieving demonstration and calibration data

Calibration tables are required to provide reference values of wavelength for Th-Ar arc lamp lines, atmospheric extinction or standard star fluxes.

A certain number of tables are distributed on request in complement to the Midas releases. These tables are also available on anonymous ftp at the host **ftphost.hq.eso.org** (IP number 134.171.40.2). The files to be retrieved are located in the directory /midaspub/calib and are named README.calib and calib.tar.Z. Command `SHOW/TABLE` can be used to visualize the column name and physical units of the tables. Demonstration data required to execute the tutorial procedure `TUTORIAL/ECHELLE` are also located on this ftp server in the directory /midaspub/demo as echelle.tar.Z. FTP access is also provided on the World Wide Web URL:

http://http.hq.eso.org/midas-info/midas.html

The calibration directory contains other information such as characteristic curves for ESO filters and CCD detectors, which can be visualized with the Graphical User Interface XFilter (command `CREATE/GUI FILTER`).

7.1.3 General Description

The first problem in the reduction of echelle spectra is, of course, the solution of the dispersion relation. That is the mapping between the space (λ, m) wavelength, spectral order and the space (x, y) sample x, line y in the raw image. This relation gives the position of the orders on the raw image, and defines the wavelength scale of the extracted spectrum. The mapping is performed in two steps:

- A first operation (order definition), gives the position of the orders in the raw image. In figure 7.1, this operation corresponds to the step "Find Order Position". The required input is an order reference frame (usually `FLAT` or `STD`) and the output is a set of polynomial coefficients. These coefficients are an input of the step "Extract Orders".

- A second operation (wavelength calibration) defines the wavelength scale of the extracted spectrum. The successive steps of this operation are shown in the second column of figure 7.1. The output is a set of dispersion coefficients required by the step "Sample in Wavelength".

Sections 7.2 and 7.6 describe the solution of this mapping.

The second step in the reduction, described in Section 7.4, is to estimate the image background. The background depends mainly on the characteristics of the detector, but includes the additional components of the scattered light in the optics and spectrograph. This operation corresponds to the step "Subtract Background" in fig. 7.1.

`FLAT`	`WLC`	`STD`	`OBJECT`
$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$
FIND ORDER POSITIONS	EXTRACT ORDERS	*SUBTRACT BACKGROUND*	SUBTRACT BACKGROUND
$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$
SUBTRACT BACKGROUND	IDENTIFY LINES	*FLAT FIELD CORRECTION*	*FLAT FIELD CORRECTION*
$\Downarrow$	$\Downarrow$	$\Downarrow$	$\Downarrow$
DEFINE BLAZE	COMPUTE DISP.COEFFS.	*EXTRACT ORDERS*	EXTRACT ORDERS
		$\Downarrow$	$\Downarrow$
		SAMPLE IN WAVELENGTHS	SAMPLE IN WAVELENGTHS
		$\Downarrow$	$\Downarrow$
		COMPUTE RESPONSE	*MULTIPLY BY RESPONSE* or *FIT BLAZE*
			$\Downarrow$
			MERGE ORDERS

Figure 7.1: Echelle Reduction Scheme

A particular problem in the CCD–detector used by the two echelle instruments is the appearence of interference fringes produced within the silicon, which can be especially important in the long wavelength range of the instrument. By processing the flat-field (first column of fig. 7.1), correction frames are prepared and used for the standard star and the object reduction. A method to correct for this effect is described in Section 7.7.

After the corrections for all these effects, the information in the spectral orders is extracted using the methods described in Section 7.5. The extracted flux, used in conjunction with the dispersion relation, gives the photometric profiles of the spectral orders. Two instrumental effects are still present in these profiles: first, due to the blaze effect of the echelle grating, the efficiency of the spectrograph changes along each order; second, the efficiency of the whole instrument is not uniform with wavelength. In Section 7.8 we describe how to correct both effects, to normalize the fluxes and, if the input data includes calibration stars, to convert the fluxes into absolute units.

Note

Taking a standard star exposure (STD) is a recommended observation strategy which can make easier the order definition in the blue part of the spectrum as well as the correction of individual orders for the variations of grating efficiency (blaze function).

The steps summarised above comprise the `STANDARD` reduction. Alternatively, it is possible to correct the variation in sensitivity along the spectral orders using a suitable model for the blaze function as described in Section 7.8.2. Figure 7.1 displays the process scheme in a typical reduction session; slanted fonts indicate optional operations. In the rest of this Section the algorithms used in each step of the reduction are described.

7.2 Order Definition

The dispersion relation is defined by the following equations:

$$\begin{aligned} y &= f_1(x, m) \\ \lambda &= f_2(x, m) \end{aligned} \tag{7.1}$$

The first of the equations 7.1 defines the position of the spectral orders, m, in the raw image, while the second equation gives, for each order, the dispersion relation in one dimension. The mapping between the spaces (λ, m) and (x, y) is separated into two different equations; the first one will be discussed in this Section, while the description of the second equation will be postponed to Section 7.6.

The function f_1 is approximated by a polynomial of the form

$$y = f_1(x, m) \approx \sum_{j=0}^{J} \sum_{i=0}^{I} a_{ij} x^i m^j \tag{7.2}$$

where the coefficients a_{ij} are computed using least squares techniques on a grid (x_k, y_k), i.e. sample number and line number of points located within the spectral orders of the image. These points in the grid are found automatically by an order–following algorithm, normally using the FLAT or STD image.

- A first guess of the position of the orders is found on a trace perpendicular to the dispersion direction done in the middle of the flat field image, in this way we define the set of points (x_0, y_{0m}), m being the relative order number.

- For each order, the order–following algorithm finds the series of points located on the order at $x_n = x_0 + n \times \Delta x$ for points on the right half of the order, and at $x_{-n} = x_0 - n \times \Delta x$ for points on the left half of the order, $n = 1, 2, \ldots$ integer and Δx is the step of the grid.

This set of points forms the basic grid with the geometric positions of the orders. Typical values of the standard deviation of the residuals of this approximation are about 0.3 to 0.1 pixel.

It is worth mentioning here that the order following algorithm finds the center of the orders by taking the middle point with respect to the edges of the orders. The edges of the orders are detected automatically by thresholding the order profiles, perpendicular to the dispersion direction; the level of the threshold is a function of the signal in the order. The command DEFINE/ECHELLE performs the automatic order detection.

An alternative method is available, based on the Hough transform to perform the order detection and involving a tracing algorithm able to estimate an optimal threshold for each order independently. The order definition is performed as follows:

- A preprocessing of the frame is performed, including a median filtering (radx,y=2,1) to remove hot pixels and bad rows from the image. Then the background value is measured in the central area of the image and subtracted. This preprocessing assumes that the defaults are small enough to be corrected by a simple median filtering and that the interorder background is basically constant all over the image. If the above conditions are not respected, the frame must be processed by the user. The echelle command BACKGROUND/SMOOTH enables performance of a background correction at this early stage of the calibration.

- A first guess of the position and the slope of the orders is found by processing the Hough transform of a subset of columns of the input image. The order detection by Hough transform is described in (Ballester, 1994).

- For each order, an initial threshold is estimated by measuring the pixel values in the middle of the order. The order following algorithm finds the series of points located on the order at regular steps on the grid, as describd above. The threshold is optimised in order to follow the order on the longest possible distance. If the trace of the order is lost, the algorithm extrapolates linearly the positions and attempts to skip the gap.

- For each position, the center of the order is defined as the first moment of the pixel values above the threshold:

$$y_{center} = \frac{\sum_{y=y_{min}}^{y_{max}} y * (I_y - threshold)}{\sum_{y=y_{min}}^{y_{max}} y}$$

  This algorithm is implemented in the command DEFINE/HOUGH. The algorithm can run in a fully automatic mode (no parameters are required apart from the name of the input frame). It is also possible to set the following parameters to enforce a given solution:

  - numbers of orders to be detected.
  - half-width of orders
  - threshold

A practical decription of the way to use this algorithm and to optimise the parameters is described in the Appendix D

7.3 Removal of particle hits

Cosmic ray events pose a serious problem in long CCD exposures. Their removal is a rather delicate step, because in high-contrast images (such as well-exposed echelle spectra) there is always a danger of damaging the scientific contents of the frame. Particle hits can be removed from scientific exposures by splitting the exposure and comparing spectra of the same target obtained under the same instrumental configuration. Offsets of the target resulting from the positioning of the target on the entrance slit of the spectrograph and variations of exposure time must be accounted for. Commands AVERAGE/IMAGE and AVERAGE/WEIGHT offer number of options to compare the images and reject particle hits. In the case of echelle spectra of sources with very little variation of the spectral information along the slit, one can also exploit the knowledge provided by the order definition as to where in the frame the relevant data is located.

The removal of unwanted spikes, above an otherwise featureless background such as the inter-order space of echelle spectra, is done most easily with a median filter. Therefore, in a first step a median filter is applied to the entire frame. This then enables the true background to be determined as described in Section 'Background Definition' of this chapter. The subtraction of the background calculated completes the second step, and, as far as the inter-order space is concerned, the final result is reached already. The removal of cosmics from the object spectrum forms the third step and is restricted to the regions covered by the spectral orders in the background-corrected, but otherwise raw frame. This step comprises the following operations performed within a sliding (along and separately for each spectral order) window of user-specified width:

- For all x_i of the window, normalize the spatial profile to the total flux in the associated slice (i.e. all y_j of the order considered).

- Form the 'true' spatial profile as the median over the individual profiles at all x_i in the window.

- For all pixels (x_c, y_j) in the central slice, c, of the window compare their re-normalised flux, $f_{c,j}$, with the properly scaled contents m_j of pixel j in the median profile. If the difference exceeds the expected statistical error of $f_{i,j}$ (calculated from the number of photons detected and the readout noise) by a user-specified factor, replace $f_{c,j}$ with m_j.

If the threshold for substitution by the median is set properly ($\sim$4 σ) and the spectral information within the spatial profile does not change (point sources are best), this procedure does not redistribute the flux or dilute the point spread function.

These three steps are the backbone of command `FILTER/ECHELLE`. The final output frame is the merger of the median-filtered inter-order domains with the spectral orders after having been subjected to step three. Note that the background has been subtracted already. A keyword `BACKGROUND` with contents `SUBTRACTED` is appended to the frame as a flag to subsequent high-level procedures so as not to have to go through the very time consuming step of the background modeling again. Delete that descriptor or change its contents if re-modeling of the residual background is desired.

7.4 Background Definition

The estimation of the background is one of the critical points in the reduction of echelle spectra for two reasons. On one side, a correct estimate of the background level is necessary to compute the true flux of the object spectrum; on the other side, a wrong estimate of the background in either the flat field image (`FLAT`), the object (`OBJ`) or (optionally) the standard star (`STD`), will severely affect the accuracy with which instrumental effects – such as the blaze – can be corrected for. The background in an echelle image consists of:

- a constant offset introduced by the electronics (bias),
- an optional constant pedestal due to the pre–flashing of the CCD,
- the dark current,
- general scattered light,
- diffuse light in the interorder space coming from adjacent orders.
- sky background spectrum

The first three components are removed during the preprocessing as described in Appendix D. Correction for the general scattered light and diffuse light background is presented in the three following sections. Correction for the sky background is presented in Section 7.4.4.

The remaining background due to scattered light is estimated from points located in the interorder space. These locations are defined when performing the order definition (command `DEFINE/ECHELLE` or `DEFINE/HOUGH`) and can be displayed by command `LOAD/ECHELLE`. The order definition is used to create a table back.tbl containing the background positions. Unscanned areas of the `CCD` can be avoided in the background estimate by using the command `SCAN/ECHELLE`. If bright features (e.g. sky lines) are located at the same location as background points, these locations must be unselected from table back.tbl using `SELECT/BACKGROUND`. Selection of the method is possible by assignment of a value to the echelle keyword `BKGMTD` and the background estimate, subtraction and update of the descriptor `BACKGROUND` is performed by the command `SUBTRACT/BACKGROUND`

7.4.1 Bivariate polynomial interpolation

Background points are used to approximate the observed background by a polynomial of two variables, sample and line numbers, as:

$$B(x, y) \approx \sum \sum b_{ij} x^i y^j \tag{7.3}$$

The background of flat field images is usually well modelled by a 2D polynomial of degrees 3 and 4 in variables sample and line respectively. The agreement of the model is typically better than 1% of the background level. For object exposures the signal–to–noise ratio is normally much lower, as is the actual background level. A polynomial of lower degree, for example linear in both dimensions or a constant background should be enough. Because small errors in the determination of the background are carried through the whole rest of the reduction and are even amplified at the edges of the orders, care should be taken in the background fitting.

If no `DARK` or `BIAS` frames are available, the background definition might be slightly less accurate because the modelling procedure has to take into account these contributions as well. In some cases the degree of the polynomial has to be increased. As a rule of thumb, one should try to fit the background with a polynomial of the lowest possible degree.

This method gives good results when the main contribution to the background is due to global scattered light.

7.4.2 Smoothing spline interpolation

An alternative method performs the interpolation of interorder background using smoothing spline polynomials. Spline interpolation consists of the approximation of a function by means of series of polynomials over adjacent intervals with continuous derivatives at the end-point of the intervals. Smoothing spline interpolation enables to control the variance of the residuals over the data set, as follows:

$$\delta = \sum_{i=1}^{m} (y_i - \hat{y}_i)^2$$

where y_i is the i^{th} observed value and $\hat{y}_i$ the i^{th} interpolated value is the sum of the squared residuals and the smoothing spline algorithm will try to fit a solution such as:

$$\delta \leq S * \alpha$$

where S is the smoothing factor and $\alpha = 0.001$ is the tolerance.

One must retain two particular values of S:

- S = 0. The interpolation pass through every observation value.
- S very large. The interpolation consists of the one-piece polynomial interpolation.

The solution is estimated by an iterative process. Smoothing spline interpolation is designed to smooth data sets which are mildly contaminated with isolated errors. Convergence is not always secured for this class of algorithms, which on the other hand enables to control the residuals. The median of pixel values in a window surrounding the background reference position is computed before spline interpolation. The size of the window (session keyword BKGRAD) is defined along the orders and along the columns of the raw spectrum.

7.4.3 Background estimate by filtering

The command BACKGROUND/SMOOTH enables to define the background without previous order definition. This feature is useful for example to correct for the background the image required for the order definition. This command involves an iterative algorithm which performs the following operations:

- the input frame is heavily smoothed in the direction perpendicular to the orders.
- the original frame is divided by the smoothed one and all pixels which ratio is greater than one are replaced by the smoothed value.
- the corrected frame becomes the new input frame and the two previous steps are repeated until a satisfying solution is obtained.

A more elaborated scheme is required if the contribution to the background from adjacent orders is important, this occurs when the distance between orders is small. All above methods are implemented in command BACKGROUND/ECHELLE and selected by the echelle keyword BKGMTD.

7.4.4 Sky background definition

The previous methods allow to correct for the interorder scattered light. The sky background component can be measured in spectra taken with an extended slit using the two commands DEFINE/SKY and EXTRACT/SKY. The command DEFINE/SKY allows to define the offset limits of up to two sky windows, usually on both sides of the spectrum. The command EXTRACT/ECHELLE performs an average extraction of the sky background using these offsets, optionally fiters for cosmics, and provides an extracted spectrum in a format similar to the one resulting from EXTRACT/ECHELLE. The two extracted images can be subtracted for sky background correction. It can be noted that the background measured by the command `EXTRACT/SKY` includes also the interorder scattered light components and makes in principle unnecessary the correction described in the previous Section.

7.5 Order Extraction

Individual echelle orders are extracted by adding the pixel values over a numerical slit running along the orders, with the position of the slit center defined by equation 7.2. The width of the slit is one pixel and its length, as well as an optional offset to shift the slit prependicular to the dispersion direction, are defined by the user.

The pixel values in the numerical slit are found by linear interpolation of the values in the image. The extracted flux number is the weighted average of these interpolated pixel values. There are three types of weights (w) depending on the selected option:

- option `LINEAR`: $w = 1$,
- option `AVERAGE`: $w = 1/L$ where L is the length of the slit,
- option `OPTIMAL`: weights optimising the signal to noise ratio of the extracted spectrum. This algorithm is based on (Mukai, 1990)

There are several effects to consider when defining the length of the extraction slit. If the length is too small, the orders are only partially extracted and they present a periodic variation due to the inclination of the orders with respect to the lines in the image. On the other side, if the slit is too large, the extracted flux will include noisy pixels from the flatfielded background, when the flat field correction is applied.

The command `EXTRACT/ECHELLE` is used for the order extraction. The method is selected using echelle keyword `EXTMTD`.

7.6 Wavelength Calibration

7.6.1 General Description

A preliminary step to the wavelength calibration consists of extracting the orders of the `WLC` image which can then be used to determine the dispersion relation in two steps:

- The calibration lines are detected on the extracted orders by means of a simple thresholding algorithm. The center of the line is estimated by its center of gravity (`GRAVITY` method) or by a gaussian fit to the line profile (`GAUSSIAN` method). This is done with the command `SEARCH/ECHELLE`.
- A few lines are identified interactively on the 2D image display and a set of global dispersion coefficients are derived by comparing the identified lines with the line catalogue available in the system. This global model for the dispersion is a function of the wavelength and the spectral order number. Finally, dispersion coefficients

for each order are computed using the global coefficients as a first approximation. A polynomial of degree 2 or 3 is sufficient to obtain, for each order, a good approximation of the wavelength scale.

The command `IDENTIFY/ECHELLE` involves the echelle relation and requires the identification of two lines in overlapped regions of adjacent orders (method `PAIR`). The calibration can as well be performed for spectra which orders are not overlapped, this time requiring a minimum of four identifications (method `ANGLE`). Both methods are based on the echelle relation and therefore are not applicable if the disperser is not an echelle grating, as it is the case for `EFOSC` which involves a grism disperser. The method `TWO-D` allows to start directly the calibration with a two-dimensional fitting polynomial and requires more initial identifications. In case of several observations with the same, or near the same instrumental configuration, it is possible to use the global dispersion model from a previous calibration. The method `GUESS` implements this mode of operation. Two additional methods `RESTART` and `ORDER` are available. The selection of the method is performed by assigning a value to the echelle keyword `WLCMTD`.

Solutions are computed either for each independent order (`WLCOPT=1D`) or using a global bivariate polynomial (`WLCOPT=2D`).

7.6.2 The Echelle Relation

The wavelength calibration involves a physical equation, the echelle relation and regression analysis to achieve estimates of the dispersion relation. Provided that the echelle dispersion is performed with a grating, any echelle spectrum can be calibrated usually with four lines used as pre-identifications and a catalog of laboratory wavelengths associated to the calibration lamp. The achieved accuracy is usually in the range 0.2 - 0.02 pixel. Accuracy can be improved by selecting lines of a sufficient signal-to-noise ratio and using a line catalog sorted for blends for the specific spectral resolution of the instrument.

The echelle relation derives from the grating dispersion relation :

$$\sin i + \sin \theta = k.m.\lambda$$

with k the grating constant, m the order number, and λ the wavelength. The cross-disperser displaces successive orders vertically with respect to one another. For a given position x on the frame, we have :

$$m.\lambda = cste(x) \text{ (Echelle Relation)}$$

The acurracy of this relation is limited by optical aberrations and optical misalignments, which make it only useful to initialise the calibration process by reducing the number of identifications necessary to determine this one-dimensional relation, expressed as a polynomial of low degree N like:

$$\lambda(m, x) = \frac{1}{m}.\sum_{i=0}^{N} a_{mi}.x^i$$

The two major limits of accuracy of the echelle relation are:

- **Optical aberrations:** the echelle relation does not include the effect of optical aberrations which will displace the lines in the frame and then become a source of unaccuracy when attempting to estimate the echelle relation parameters from a calibration frame. This contributor however will be partially removed by using an appropriate model to fit the echelle relation, like a polynomial of sufficient degree.

- **Optical misalignments:** Optical misalignments occur between echelle grating and cross-disperser between this latter and detector. The effective misalignment angle can be up to a few degrees (usually less than 3). Over many hundreds pixels, the misalignment error amounts to systematic errors of many pixels, far beyond the seeked accuracy. it is therefore necessary to correct for any rotation of the detector.

7.6.3 Estimating the angle of rotation

As a consequence of the cross-disperser dispersion relation, a given line repeated in two overlapped regions of the spectrum must be found at the same y position if spectrum and detector are perfectly aligned.

In the following, we will call a pair two occurences of the same line in the overlapped parts of two adjacent orders.

The above condition provides a geometrical way to estimate the angle, as: $\alpha = \Delta y/\Delta x$, with Δy the difference in y position of the two occurences of the pairs and Δx the difference of their x positions. This method requires overlaps between orders and is used in the calibration method `PAIR`.

Another approach consists of estimating the rotation angle as the parameter for which regression analysis provides the smallest residual for a given set of observations.

- $x_r = x \cos\alpha + y \sin\alpha$
- $m.\lambda = \sum_{i=0}^{N} a_i.x_r^i$
- α such as the standard-error is minimized

The determination of the optimum is performed analytically and is involved in the calibration method `ANGLE`. This one-dimensional representation of the dispersion relation is used as a starting point in the loop and is replaced by a bivariate solution $m.\lambda = f(x, m)$ as soon as a sufficient number of identifications has been performed.

7.6.4 Identification loop

The identification criterion combines estimate of the wavelength of a line and an estimate of the error as well as a list laboratory wavelengths to determine and guarantee the identification of a given line. One could involve the additional knowledge of line strengths. But in practice this information of limited use, in reason of variations of relative line intensities caused by impurities, lamp ageing, pressure variations, a.s.o. Accordingly, the identification criterion is:

$$\lambda_c \equiv \lambda_{cat} \text{ if } \exists! \ \lambda_{cat} \ / \parallel \lambda_c - \lambda_{cat} \parallel < \delta\lambda$$

with λ_c, computed estimated wavelength, λ_{cat} the catalog wavelength and $\delta\lambda$, a majorant of the error of the computed wavelength, taken as the distance of the closest neighbor in the line catalog or in the arc spectrum divided by a coefficient α which value does not exceed 1 (this parameter is controlled by the session keyword `WLCLOOP(2)`).

7.6.5 Resampling and checking the results

The extracted orders in the pixel domain can be resampled into wavelengths with the command `REBIN/ECHELLE`. Several quality checks are provided by the command `IDENT/ECH`. Residuals are visualized with the command `PLOT/RESIDUAL`. A method to verify the wavelength calibration consists of extracting and resampling the wavelength calibration frame and displaying the resampled image with a large scaling factor on the Y-axis. The variation of wavelength coverage from one order to the next should be smooth. Different regions of the resampled image and in particular the overlaps can be verified with the command `PLOT/SPECTRUM`.

7.7 Flat Field Correction

The main disadvantage of the thin CCD–chips used currently as detectors in some instruments is the generation of interference fringes, that is, intensity fluctuations in the spectra which can be as high as 30% at $\lambda > 6000$Å (York, 1981). These fringes arise from interferences within the silicon for long wavelengths, while for shorter wavelengths they can be due to the interfaces silicon–glass on the back side of the chip. This effect is constant for a given setting and it can be effectively corrected by dividing the object image by a flat–field exposure taken with the same instrument configuration. Before the actual division is carried out, the background levels, both in the object image and flat–field, are subtracted and the flat–field is normalised.

The flat–field correction is done with the command `COMPUTE/IMAGE`, this command divides the background subtracted `OBJ` by the normalised flat–field as computed by the command `FLAT/ECHELLE`.

7.8 Instrument Response Correction

7.8.1 Using a Standard Star

The extracted orders, together with the dispersion relation, define the observed flux as a function of the wavelength for each order:

$$F = F_m(\lambda) \tag{7.4}$$

This flux has to be corrected for two effects in order to get absolute fluxes: first, for the echelle blaze effect, and second, for the chromatic response of the instrument. For a given configuration, the blaze effect is a function of the position in the order, while the instrument response is, essentially, a function of the wavelength.

The solution adopted in the reduction, using the standard star, is to correct for both the blaze effect and the instrument response simultaneously. This is done by comparing a standard star, observed with the same configuration as the object, to a table of absolute fluxes. The standard star is reduced exactly as the object and then correction factors are calculated by comparing the flux values in the table to the observed counts sampled at the same wavelength intervals as the fluxes in the table. The resulting response is normalised to an exposure time of one second. There is no effect due to differences between the flatfield of the object and the one corresponding to the standard star given that the flatfields are normalized (see Section 7.7).

If, as usually is the case, OBJ and STD were observed through different airmasses, the spectra have to be corrected for extinction using command `EXTINCTION/SPECTRUM`. More information about this command is available in Vol.2, Chapter L (Spectral Data). The command `RESPONSE/ECHELLE` is used to compute the instrument response as described here. Southern spectrophotometric standards have been published by Hamuy and al. (1992, 1994).

7.8.2 Fitting the Blaze Function

A different approach is also available at this stage, as an alternative to the method described in the last Section. It consists of a correction for the blaze function by using a suitable model of the blaze effect introduced by the echelle grating. In this approach, no correction for the chromatic response of the instrument is applied. It is noteworthy however to say that the standard star correction is a much more efficient way to perform the instrumental response correction. The model assumes a plane grating, used in near–Littrow mode. The blaze function R at wavelength λ is approximated by

$$R(\lambda) = \frac{\sin^2 \pi\alpha X}{(\pi\alpha X)^2} \tag{7.5}$$

where α is a grating 'constant' with value between 0.5 and 1, and $X = m(1 - \lambda_c(m)/\lambda)$, in which m is the order number, and $\lambda_c(m)$ is the central wavelength of order m. Both parameters are related through the grating 'constant' k by $k = m\lambda_c(m)$. This correction is done with the command `RIPPLE/ECHELLE`; the command includes three methods to compute the parameters k and α:

The first one, method `SINC`, is a modification of the method suggested by Ahmad, 1981, *NASA IUE Newsletter*, **14**, 129. This algorithm approximates the blaze function by a sinc square and finds the function parameters by a *non–linear least squares fit to the order profile*. The method is suitable for objects without strong emission or absorption features and can be used to get a first estimation of the blaze parameters.

The second method, named `OVER`, is based on Barker, 1984, *Astron.J.*, **89**, 899. This method uses the overlapping region of adjacent orders to estimate, in a few iterations, the parameter k of the blaze function which is, as before, assumed to be a sinc square. The method works well, provided that orders are overlapping and that there is a very good estimation of the parameter α, assumed to be a contant.

The third method, `FIT`, is an extension of the previous one. It uses, as before, the overlapping region of the adjacent orders but has the advantage of assuming that both parameters k and α can vary. The method minimises the difference of the corrected orders in each of the overlapping intervals.

7.9 Order Merging

Finally, the extracted orders, sampled at constant wavelength steps and corrected for the blaze effect, can be merged into a one dimensional spectrum which is suitable for further analysis. The merging algorithm computes a weighted average in the overlapping region of adjacent orders. The normalised weight is a linear ramp changing from 0 to 1 in the overlapping region for each of the adjacent orders. Therefore, in the overlapping region of two consecutive orders, the ramp decreases linearly for the 'blue' order while it increases linearly for the 'red' order. This gives less weight to points near the edges of the orders. It is also possible to extract individual orders and store them in different spectral files for further analysis. The command `MERGE/ECHELLE` performs the merging of the orders.

7.10 Implementation

In this Section we describe the different data formats related to the echelle reduction. Both images and tabular information are used to store intermediate results of the commands in the reduction procedure. We also include a summary of the echelle commands and a detailed description of the parameters used in a reduction session. In the command description we use upper case letters for fixed parts of the command, while names in lower case are variable parameters. Optional parameters are enclosed in square brackets.

7.10.1 The Session Manager

Input data observed with the same configuration of the instrument and the parameters needed for the reduction define a session. Session parameters are listed by the command `SHOW/ECHELLE`. It is recommended to use this command to control the actual status before executing any further reduction step. Current parameters are saved with the command `SAVE/ECHELLE name`, where `name` is the session name. This command will be used whenever you want to interrupt a session which then can be restarted at any other time. Current parameter values are set to the default value with the command `INIT/ECHELLE`, or set to the values of a previously saved session with `INIT/ECHELLE name`.

Relevant session parameters can be defined for each command in the usual way:

```
command/qualifier parameters
```

or can be defined in explicit form as

```
SET/ECHELLE param=value [param=value ...]
```

where `param` is the parameter name and `value` is the assigned value. The assigned values will be maintained until you save them for later reference. Current parameter values are re–assigned either by `INIT/ECHELLE` or by another `SET/ECHELLE` command.

Please note that the session concept is part of the high level command structure (level 1 and above). If level 0 commands are used one has to specify explicitely ALL the parameters required by the level 0 commands, despite the fact that some of them may already have been set via `SET/ECHELLE`.

7.10.2 Image Formats

One and two dimensional images are produced by echelle commands. These images are standard MIDAS frames, sampled in the following spaces:

- pixel–pixel space: corresponds to 2D raw images, with the sampling units `PIXEL` in both dimensions.
- pixel–order space: corresponds to 2D extracted images, produced by the command `EXTRACT/ECHELLE`. Unit in the x–axis is `PIXEL`, unit in the y–axis is `ORDER`, sequential echelle order number.
- wavelength–order space: corresponds to 2D extracted images, with uniform sampling steps in wavelength, produced by the command `REBIN/ECHELLE`. Unit in the x–axis is Ångstrøm , unit in the y–axis is `ORDER`, sequential echelle order number. These images *are not standard*, in the sense that the descriptors `START(1)` and `NPIX(1)` are meaningless. The starting position for each order is defined in the descriptor `WSTART`, and the number of pixels per order is given by `NPTOT`, both descriptors are arrays of `NPIX(2)` elements. This deviation from the standard is due, obviously, to the different spectral range of each echelle order.
- wavelength space: corresponds to 1D images, sampled at constant wavelength steps. These images are produced by the command `MERGE/ECHELLE`. Unit in the x–axis is Ångstrøm .

7.10.3 Table Formats

MIDAS table files are used to store relevant information in tabular form. Four types of tables are considered. The first two, tables order.tbl and line.tbl, are operational tables generated by the user during the session. The other two types of tables are provided by the system to calibrate the data in wavelength and flux.

order.tbl — Contains echelle orders. This table contains the coefficients a_{ij} in relation 7.2 stored as descriptors. The table is created by the command `DEFINE/ECHELLE` or `DEFINE/HOUGH`

back.tbl — Contains information related to the background reference positions. This table is created by the command `PREPARE/BACKGROUND` which is called by `DEFINE/ECHELLE` and `DEFINE/HOUGH`.

line.tbl — Contains information related to the position of the calibration lines. This table contains the dispersion coefficients for each spectral order, stored as descriptors after the line identification process. It is generated by the command `SEARCH/ECHELLE` and extended and updated by the command `IDENTIFY/ECHELLE`.

Line Catalogue — Contains the wavelength calibration lines. There are several line catalogues available in instrument related system area, like `MID_CASPEC` and `MID_EFOSC`.

Standard Stars — Contains the fluxes of standard stars in different units. These tables are copied automatically from the area `MID_STANDARD` into the user work space with the command `SET/ECHELLE FLUXTAB=name`

Table order.tbl		
Label	**Unit**	**Description**
ORDER	–	sequential order number
X	PIXEL	sample (x–axis) position of the order
Y	PIXEL	line (y–axis) position of the order
YFIT	PIXEL	fitted line (y–axis) position of the order
RESIDUAL	PIXEL	residual (Y-YFIT)

Table back.tbl		
Label	**Unit**	**Description**
ORDER	–	sequential order number
X	PIXEL	sample (x–axis) position of the order
YBKG	PIXEL	line position of the background above the order
BKG	DN	value of the background

Table line.tbl		
Label	**Unit**	**Description**
X	PIXEL	sample (x–axis) position of the line
Y	PIXEL	relative order number
PEAK	DN	estimated line maximum
YNEW	PIXEL	line (y–axis) position of the line
ORDER	–	spectral order number
IDENT	ANGSTROM	manual identification
WAVEC	ANGSTROM	computed wavelength
RESIDUAL	ANGSTROM	residual (WAVEC-WAVE)

Line Catalogue		
Label	**Unit**	**Description**
WAVE	ANGSTROM	wavelength

Standard Star Atlas		
Label	**Unit**	**Description**
MAGNITUDE	-	magnitude
WAVE	ANGSTROM	wavelength
BIN_W	ANGSTROM	bin width
FLUX_W	ERGS/S/CM/CM/ANG	flux

Table 7.1: Auxiliary Tables

7.10.4 MIDAS Commands

A full description of the echelle commands is given in the Appendix D. We include here a brief summary for quick reference. The echelle package is hierarchically organised from low–level commands (level 0) to high–level commands (level 3). The organization is a result of the following classification:

- Level 0.
  Apart from the level 0 command `LOAD/ECHELLE`, the user will make seldom use of level 0 commands. All parameters of these commands must be provided on the command line. The user may use these commands to benefit from options non available from higher level commands.

- Level 1.
  Level 1 commands perform the individual steps of the reduction. Parameters may be provided on the command line (thus updating the echelle keywords) or will be read from the echelle keywords (set by command `SET/ECHELLE`). Level 1 command enable to check individual steps of the reduction.

- Level 2.
  Level 2 commands perform high level steps of the reduction. The level 2 set of commands is self–consistent and enables to perform a complete reduction, with the optional use of verification lower level commands `PLOT/ECHELLE, PLOT/IDENT, LOAD/IDENT, PLOT/RESIDUAL, LOAD/ECHELLE`. Apart from method keywords and input/output images, no parameter value is required on the command line, all keywords being updated by `INIT/ECHELLE` and `SET/ECHELLE` commands.

- Level 3.
  The higher level 3 includes only two very general commands. The `SET/CONTEXT` initializes echelle keyword values and `TUTORIAL/ECHELLE` provides a demonstration of the package.

SET/CONTEXT echelle
TUTORIAL/ECHELLE

Table 7.2: Echelle Level–3 Commands

Echelle reduction commands	
CALIBRATE/ECHELLE	[defmtd] [wlcmtd]
FLAT/ECHELLE	[flat] [correct] [blazeff]
FILTER/ECHELLE	input output
PREPARE/WINDOW	catalog flatbkg lhcuts
RESPONSE/ECHELLE	[std] [fluxtab] [response]
REPEAT/ECHELLE	[scalx,scaly] [response]
REDUCE/ECHELLE	input output [bkcor]
ROTATE/ECHELLE	catalog root-name [mode]
SELECT/BACKGROUND	[all]
SCAN/ECHELLE	frame [scan-par]
Session manager commands	
HELP/ECHELLE	[param]
INIT/ECHELLE	[name]
SAVE/ECHELLE	name
SET/ECHELLE	par=value
SHOW/ECHELLE	

Table 7.3: Echelle Level–2 Commands

BACKGROUND/SMOOTH	input output [radx,rady] [niter] [visu]
BACKGROUND/ECHELLE	in out [radx,rady,step] [degree] [smooth] [method]
DEFINE/ECHELLE	[ordref] [width1,thres1,slope] [defmtd] [defpol]
DEFINE/HOUGH	[ordref] [nbord] [hwid] [hough_par] [thresh] [degx,degy] [hot_thres,step]
DEFINE/SKY	ima [nsky] [possky] [half-width]
EXTRACT/ECHELLE	input output slit[,offset] [method]
EXTRACT/SKY	in out [mode]
LOAD/IDENTIFICATIONS	
MERGE/ECHELLE	input output [params] [method]
IDENTIFY/ECHELLE	[wlc] [lincat] [dc] [tol] [wlcloop] [wlcmtd] [guess]
PLOT/ECHELLE	frame [ord1,ord2] [printer]
PLOT/IDENT	frame [ord1,ord2] [printer]
PLOT/RESIDUALS	[ord1,ord2]
PLOT/SPECTRUM	in [start,end]
REBIN/ECHELLE	input output [sample]
RIPPLE/ECHELLE	input output [params] [method] [option]
SEARCH/ECHELLE	input [width2,thres2]
SUBTRACT/BACKGR	input backgr output [bkgmtd] [bkgvisu]

Table 7.4: Echelle Level–1 Commands

AVERAGE/TABLE	frame table columns outcol rad (No on--line help)
EXTRACT/ORDER	in out slit,angle,offset meth table coeffs [ord1,ord2] (No on--line help)
EXTRACT/OPTIMAL	
HOUGH/ECHELLE	input [scan] [step,nbtr] [nbord] [flags] [hwid] [thres]
LOAD/ECHELLE	
PREPARE/BACKGROUND	input [step] [init] [back_tab] [order_tab] [descr]
REGRESSION/ECHELLE	[defpol] [niter] [absres] [kappa]
SEARCH/ORDER	[ordref] [w,t,s] [outtab] [defmtd]
VERIFY/ECHELLE	file [type]

Table 7.5: Echelle Level–0 Commands

7.11 Session Parameters

Parameters: CALIBRATE command (See also next table)	
Parameter	**Description**
INSTR	Defines the spectrograph (e.g. CASPEC, EFOSC).
GRATING	Defines the grating or instrument configuration.
CCD	Defines the CCD.
CCDBIN	Binning factor along X and Y. This parameter has impact on the wavelength calibration.
SCAN	Limits of the scanned area of the CCD. This parameter has impact on order definition (method Hough) and background estimates.
ORDREF	Order reference frame
DEFMTD	Order definition method (STD, COM, HOUGH).
DEFPOL	Degree of the bivariate polynomial used in the definition of the orders, see Section 7.2.
WIDTH1	Defines the width in pixels of the orders perpendicular to the dispersion direction. It is used to detect the orders as described in Section 7.2 (methods STD, COM). Typical values are between 2 and 15, depending on the observing slit.
THRES1	Defines the threshold to detect orders on the order reference image as described in Section 7.2 (methods STD, COM).
SLOPE	Mean slope of the orders in pixel space (methods STD, COM).

Table 7.6: Command parameters (1)

Parameters: CALIBRATE command (Continued)	
Parameter	**Description**
NBORDI	Number of orders to be detected (method HOUGH).
WIDTHI	This parameter is used to remove the traces of the orders in Hough space during the detection. Its minimum value is the half-width in pixels of the orders perpendicular to the dispersion direction. Its maximum value is the interorder distance minus the half-width of the orders (method HOUGH).
THRESI	Defines the threshold for the order detection (equivalent to THRES1)
WLC	Raw wavelength calibration image.
LINCAT	System table with comparison lines.
EXTMTD	Extraction method (AVERAGE, LINEAR, OPTIMAL).
SLIT	Width of the extraction slit in pixels.
OFFSET	Offset of the extraction slit. The offset is given in pixels, positive values are above the center and negative offsets are below the center of the orders as shown in the image monitor (command LOAD/ECHELLE).
SEAMTD	Searching method (GAUSSIAN, GRAVITY). This parameter controls the definition of the center of the calibration lines.
WIDTH2	Defines the width of the calibration lines in pixels.
THRES2	Defines the threshold above the local background to detect comparison lines. The actual value should be chosen to detect about 10 to 20 lines per order.
WLCMTD	Wavelength calibration method (PAIR, ANGLE, TWO-D, GUESS, RESTART, ORDER). This parameter controls the execution of IDENTIFY/ECHELLE.
WLCOPT	Dispersion relation option (1D, 2D)
GUESS	Optional reference to a previous session with the same instrument configuration, to be used as a guess for the dispersion coefficients (required if WLCMTD=GUESS).
WLCVISU	Visualisation of intermediate results (YES/NO).
DC	Is the degree of the polynomial used in the dispersion relation, see Section 7.6.
TOL	Defines a tolerance window for the last step of single-order computation of the dispersion relations.
WLCLOOP	Three parameters to control the iterative identification of lines by improvement of a global solution. • WLCLOOP(1) = Minimum initial accuracy of the solution (pixels) • WLCLOOP(2) = Tolerance on the distance of the nearest neighbours. A value of e.g. 0.2 means that the nearest neighbour must be found at least at 5 times (=1/0.2) the residual to confirm the identification. Optimal values of this parameter are in the range 0. to 0.5. • WLCLOOP(3) = Maximal allowed accuracy of the loop.
WLCNITER	Two parameters for the minimum and maximum number of iterations of the identification loop.

Table 7.7: Command parameters (2)

Parameters: FLAT command	
Parameter	**Description**
FFOPT	Flat-Fielding option (`YES/NO`). If the value `NO` is assigned to this paramter, no Flat-Field correction is performed
FLAT	Raw flat field image.
CORRECT	Flat field correction image.
BLAZE	Smoothed flat field used in the normalisation of the flat field.
BKGMTD	Background estimation method (`POLY, SPLINE, SMOOTH`).
BKGVISU	Visualisation of intermediate results (`YES/NO`).
BKGSTEP	Step in pixels of the grid of background reference positions.
BKGPOL	Degree of the bivariate polynomial for background fiting (method `POLY`).
BKGRAD	Radius (radx, rady) in pixels of the window for local estimate of the background. The window is parallel to the orders (radx is measured along the orders, rady is parallel to the columns). (method `SPLINE`)
BKGDEG	Degree of spline polynomials (method `SPLINE`).
BKGSMO	Smoothing factor for smoothing spline interpolation. See Section 7.4 (method `SPLINE`).
EXTMTD	(See definition in Table 7.7)
SLIT	(See definition in Table 7.7)
OFFSET	(See definition in Table 7.7)
SAMPLE	Defines the wavelength step of the spectrum sampled in wavelengths. It can either be a real number indicating the step in units of Ångstrøm or a reference file corresponding to an image sampled in the space order–wavelength.
Parameters: FILTER command	
Parameter	**Description**
BKGxxx	All background parameters : see definitions above.
MEDFILT	widx,widy,no_iter. See help of command `FILTER/ECHELLE`.
CRFILT	radx,rady,mthresh.
CCDFILT	read-out noise (in e-), inverse gain factor (e-/ADU), threshold (in units of standard deviation).

Table 7.8: Command parameters (3)

Parameters: `RESPONSE` command	
Parameter	**Description**
STD	Raw Standard star, in `STANDARD` reduction mode.
RESPONSE	Computed instrument response in `STANDARD` reduction. If the name `NULL` is assigned to this parameter no response correction is applied in the `REDUCE` command. Instead, the blaze function is fitted.
FLUXTAB	Table with absolute fluxes for the Standard star, in `STANDARD` reduction mode. The tables are in the area `MID_STANDARD`
FILTMED	Radius in x and y, threshold, as in command `FILTER/MEDIAN` used to smooth the response function.
FILTSMO	Radius in x and y, threshold, as in command `FILTER/SMOOTH` used to smooth the response function.
PIXNUL	Number of pixels to set to zero at the edges of each order.
BKGxxx	All background parameters : see definitions in Table 7.8)
FFOPT	Flat-Fielding option (`YES/NO`)
CORRECT	Flat field correction image (required if `FFOPT=YES`).
BLAZE	Smoothed flat field (required if `FFOPT=YES`).
EXTMTD	(See definition in Table 7.7)
SLIT	(See definition in Table 7.7)
OFFSET	(See definition in Table 7.7)
SAMPLE	(See definition in Table 7.7)
Parameters: `REDUCE` command	
Parameter	**Description**
BKGxxx	All background parameters : see definitions in Table 7.8)
FFOPT	Flat-Fielding option (`YES/NO`)
CORRECT	Flat field correction image (required if `FFOPT=YES`).
BLAZE	Smoothed flat field (required if `FFOPT=YES`).
EXTMTD	(See definition in Table 7.7)
SLIT	(See definition in Table 7.7)
OFFSET	(See definition in Table 7.7)
SAMPLE	(See definition in Table 7.7)
RESPOPT	Option for the response corection (`YES/NO`).
RESPMTD	Method for the instrumental response correction (`STD, IUE`).
RESPONSE	Name of the response image as produced by `RESPONSE/ECHELLE` (required if RESPMTD=STD).
RIPMTD	Defines the ripple correction algorithm as `SINC` for the method fitting the blaze function, described by Ahmad(1981), and as `OVER` for the method using the overlapping region of the orders, proposed by Barker (1984) (required if `RESPMTD=IUE`).
RIPK	Defines the initial guess for the parameter k in Equation 7.5. The default value is updated during the wavelength calibration.
ALPHA	Defines the initial guess for the parameter α in Equation 7.5.
MGOPT	Merging option (`YES/NO`).
MRGMTD	Merging method (`AVERAGE, NOAPPEND`).
DELTA	Interval (in wavelength units) to be skipped at the edges of each order.

Table 7.9: Command parameters (4)

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