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VERY LARGE TELESCOPE

ESPRESSO DAS User Manual

VLT-MAN-ESP-13520-274

Issue 1.4.0

Date Mar 12, 2025

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1 Introduction

1.1 Purpose

The ESPRESSO Data Analysis Software (DAS) is a subsystem of the *VLT Data Flow System* (DFS). Its target user is *ESO Data Products Department* (DPD). It should also serve as a quick look tool for *Paranal Science Operations* (PSO). Additionally, the ESPRESSO DAS recipes are made public to the user community, to allow the analysis and the computation of scientific quantities from the instrument reduced data. The purpose of this document is to describe a set of typical ESPRESSO data analysis session with the ESPRESSO DAS.

This manual is a complete description of the data analysis recipes implemented by the ESPRESSO DAS, reflecting the status of the ESPRESSO DAS as of Mar 12, 2025 version 1.4.0.

1.2 Scope

This document describes the ESPRESSO DAS used at ESO-Garching and ESO-Paranal for the purpose of data analysis and data quality control.

The examples on running individual pipeline recipes in this manual use the `esorex` command and manually created list of input files. Several interfaces to automatically organise the data, create the list of input files and execute the pipeline recipes in the proper sequence are available, see the [ESO pipeline page](#) for details.

Please note that the use of Gasgano as a GUI for processing data is deprecated. Its use is no longer recommended and the related section in this manual, as well as support for Gasgano as a data processing GUI application in general will be dropped entirely in a future release.

Updated versions of the present document may be found on [11]. For general information about the current instrument pipelines status we remind the user of [4]. Quality control information are at [3].

Additional information on the Common Pipeline Library (CPL) and ESOREX can be found respectively at [8], [10]. The Gasgano front end is described in [12]. A description of the instrument is in [5]. The ESPRESSO instrument user manual is in [6].

1.3 Acknowledgements

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1.4 Reference documents

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2 Overview

In collaboration with instrument consortia, the Pipeline Systems Department (PSD) of the Software Development Division is implementing data reduction pipelines for the most commonly used VLT/VLTI instrument modes. In the case of the ESPRESSO instrument, ESO has decided to offer to the community also a suite of dedicated recipes to carry out the scientific analysis of the reduced spectra.

The data analysis software consists of a set of data processing modules that can be called from the command line or from the automatic data management tools available on Paranal.

ESO offers a front-end applications for launching pipeline recipes, *EsoRex* [10], included in the DAS distribution (see Appendix 11, page 60). This application can also be downloaded separately from www.eso.org/cpl/esorex

The ESPRESSO instrument and the different types of ESPRESSO reduced frames are described in Sections 4 and 7.

A brief introduction to the usage of the available reduction recipes using *EsoRex* is presented in Section 5. In section 6 we advice the user about known data analysis problems providing also possible solutions.

An overview of the data analysis, what are the input data, and the recipes involved in the analysis cascades is provided in section 8.

More details on what are inputs, products, quality control measured quantities, and controlling parameters of each recipe is given in section 9.

More detailed descriptions of the data analysis algorithms used by the individual pipeline recipes can be found in Section 10.

In Appendix 11 the installation of the ESPRESSO DAS recipes is described and in Appendix 12 a list of used abbreviations and acronyms is given.

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3 Recent improvements

This pipeline release implements –with respect to release 1.2.0– the following improvements:

- Added support for input ESPRESSO pipeline products in Phase 3 standard format.

This pipeline release implements –with respect to release 1.0.3– the following improvements:

- The QSO workflow has been split in two. The QSO I workflow carries out the coaddition of the spectra, the line detection, the continuum fitting, the identification of the lines and the creation of the absorption systems. The QSO II workflow starts from the identified absorption systems and gives the possibility to choose which ones to fit with Voigt profiles. In a future release, it will be possible also to repeat the fit of the continuum using the improved fit of the lines.
- In the interactive windows of the QSO I workflow steps: Coadd spectrum, Detect lines and fit continuum, sliding cursors have been added to simplify the inspection of the spectra.
- In the interactive window of the QSO I workflow: Mask spectrum it is now possible to apply different masks to different input frames.
- The names and definitions of the parameters of the recipe `espda_iden_sys` have been modified to clarify their use.
- It is now possible for the user to add interactively new knots to improve the spline fitting of the continuum in the QSO I workflow. This new feature allows to obtain very good results also in those region that in general were not well fitted by the automatic algorithm (e.g. the region severely affected by telluric absorptions or in general by strong absorption lines).
- The STAR III workflow is now operative. It computes the radial velocity in stellar spectra with the same algorithm adopted by the science recipe at the end of the data reduction cascade. Then it computes also the stellar indexes based on the Ca II lines: R’HK and S.
- Updated 3rd library dependency to CPL-7.1.3

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4 ESPRESSO Instrument Description

ESPRESSO has been developed by a consortium led by the Observatoire de Genève, including Trieste and Brera INAF Observatories (Italy), the Instituto de Astrofísica de Canarias (Spain), the Universidade de Porto and Lisboa (Portugal) and in collaboration with ESO. The instrument has been made available to the community and started operations in Paranal on October 1st, 2018.

In this chapter a brief description of the ESPRESSO instrument is given. A more complete documentation can be found in the ESPRESSO Instrument description web page

www.eso.org/sci/facilities/paranal/instruments/espresso/inst)

and User Manual, downloadable from

www.eso.org/sci/facilities/paranal/instruments/espresso.

4.1 Instrument overview

ESPRESSO is the ESO/VLT high-resolution spectrograph for measuring precise radial velocities on a long timespan with the main scientific aim to detect and characterise Earth twins in the inhabitable zone of solar-like stars [19].

ESPRESSO is a highly-stabilized fibre-fed échelle spectrograph that can be fed with light from either one or the four Unit Telescopes of the VLT. The instrument is installed at the incoherent combined Coudé focus (ICCF) of the VLT. The light from the astronomical source is redirected from the telescopes to the detectors through three components of the ICCF facility: the Coudé trains, the front ends, and the spectrograph. The Coudé Trains (CT) bring the light from each telescope to the Combined Coudé Lab (CCL) through 13 optical elements, including mirrors, lenses, and prisms. The four Front Ends (one for each UT) receive the light from the CTs and feed the entrance fibres. The Fibre Link transports the light from the Front Ends to the vacuum vessel. The latter is thermally stabilized at the mK level. The light is then going through the different optical elements of the spectrograph and splitted up into a red and a blue spectrum recorded on the corresponding red and blue cameras.

The spectrograph is fed by two fibres, one for the target itself and the other for simultaneous calibration (either sky or simultaneous reference: Laser Frequency Comb, Fabry-Perot or Thorium-Argon lamp). The light from the two fibres is recorded onto a blue (378 – 520 nm) and a red (520 – 779 nm) detector. The instrument can operate in three different modes: High Resolution 1UT (HR), Ultra High-Resolution 1UT (UHR), and Medium Resolution 4UTs (MR). The main characteristics of these modes are summarised below.

	HR (1UT)	UHR (1UT)	MR (4UTs)
Wavelength range	380-780 nm	380-780 nm	380-780 nm
Resolving power (median)	140,000	190,000	70,000
Aperture on the sky	1".0	0".5	4 × 1".0
Global efficiency @ 550nm	9 %	4 %	9 %
RV precision (requirement)	< 10 cm/s	< 5 m/s	< 5 m/s
Limiting V-band magnitude ¹	~ 17	~ 16	~ 20
Binning (spatial × spectral)	1x1, 2x1	1x1	4x2, 8x4
Spectral sampling (average)	4.5 px	2.5 px	5.5 px (binned ×2)
Spatial sampling per slice	9.0 (4.5) px	5.0 px	5.5 px (binned ×4)
Number of slices	2	2	2

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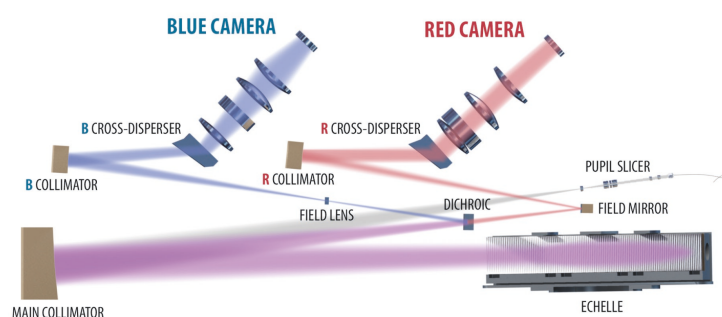


Figure 4.1.0: An inside view of ESPRESSO vacuum vessel: at the entrance of the spectrograph, an anamorphic pupil slicing unit (APSU, not shown) shapes the beam in order to compress the beam in cross-dispersion direction but not in main-dispersion direction, where high resolving power needs to be achieved. In the latter direction, the pupil is sliced and superimposed on the echelle grating to minimize its size. Then, a dichroic beam splitter separates the beam in a blue and a red channel optimized for image quality and optical efficiency. The cross-disperser separates the dispersed spectrum in all its spectral orders and before arriving on the camera, an anamorphism is re-introduced to make the pupil square and to compress the order width in cross-dispersion direction, such that the inter-order space is maximized.

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5 Quick start

This section describes the most immediate usage of the ESPRESSO DAS recipes.

5.1 ESPRESSO DAS recipes

The current ESPRESSO DAS is based on a set of 13 stand-alone recipes involved in six data analysis cascades (or branches), one for the quick verification of the SNR of the coadded spectrum (COADD, to be used in particular at the telescope), two for the analysis of quasar spectra (QSO I and QSO II) and three for the analysis of stellar spectra (STAR I, STAR II and STAR III).

espda_coadd_spec to combine multiple spectra of the same object, the individual pixels are kept independent for a more reliable computation of the noise .

espda_mask_spec to mask regions of the spectrum that do not have to be used in the subsequent analysis. Interactive.

espda_create_linelist to detect the absorption lines present in a quasar spectrum. Interactive.

espda_fit_qsocont to fit the quasar intrinsic continuum after the removal of the detected lines.

espda_iden_syst to carry out a preliminary identification of the absorption lines and the creation of absorption systems by coincident redshift. Interactive.

espda_fit_line to fit the lines with Voigt profiles taking into consideration the identification and the division in systems carry out before. Interactive.

espda_compu_eqwidth to compute the equivalent width of a set of predefined lines in a stellar spectrum.

espda_compu_starpar to estimate the effective temperature, T_{eff} , and the metallicity, [Fe/H], of a stellar spectrum comparing the previously determined equivalent widths with static calibration tables.

espda_fit_starcont to compute the stellar continuum level order by order by fitting a polynomial function.

espda_synth_spec to derive the closest synthetic spectrum to the observed one based on a set of input stellar parameters (effective temperature, surface gravity and metallicity) and broadening parameters (instrumental broadening, rotation velocity and macroturbulence).

espda_rv_synth to compute the radial velocity of the star by cross-correlating the observed 1D stellar spectrum normalized to the continuum with the synthetic spectrum selected by the previous recipe already interpolated and convolved.

espda_compu_radvel to compute the cross-correlation function (CCF) of the stellar 2D spectrum (in the wavelength-order space) using a given stellar type line mask, and then fits a Gaussian function to the CCF to obtain CCF parameters including radial velocity.

espda_compu_rhk to compute the Ca II H&K activity index as $\log(R'_{\text{HK}})$.

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5.2 An introduction to Reflex and EsoRex

Before being able to call the DAS recipes to process a set of data, the data must be correctly classified. This operation is simpler for the DAS than for the Data Reduction because there are no calibrations to associate with the frames.

Typically, a set of frames can be associated if they share a number of properties, such as instrument and detector configuration. Since all the required information is stored in the FITS headers, data association is based on a set of header keywords (called "association keywords") and the process is specific to each data analysis branch. The process of data classification and association is known as data organisation.

An instrument pipeline consists of a set of data processing modules that can be called from different host applications, namely:

- *Reflex* is a graphical tool that helps the user to execute data reduction/analysis workflows which contain several recipes. This dramatically decreases the time the user needs to run a whole reduction/analysis chain. *Reflex* takes care of grouping the different data sets, associating the calibration frames and managing the interdependencies between recipes. **Reflex is the recommended software tool for reducing/analysing your data.**
- *EsoRex* is a command line tool used to run the DAS recipes. *EsoRex* commands can be easily scripted.

5.2.1 Using Reflex

Reflex is the recommended tool to reduce/analyse complete data sets that include all the calibration frames. It is an advanced tool, and yet easy to use, that is geared towards maximum scientific return. It is based on the workflow engine *Kepler* [26].

This manual does not cover the installation of *Reflex*. Please refer to [13] for the installation procedure which also contains a detailed description of the *Reflex* application. What follows is a very brief summary of it.

Once installed, *Reflex* can be executed with the command:

```
user@host# reflex &
```

Reflex main concepts are workflows and actors. Workflows are canvasses which show the interdependence of the pipeline recipes, allowing the user to easily obtain an overview of the reduction/analysis steps. Workflows have the advantage of requiring a small learning curve in order to get the pipeline running.

Actors are the entities which actually perform some kind of operation. In *Reflex*, to each main actor corresponds a pipeline recipe, which performs the data reduction/analysis steps, but there are other actors such as the DataOrganizer, or the FitsRouter that are useful to manage the data files. Each actor can be configured by right-clicking on it and selecting *Configure Actor* as shown in Figure 5.2.1. In the case of the recipe actors, the recipe parameters are part of the actor and make up the second group of parameters.

In addition to those elements, the workflow contains variables that contain the most important settings, such as the directories where data is located and will be saved.

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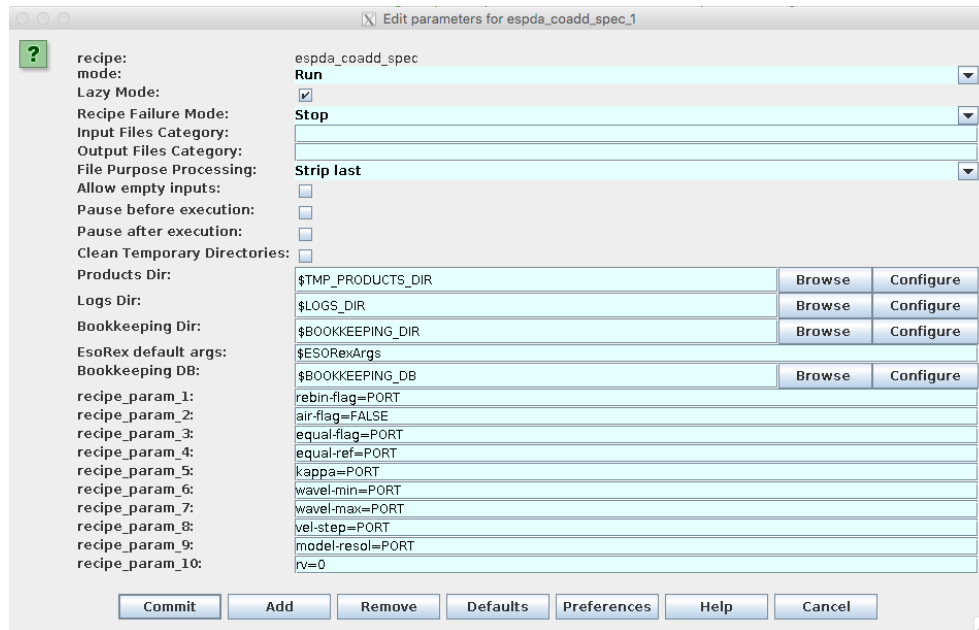


Figure 5.2.1: Parameters of a recipe actor. The first group of parameters affect the execution of the pipeline recipe and are common to all recipe actors. The second group of parameters are specific to the pipeline recipe to be called and they are identical to those that can be configured in EsoRex (see 5.2.3).

To start using *Reflex* with this pipeline, please refer to [13].

5.2.2 Example of data analysis using the Reflex-based ESPRESSO DAS workflow

For the user who is keen on starting data analysis without being distracted by detailed documentation, we describe the steps to be performed to analyze the science reduced data provided in the ESPRESSO DAS demo data set supplied with the *Reflex* 2.11.5 release. By following these steps, the user should have enough information to attempt an analysis of his/her own data without any further reading. We will present only the steps necessary to run the *STAR I* workflow, for the information on all the other DAS workflows please refer to the DAS tutorial document [13].

Start the *Reflex* application:

```
reflex &
```

The empty *Reflex* canvas as shown in Figure 5.2.2 will appear.

Now open the ESPRESSO DAS workflow by clicking on *File* -> *Open File*, selecting first *espda-1.4.0* and then one of the files *.xml* in the file browser.

If you choose e.g. the *starI.xml*, you will be presented with the workflow canvas shown in Figure 5.2.3. Note that the workflow will appear as a canvas in a new window.

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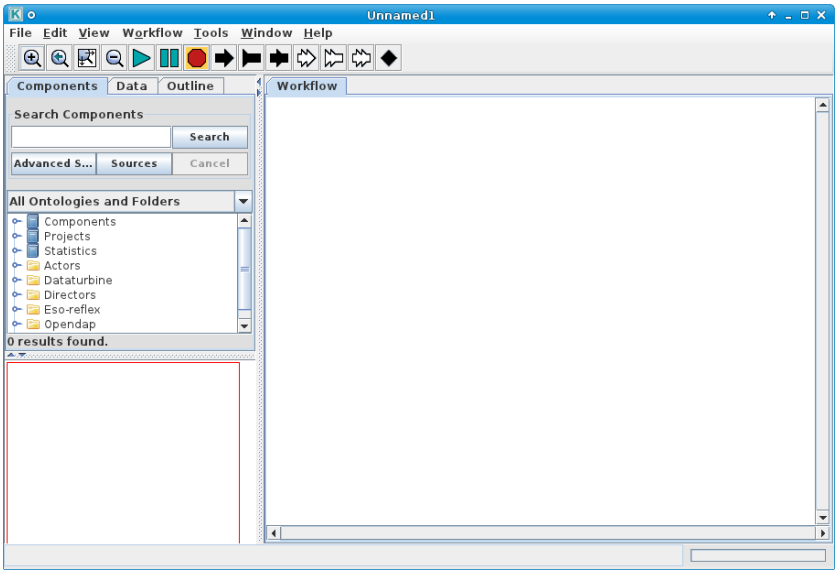


Figure 5.2.2: Fresh Reflex canvas.

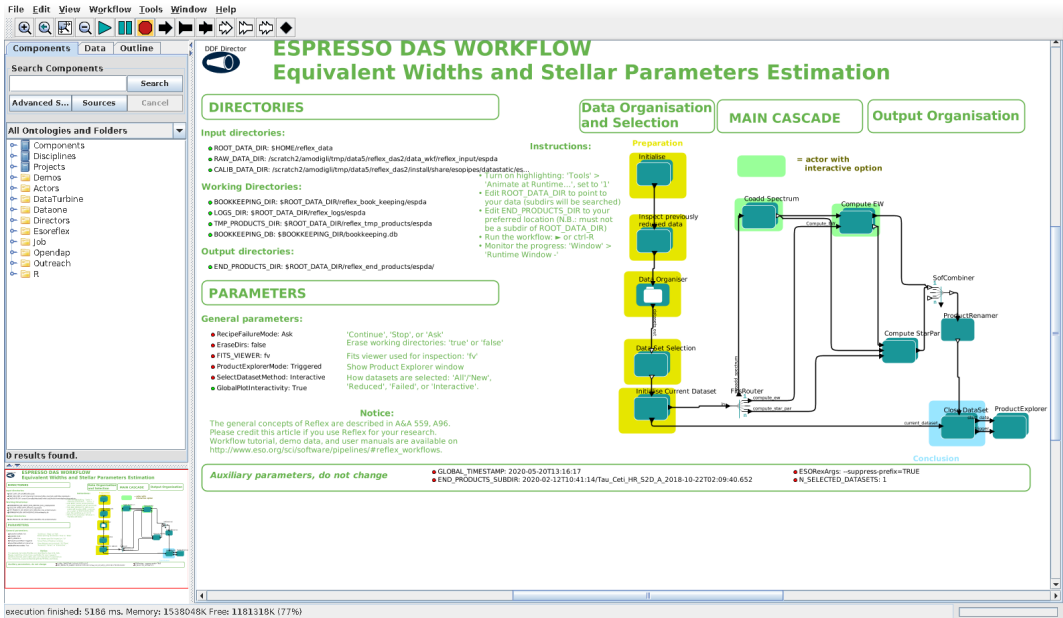



Figure 5.2.3: ESPRESSO DAS STAR I workflow general layout.

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To aid in the visual tracking of the reduction cascade, it is advisable to use component (or actor) highlighting. Click on **Tools** -> **Animate at Runtime**, enter the number of milliseconds representing the animation interval (100 ms is recommended), and click **OK**.

1. Under “Setup Directories” in the workflow canvas there are seven parameters that specify important directories (green dots). Setting the value of `ROOT_DATA_DIR` is the only necessary modification if you want to process data other than the demo data², since the value of this parameter specifies the working directory within which the other directories are organised. Double-click on the parameter `ROOT_DATA_DIR` and a pop-up window will appear allowing you to modify the directory string, which you may either edit directly, or use the **Browse** button to select the directory from a file browser. When you have finished, click **OK** to save your changes.
2. Click the  button to start the workflow
3. The workflow will highlight the `Data Organiser` actor which has recursively scanned the raw data directory (specified by the parameter `RAWDATA_DIR` under “Setup Directories” in the workflow canvas) and constructs the `DataSets`. Note that the calibration and reference data must be present either in `RAWDATA_DIR` or in `CALIB_DATA_DIR`, otherwise `DataSets` may be incomplete and cannot be processed. However, if the same reference file was downloaded twice in different places this creates a problem as `Reflex` cannot decide which one to use.
4. The `Data Set Chooser` actor will be highlighted next and will display a “Select Datasets” window that lists the `DataSets` along with the values of a selection of useful header keywords³. The first column consists of a set of tick boxes which allow the user to select the `DataSets` to be processed, and by default all complete `DataSets` are selected.
5. Click the **Continue** button and watch the progress of the workflow by following the red highlighting of the actors. A window will show which `DataSet` is currently being processed.
6. When the workflow has finished executing the recipe `espda_coadd_spec` in the `Coadd Spectrum` actor for the first `DataSet`, an interactive window will appear which shows a plot of the coadded, rebinned, equalized spectrum (in blue). The bottom panel shows the SNR computed pixel-by-pixel for the rebinned spectrum. Using the buttons at the top of this window, one may pan and zoom in on the spectrum in order to inspect absorption/emissions lines and other interesting spectral features. In the right part of the panel, the recipe input parameters are shown with their default values. You can change those parameters and re-run the recipe or click the **Continue Wkf** button and go on to the next DA step.
7. The output of the previous recipe will be a one dimensional spectrum corrected by the radial velocity. This spectrum goes to the recipe `espda_compu_eqwidth` which identifies the lines in their rest frame in order to measure the equivalent widths. The recipe will enter a loop on a line by line procedure reading the input line list and measuring the equivalent widths of the corresponding lines in the observed spectrum. The output of the recipe will be the list of lines with the computed equivalent widths and respective errors for

²If you used the install script `install_reflex`, then the value of the parameter `ROOT_DATA_DIR` will already be set correctly to the directory where the demo data was downloaded.

³The keywords listed can be changed by right-clicking on the `DataOrganiser` Actor, selecting `Configure Actor`, and then changing the list of keywords in the second line of the pop-up window. Make sure that the `Lazy Mode` is not active and then click on **Commit** to save the change.

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each line. The `Compute EW` actor opens an interactive window showing in the top panel the fitted lines: all detected and fitted lines can be inspected using the sliding cursor that moves through the list of lines. The bottom panel shows a scatter plot with the measured equivalent widths as a function of wavelength.

8. The product with the measurements of the equivalent widths for the lines is the input to the next actor, `Compute Starpar`. The implemented recipe is `espda_compu_starpar`, which will make use of static calibrations to estimate the effective temperature and metallicity [Fe/H] of the observed star.
9. When the analysis of the current DataSet finishes, a pop-up window will appear showing the directory where the final products have been saved.
10. The workflow will continue with the remaining DataSets following the same steps described above.
11. After the workflow has finished, all the products from all the DataSets can be found in a directory under `END_PRODUCTS_DIR` with the named with the workflow start timestamp. Further subdirectories will be found with the name of each DataSet.

5.2.3 Using EsoRex

EsoRex is a command line utility for running pipeline recipes. It may be embedded by users into data reduction/analysis scripts for the automation of processing tasks. On the other side, *EsoRex* doesn't offer all the facilities available with *Reflex*, and the user must classify and associate the data using the information contained in the FITS header keywords (see Section 7). The user should also take care of defining the input set-of-frames and the appropriate configuration parameters for each recipe run:

The set-of-frames: Each pipeline recipe is run on a set of input FITS data files. When using *EsoRex* the filenames must be listed together with their DO category ⁴ in an ASCII file, the *set-of-frames* (SOF), that is required when launching a recipe.

Here is an example of SOF, valid for the `espda_compu_eqwidth` recipe:

```

/file_path/      FSPEC_PRE
/file_path/      RSPEC_PRE
/file_path/      LINE_STARPAR
```

It contains for each input frame the full path file name and its DO category. The DAS recipe will access the listed files when required by the analysis algorithm.

Note that the ESPRESSO DAS recipes do not verify in any way the correctness of the classification tags specified by the user in the SOF. In the above example, the recipe `espda_compu_eqwidth` will treat the frame `/file_path/.fits` as a `FSPEC_PRE`, the frame `/file_path/.fits` as a `LINE_STARPAR`, etc., even when they do not contain this type of data. The recipe will also assume that all frames are associated correctly, *i.e.*, that they all come from the same instrument configuration.

The reason of this lack of control is that the ESPRESSO DAS recipes are just the components of the four DAS workflows, where the task of data classification and association is carried out by separate applications.

⁴The indicated *DO category* is a label assigned to any data type after it has been classified, which is then used to identify the frames listed in the *set-of-frames*

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A recipe handling an incorrect SOF may stop or display unclear error messages at best. In the worst cases, the recipe would apparently run without any problem, producing results that may look reasonable, but are actually flawed.

EsoRex syntax: The basic syntax to use ESOREX is the following:

esorex [esorex_options] recipe_name [recipe_options] set_of_frames

To get more information on how to customise ESOREX (see also [10]) run the command:

esorex - -help

To generate a configuration file `esorex.rc` in the directory `$HOME/.esorex` run the command:

esorex - -create-config

A list of all available recipes, each with a one-line description, can be obtained using the command:

esorex - -recipes

All recipe parameters (aliases) and their default values can be displayed by the command

esorex - -params recipe_name

To get a brief description of each parameter meaning execute the command:

esorex - -help recipe_name

To get more details about the given recipe give the command at the shell prompt:

esorex - -man-page recipe_name

Recipe configuration: Each DAS recipe may be assigned an *EsoRex* configuration file, containing the default values of the parameters related to that recipe. The configuration files are normally generated in the directory `$HOME/.esorex`, and have the same name as the recipe to which they are related, with the filename extension `.rc`. For instance, the recipe `espda_compu_eqwidth` has its *EsoRex* generated configuration file named `espda_compu_eqwidth.rc`, and is generated with the command:

esorex - -create-config espda_compu_eqwidth

The definition of one parameter of a recipe may look like this:

```
# --ew_min
# ew min:  (2., 0., 400.)
espda.ew_min=4.0
```

In this example, the parameter `espda.ew_min` is set to the value `4.0`. In the configuration file generated by *EsoRex*, one or more comment lines are added containing information about the possible values of the parameter, and an alias that could be used as a command line option.

The command

esorex - -create-config recipe_name

generates a default configuration file **recipe_name.rc** in the directory **`$HOME/.esorex`**⁵.

A recipe configuration file different from the default one can be specified on the command line:

⁵If a number of recipe parameters are specified on the command line, the given values will be used in the created configuration file.

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esorex - -recipe-config=my_alternative_recipe_config

Recipe parameters are provided in section 9 and their role is described in Section 10.

More than one configuration file may be maintained for the same recipe but, in order to be used, a configuration file not located under `$HOME/.esorex`, or having a name different from the recipe name, should be explicitly specified when launching a recipe.

Recipe execution: A recipe can be run by specifying its name to *EsoRex*, together with the name of a set-of-frames. For instance, the following command line would be used to run the recipe *espda_compu_eqwidth* for processing the files specified in the set-of-frames *espda_compu_eqwidth.sof*:

esorex espda_compu_eqwidth espda_compu_eqwidth.sof

The recipe parameters can be modified either by editing directly the used configuration file, or by specifying new parameter values on the command line using the command line options defined for this purpose. Such command line options should be inserted after the recipe name and before the SOF name, and they will supersede the system defaults and/or the configuration file settings. For instance, to set the *espda_compu_eqwidth* recipe *ew_min* parameter to `4.0`, the following should be typed:

esorex espda_compu_eqwidth - -ew_min=4.0 espda_compu_eqwidth.sof

For more information on *EsoRex*, see www.eso.org/cpl/esorex.html.

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6 Known problems

We suggest the user to execute the DAS recipes using default parameters and all the reference calibrations indicated in this manual. The following is a list of currently-known issues with ESPRESSO DAS recipes, and workarounds, if available:

- **WARNING:** The recipe `espda_coadd_spectrum` can take from a few to several minutes to create the rebinned spectrum, depending on the number of input frames and on the size of the adopted rebinning step.
- The recipe `espda_coadd_spectrum` produces line profiles with small steps, visible in particular when the signal-to-noise ratio (SNR) is large. The issue is due to the kappa-sigma clipping: input pixels are not weighted properly. If the clipping is skipped, the problem disappears, but in this case the order merging is not effective when the SNR is low. The issue will be fixed in the next DAS release. A temporary workaround is provided: for high-SNR spectra, the user must choose a high value of kappa (> 5) in `espda_coadd_spec` to minimize the effect of kappa-sigma clipping, while for low-SNR spectra the user must keep the default value ($\text{kappa} = 3$) to obtain a proper order merging.
- In the STAR III workflow the recipe `espda_compu_radvel` does not compute the correct radial velocity with the default parameters if the minimum of the CCF does not fall in the range **rv-center** \pm **rv-window**. If, in the plot created by the recipe, you don't see the minimum, increase the value of **rv-window** to e.g. 100 km s^{-1} and run the recipe again. Then modify the value of **rv-center** to the approximate center of the observed CCF and decrease again the size of **rv-window**. Run again the recipe to have a more precise determination of the radial velocity.
- In the QSO I workflow the data organizer will present for a single object one dataset with the sky-subtracted spectrum and one for the non-sky-subtracted spectrum. If the dataset has been reduced with the "smoothed" sky subtraction method then it is preferable to use the sky-subtracted spectrum otherwise, use the non-sky-subtracted one.
- In the QSO I and II workflows the continuum fitting procedure (`espda_fit_qsocont`) can take a long time. To avoid this long processing time it is possible to select smaller regions of the spectrum at the coaddition step (`espda_coadd_spec`).
- In the QSO II workflow the line fitting procedure (`espda_fit_line`) sometimes fail to fit complex systems with many components. The issue will be fixed in a later release.
- In the QSO II workflow the continuum fitting recipe (`espda_fit_qsocont`) and the system identification recipe (`espda_iden_system`) are currently unable to handle input from the line fitting recipe (`espda_fit_line`), and are therefore disabled.

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7 Instrument Data Description

In the following sections the reduced ESPRESSO data frames are listed, together with the relevant FITS keywords (omitting the prefix HIERARCH ESO) used for their classification and correct association. The indicated *DO category* is a label assigned to any data type after it has been classified, which is then used to identify the frames listed in the *Set of Frames* (see Section 5.2.3, page 20). Only the reduced ESPRESSO frames which are the input data of the analysis workflows are described, for a complete description of all reduced frames refer to the DRS User Manual.

- **One-dimensional spectrum:**

One-dimensional spectrum for fiber A or B, where A is the fiber dedicated to the target observation, while in fiber B there can be either the sky or a calibration source (Th-Ar lamp, Fabry-Perot or Laser Frequency Comb).

DO category: S1D

Classification keywords:

PRO CATG = S1D_fiber
PRO TYPE = REDUCED
PRO TECH = ECHELLE

Association keywords:

INS MODE, DET BINX, DET BINY

- **Sky subtracted one-dimensional spectrum:**

This product is generated by the DRP when fiber B observes the sky.

DO category: S1D

Classification keywords:

PRO CATG = S1D_SKYSUB_A
PRO TYPE = REDUCED
PRO TECH = ECHELLE

Association keywords:

INS MODE, DET BINX, DET BINY

- **Sky-subtracted, flux-calibrated, one-dimensional spectrum:**

This product is generated by the DRP when fiber B observes the sky.

DO category: S1D

Classification keywords:

PRO CATG = S1D_SKYSUB_FLUXCAL_A
PRO TYPE = REDUCED
PRO TECH = ECHELLE

Association keywords:

INS MODE, DET BINX, DET BINY
DET BINX

- **Flux-calibrated, one-dimensional spectrum:** This product is generated by the DRP when in fiber B there is a calibration source.

DO category: S1D

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Classification keywords:

PRO CATG = S1D_FLUXCAL_A
PRO TYPE = REDUCED
PRO TECH = ECHELLE

Association keywords:

INS MODE, DET BINX, DET BINY

- **Two-dimensional spectrum:** Spectrum in the wavelength-order space. This product is generated by the DRP for fiber A or B, where A is the fiber dedicated to the target observation, while in fiber B there can be either the sky or a calibration source (Th-Ar lamp, Fabry-Perot or Laser Frequency Comb).

DO category: S2D

Classification keywords:

PRO CATG = S2D_fiber
PRO TYPE = REDUCED
PRO TECH = ECHELLE

Association keywords:

INS MODE, DET BINX, DET BINY

- **Sky-subtracted, two-dimensional spectrum:** Spectrum in the wavelength-order space. This product is generated by the DRP when fiber B observes the sky.

DO category: S2D

Classification keywords:

PRO CATG = S2D_SKYSUB_fiber
PRO TYPE = REDUCED
PRO TECH = ECHELLE

Association keywords:

INS MODE, DET BINX, DET BINY

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8 Data Analysis

In this section, we overview the main steps the data analysis for quasar and stellar spectra has to go through and we list the required data and the recipes which allow to perform them. The reported name of the frames are the standard names assigned to the DAS to that kind of frames.

Note that the `WAVE_MATRIX` frames in air and vacuum corrected to the barycentric reference frame and the `DLL_MATRIX` frames containing the sizes of the pixels are extensions of the reduced scientific frame, as a consequence it is not necessary to provide them as separate input frames to the DAS workflows. On the other hand the `BLAZE` frame has to be recovered from the directory `reflex_book_keeping` because it is an output product of the recipe `espdr_mflat`.

8.1 Overview of stellar spectrum analysis

The ESPRESSO data analysis of stellar spectra offers three possible paths, one for the determination of the stellar parameters (effective temperature and metallicity), one for the rough estimate of the radial velocity from a comparison of observed and synthetic spectra and one for the precise determination of the radial velocity and of activity indexes.

In the following we report the steps of each analysis path.

8.1.1 STAR I

- Combine multiple spectra of the same star and correct for radial velocity, running the recipe `espda_coadd_spectrum`.
- Determine the equivalent width of predefined absorption lines carrying out a local determination of the continuum with the recipe `espda_compu_eqwidth`.
- Compare the measured equivalent widths with static calibrations to determine the effective temperature and the metallicity ($[Fe/H]$) of the star with the recipe `espda_compu_starpar`.

Required input data

- Reference files:
 - The `LINE` table as input of `espda_compu_eqwidth` with the wavelengths of the lines for which the equivalent widths have to be computed. The user can adopt a personal `LINE` table, however, this may affect the precision of the estimation of the stellar parameters.
 - The `LINE_RATIO_CALIB` table as input of `espda_compu_starpar` with the equivalent width ratios to be compared with the observed ones for the determination of the effective temperature.
 - The `LINE_FEH_CALIB` table as input of `espda_compu_starpar` containing the Fe lines and respective calibrations including the limits of the parameter space where they can be applied.
- Reduced frames:

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- Science spectra of one fiber in the [extracted pixel, spectral order] space corrected for the blaze function (S2D_fiber). They represent the output of the spectrum extraction algorithms that collapse the raw spectrum along the cross-dispersion direction (without resampling) or
- One-dimensional spectra (SID_fiber) or flux calibrated spectra (SID_FLUXCAL_fiber).
- Calibration data products.
 - The matrix which contains the size of the pixels in air (AIR_DLL_MATRIX_fiber) for the used instrument mode.

8.1.2 STAR II

- Combine multiple spectra of the same star without correcting for radial velocity, running the recipe `es-pda_coadd_spectrum`.
- Estimate the continuum level order by order fitting the spectrum with a polynomial with the recipe `espda_fit_starcont`.
- Use the recipe `espda_synth_spec` to generate an interpolated synthetic spectrum corresponding to the set of stellar (T_{eff} , $[\text{Fe}/\text{H}]$ and $\log g$) and broadening (instrumental, rotation velocity and macroturbulence) parameters in input .
- Cross-correlate the previously created synthetic spectrum with the observed one and fit the cross-correlation function to estimate the radial velocity using the recipe `espda_rv_synth`.

Required input data

- Reference files:
 - The SYNTH_SPEC library of synthetic spectra as input of `espda_synth_spec`
- Reduced frames:
 - Science spectra of one fiber in the [extracted pixel, spectral order] space corrected for the blaze function (S2D_fiber). They represent the output of the spectrum extraction algorithms that collapse the raw spectrum along the cross-dispersion direction (without resampling).
- Calibration data products.
 - The matrix which contains the size of the pixels in air (AIR_DLL_MATRIX_fiber) for the used instrument mode.

8.1.3 STAR III

- Estimate the star radial velocity by cross-correlating the spectrum in the wavelength-order space with a predefined stellar-type mask and correct the spectrum to the rest frame with the recipe `espda_compu_radvel`.

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- Measure the integrated fluxes in predetermined passbands to estimate the stellar activity index: Mt Wilson CaII H&K R'HK index using the recipe `espda_compu_rhk`.

Required input data

- Reference files:
 - The cross-correlation masks for the given spectral type (MASK).
- Reduced frames:
 - For radial velocity computation: science spectra of one fiber in the [extracted pixel, spectral order] space, not deblazed (S2D_BLAZE_fiber). They represent the output of the spectrum extraction algorithms that collapse the raw spectrum along the cross-dispersion direction (without resampling). In separated FITS extensions they contain also the wavelength calibration matrix and the size of the pixels for the used instrument mode.
 - For R'HK index computation: one-dimensional spectra (S1D_fiber, sky subtracted or sky subtracted and flux calibrated).
- Calibration data products.
 - The blaze function (BLAZE_fiber) which contains the information on the echelle grating blaze of one fiber in the [extracted pixel, spectral order] space.

8.2 Overview of quasar spectrum analysis

The ESPRESSO data analysis for quasar spectra is split into two parts. The first one reaches to the identification of absorption systems, while the second starts from the identified systems and fit them. In a forthcoming release, the second path will also include an improvement of the continuum fitting after the systems have been fitted and a second round of system identification.

The main ESPRESSO data analysis steps in the case of quasar spectra are described in the following.

8.2.1 QSO I

- Combine multiple frames to increase the SNR with the recipe `espda_coadd_spec`. At this step, all the pixels of all considered frames are kept distinct and the following steps are performed on this big table.
- Mask the regions of the spectrum which for any reason do not have to be considered in the analysis, using the recipe `espda_mask_spec`. This is an interactive step, the user has to input the wavelength intervals that should be masked.
- The recipe `espda_create_linelist` detect absorption lines and gather them in a table. The user can add more absorprtion lines, but only when using the Reflex workflow.
- Fit the continuum level of the spectrum with a cubic spline. The identified lines are fitted and subtracted from the continuum fit. This step is performed by the recipe `espda_fit_qsocont`.

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- Identify the detected lines and combine them into systems (different ionic transitions at the same redshift) with the recipe `espda_iden_syst`. This is an interactive step (but only in the reflex workflow): the user can accept or reject the systems generated by the recipe.

Required input data

- Reference files:
 - The `VOIGT_FUNC` table containing the tabulated data as input of the recipe `espda_fit_qsocont`.
 - The `QSO_ION` table containing the rest frame wavelength, the oscillator strength, the natural damping constant and the mass of the atom for the ionic transitions generally observed in quasar spectra as input of the recipe `espda_fit_qsocont` and `espda_iden_syst`.
 - The `QSO_ION_RED` table containing a selected list of ionic transitions from table `QSO_ION`, as input of the recipe `espda_iden_syst`.
- Reduced frames:
 - Science spectra of one fiber in the [extracted pixel, spectral order] space corrected for the blaze function and sky subtracted (`S2D_SKYSUB_fiber`). They represent the output of the spectrum extraction algorithms that collapse the raw spectrum along the cross-dispersion direction (without resampling) or
 - One-dimensional spectra of one fiber sky subtracted (`S1D_SKYSUB_fiber`) or sky subtracted and flux calibrated (`S1D_SKYSUB_FLUXCAL_fiber`)
- Calibration data products.
 - None. Both the wave matrix table (`WAVE_MATRIX_fiber`) which contains the wavelength calibration and the matrix which contains the size of the pixels (`DLL_MATRIX_fiber`) for the used instrument mode are fits extensions of the science spectrum.

8.2.2 QSO II

- Fit with Voigt profiles the identified lines using the recipe `espda_fit_line`. This is an interactive step (but only in the reflex workflow): the user can modify the proposed fit by adding more components or changing the relations between different parameters.
- Fit the continuum level of the spectrum with a cubic spline. This step takes into consideration the fit of the systems carried out in the previous step and should provide an improved estimate of the continuum level. This step is performed by the recipe `espda_fit_qsocont`. **Note:** At present the recipe `espda_fit_qsocont` is not able to process output from `espda_fit_line`. It will be enabled in a later release.
- Refine the identification of the lines detected in workflow QSO I but not identified. This step takes into consideration the systems fitted in the previous step and try to associate more lines to the already known systems or to find new systems using the non-identified lines and an enlarged list of ionic transitions. **Note:** At present the recipe `espda_iden_syst` is not able to process output from `espda_fit_line`. It will be enabled in a later release.

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Required input data

- Reference files:
 - The VOIGT_FUNC table containing the tabulated data as input of the recipe `espda_fit_line`
 - The QSO_ION table containing the rest frame wavelength, the oscillator strength, the natural damping constant and the mass of the atom for the ionic transitions generally observed in quasar spectra as input of the recipe `espda_fit_qsocont` and `espda_iden_syst`.
 - Optionally, the QSO_ION_RED table containing a selected list of ionic transitions from table QSO_ION, as input of the recipe `espda_iden_syst`.
- Reduced frames:
 - A one-dimensional spectrum normalized to continuum, in table format (RSPEC_CONT).
 - A table with the lines of the system that has to be fitted (SLINE_IDEN).
 - A table with the other lines identified in the spectrum, not belonging to the system that has to be fitted (FLINE_IDEN)
 - Optionally, a table with the instrument profile sampled at the wavelength of the spectrum (RPROF). The table is produced by `espda_coadd_spec`. If it is not available, it will be re-created by `espda_fit_line` every time it is run (this increases the computation time significantly).
- Calibration data products.
 - None

8.3 Overview of the quick view COADD workflow

The ESPRESSO DAS offers a simple tool to visualize and verify the SNR of any ESPRESSO spectrum (or set of spectra of the same target): the COADD WKF. This WKF is made of only two steps.

- Combine multiple frames to increase the SNR with the recipe `espda_coadd_spec`. At this step, all the pixels of all considered frames are kept distinct and the following steps are performed on this big table.
- Mask the regions of the spectrum which for any reason do not have to be considered in the analysis, using the recipe `espda_mask_spec`. This is an interactive step, the user has to input the wavelength intervals that should be masked.

Required input data

- Reference files:
 - None
- Reduced frames:

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- Science spectra of one fiber in the [extracted pixel, spectral order] space corrected for the blaze function and (when available) sky subtracted (S2D_SKYSUB_fiber). They represent the output of the spectrum extraction algorithms that collapse the raw spectrum along the cross-dispersion direction (without resampling) or
- One-dimensional spectra of one fiber sky subtracted (S1D_SKYSUB_fiber) or sky subtracted and flux calibrated (S1D_SKYSUB_FLUXCAL_fiber)
- Calibration data products.
 - None. Both the wave matrix table (WAVE_MATRIX_fiber) which contains the wavelength calibration and the matrix which contains the size of the pixels (DLL_MATRIX_fiber) for the used instrument mode are fits extensions of the science spectrum.

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9 Pipeline Recipes Interfaces

In this section we provide for each recipe examples of the required input data (and their TAGs to be used in SOF files).

In the tables, the column “type” indicates the kind of data:

- drp, data reduction product.
- ref, reference frame.
- dap, DAS product.

The column “n” of the input table indicates the number of required input frames using the following convention:

- 1 for a single frame.
- + for 1 or more frames.
- ! for recommended input frames.
- ? for optional input frames.

We also provide a list of the pipeline products for each recipe, indicating their default recipe name (eventually set by esorex to a given standard), the value of the FITS keyword HIERARCH ESO PRO CATG (in short PRO.CATG) and a short description.

For each recipe we also list in a table the input parameters (as they appear in the recipe configuration file), the corresponding aliases (the corresponding names to be eventually set on command line) and their default values. Also quality control parameters are listed. Those are stored in relevant products. More information on instrument quality control can be found on www.eso.org/qc.

9.1 espda_coadd_spec

The recipe espda_coadd_spec combines different spectra of the same object. It can be fed with 1-D merged spectra or with spectra in the [extracted pixel, spectral order] space.

9.1.1 Input

Type	TAG	short description	n	MODE	BIN
drp	S1D	One-dim. merged spectrum	+	any	any
drp	S2D	Spectrum in the [extracted pixel,spectral order] space	+	any	any

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9.1.2 Output

default recipe file name	PRO.CATG	short description
FSPEC_ORIG.fits	FSPEC_ORIG	Original spectrum in the [extracted pixel,spectral order] space
RSPEC_ORIG.fits	RSPEC_ORIG	Original merged spectrum (only if S1D in input)
FSPEC_PRE.fits	FSPEC_PRE	Spectrum in the [extracted pixel,spectral order] space, optionally equalised
RSPEC_PRE.fits	RPSEC_PRE	Rebinned merged spectrum, optionally equalised
RPROF.fits	RPROF	Rebinned instrument profile

9.1.3 Quality control

name	frames	description
DAS.Z_EM	All	Quasar emission redshift.
DAS.RV MEAN	All	Mean radial velocity (average of the input frames' CCF RV values) [km s ⁻¹]
DAS.SNR600.RMS	All	Root-mean-square of the signal-to-noise ratio of the input frame at 600 nm
DAS.VEL.STEP	All	Applied velocity step [km s ⁻¹]

9.1.4 Parameters

alias	default	range	description
rebin_flag	TRUE	[TRUE, FALSE]	Flag to rebin spectra (disregarded if only S1D frame is present)
air_flag	TRUE	[TRUE, FALSE]	Flag to use wavelengths in air instead of wavelengths in vacuum.
equal_flag	TRUE	[TRUE, FALSE]	Flag to equalize spectra.
equal_ref	1	[0, number of exposures]	ID number of the reference exposure to be used in equalization.
kappa	3.0	[1.0, 5.0]	Threshold for kappa-sigma clipping to be used in rebinning.
wavel_min	380.0	[0.0, 10 ³]	Minimum wavelength [nm].
wavel_max	780.0	[300.0, 10 ³]	Maximum wavelength [nm].
vel_step	0.5 (0.7, 1.4)	[0.3, 100]	Velocity step for the SINGLEUHR (SINGLEHR, MULTIMR) mode [km s ⁻¹].
rv	0.0		Radial velocity value, copied from keyword CCF RV if present [km s ⁻¹].
zem	0.0		Emission redshift, copied from keyword Z_EM if present.

9.2 espda_mask_spec

The recipe espda_mask_spec creates a spectral mask and it applies it to a spectrum.

9.2.1 Input

Type	TAG	short description	n
dap	FSPEC_PRE	Spectrum in the [extracted pixel,spectral order] space	1 or 0
dap	RSPEC_PRE	Rebinned merged spectrum	1 or 0

Note: One of the two spectra should be present.

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9.2.2 Output

default recipe file name	PRO.CATG	Short description
FSPEC.fits	FSPEC	masked full spectrum
RSPEC.fits	RSPEC	masked rebinned spectrum
MASK.fits	MASK	table with mask limits

9.2.3 Quality control

name	frames	description
QC.MASK.NROW	FSPEC, RSPEC	Number of masked rows.

9.2.4 Parameters

alias	default	range	description
mask-limit	0.0-0.0	None	Limits of the regions to be masked [nm].
mask-exp	0	[0, total number of exposures]	Number of the exposure to be masked, 0 meaning all exposures.

9.3 espda_create_linelist

The recipe `espda_create_linelist` creates a list of absorption lines identified in a spectrum.

9.3.1 Input

Type	TAG	short description	n
dap	RSPEC	rebinned, optionally masked spectrum	1 or 0

9.3.2 Output

default recipe file name	PRO.CATG	short description
FLINE_PRE.fits	FLINE_PRE	List of absorption lines
RSPEC_SMOOTH.fits	RSPEC_SMOOTH	Undersampled spectrum

9.3.3 Quality control

name	frames	description
QC.DET.LINE_NUM	All	Number of identified lines.

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9.3.4 Parameters

alias	default	range	description
vel-step-min	2.0	[0.0,10.0]	Minimum velocity step for undersampling [km s^{-1}].
vel-step-max	200.0	[10.0, 1000.0]	Maximum velocity step for undersampling [km s^{-1}].
accept	5	[3.,100]	Distance between a flux minimum and the adjacent maxima for the minimum to be accepted as an absorption line, as a multiple of the flux error at the continuum level.
add	0	None	Wavelengths of additional, manually-selected lines separated by commas [nm].

9.4 espda_fit_qsocont

The recipe `espda_fit_qsocont` fits the emission continuum in a quasar spectrum.

9.4.1 Input

Type	TAG	short description	n
dap	FSPEC	Full spectrum optionally equalized	0 or 1
dap	RSPEC	Rebinned spectrum	1
dap	FLINE_PRE	List of absorption lines	0 or 1
ref	QSO_ION	List of ionic transitions	1
ref	VOIGT_FUNC	Table with the Voigt function	0 or 1
ref	RPROF	Rebinned instrument profile	0 or 1

Note: `VOIGT_FUNC` is recommended (it speeds up the computation).

9.4.2 Output

default recipe file name	PRO.CATG	short description
FSPEC_CONT.fits	FSPEC_CONT	Full spectrum with continuum
FSPEC_REM.fits	FSPEC_REM	Full spectrum with lines removed
RSPEC_CONT.fits	RSPEC_CONT	Rebinned spectrum with continuum
RSPEC_REM.fits	RSPEC_REM	Rebinned spectrum with lines removed
FLINE_REM.fits	FLINE_REM	List of removed absorption lines
SPLINE_CONT.fits	SPLINE_CONT	Table with spline points

9.4.3 Quality control

name	frames	description
QC.CONT.RCHISQ	FSPEC_CONT	Reduced chi-squared of continuum fitting.
QC.LINE.RCHISQ	FSPEC_LINE	Reduced chi-squared of line fitting.
DAS.Z_EM	FLINE_REM	Quasar emission redshift.
QC.COLDEN.THRES	FLINE_REM	Lower limit of completeness in the line column density distribution used for fitting.

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9.4.4 Parameters

alias	default	range	description
hwidth	0.05	[0.025, 10.]	Half width for line grouping [nm].
par-range	[10^{-5} , 10.0, 16.0, 2.0, 50.0, 0.0, 0.0]	None	Range of line parameters (redshift max. variation, min column density, max column density, min thermal line width, max thermal line width, min turbulent line width, max turbulent line width)
peak-thres	0.8	[0.01, 1.0]	Relative threshold to cut line peaks during normalization.
vel-sampl-blue	2000	[100, 10^4]	Velocity sampling to fit a spline to the blue part [km s^{-1}].
vel-sampl-red	1000	[100, 10^4]	Velocity sampling to fit a spline to the red part [km s^{-1}].
model-resol	140000	[1000, 10^6]	Resolution of the instrument model.
iter-max	10	[-1, 1000]	Maximum number of lines fitted, -1 meaning all lines.
spline-knots	None	None	Manually-entered spline knots

9.5 espda_iden_syst

The recipe espda_iden_syst identifies absorption systems in a spectrum.

9.5.1 Input

Type	TAG	short description	n
dap	FLINE_REM	List of absorption lines	1
ref	QSO_ION	List of ionic transitions	1
ref	QSO_ION_RED	Reduced list of ionic transitions	0 or 1

9.5.2 Output

default recipe file name	PRO.CATG	short description
SLINE_IDEN_xy.fits	SLINE_IDEN	Individual absorption systems identified by a letter code (a, b, c, ..., aa, ab, ac, ..., zz)
FLINE_IDEN.fits	FLINE_IDEN	List of identified lines
FLINE_REJ.fits	FLINE_REJ	List of non-identified lines
QSO_ION_RED.fits	QSO_ION_RED	Reduced list of ionic transitions

Note: QSO_ION_RED is produced only if QSO_ION_RED is not provided in input.

9.5.3 Quality control

name	frames	description
QC.SYSTID	SLINE_IDEN	ID of the absorption system.
QC.SYSTZ	SLINE_IDEN	Redshift of the absorption system.

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9.5.4 Parameters

alias	default	range	description
comp-thres	5e-05	$[10^{-5}, 10^{-3}]$	Threshold for coincidence between multiplet components.
start-dz	0.001	[1e-5, 1.0]	Redshift difference to accept starting multiplets.
grp-num	2	[1, 10]	Minimum number of lines to define a group.
add-dv	0.0	[0.0, 1000.0]	Velocity difference to accept additional transitions $[\text{km s}^{-1}]$
peak-thres	0.9	[0.0, 1.0]	Peak threshold for starting the identification (normalized to the continuum)
vis-rej	None	None	List of visually rejected systems

9.6 espda_fit_line

The recipe `espda_fit_line` fits the identified absorption systems with Voigt profiles.

9.6.1 Input

Type	TAG	short description	n
dap	FSPEC_CONT	Full spectrum with continuum	1
dap	RSPEC_CONT	Rebinned spectrum with continuum	1
dap	SLINE_IDEN	Individual absorption system	0 or 1
dap	FLINE_IDEN	List of identified lines	0 or 1
dap	FLINE_REJ	List of non-identified lines	0 or 1
dap	RPROF	Rebinned instrument profile	0 or 1
ref	QSO_ION	List of ionic transitions	1
ref	QSO_ION_RED	Reduced list of ionic transitions	1
ref	VOIGT_FUNC	Table with the Voigt function	0 or 1

Note: `FLINE_REJ` is not considered if `FLINE_IDEN` is provided. `VOIGT_FUNC` is recommended (it speeds up the computation).

9.6.2 Output

default recipe file name	PRO.CATG	short description
FSPEC_GUESS.fits*	FSPEC_GUESS	Full spectrum with Voigt guess
RSPEC_GUESS.fits*	RSPEC_GUESS	Rebinned spectrum with Voigt guess
SLINE_GUESS.fits*	SLINE_GUESS	List of Voigt-guessed lines
FSPEC_VOIGT.fits	FSPEC_VOIGT	Full spectrum with Voigt fit
RSPEC_VOIGT.fits	RSPEC_VOIGT	Rebinned spectrum with Voigt fit
SLINE_VOIGT.fits	SLINE_VOIGT	List of Voigt-fitted lines

*Produced if `fit-flag = FALSE`

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9.6.3 Quality control

name	frames	description
QC.LINE.RCHISQ	All	Reduced chi-squared of line fitting.
QC.SYSTID	All	ID of the absorption system.
DAS SYSTZ	All	Redshift of the absorption system.

9.6.4 Parameters

alias	default	range	description
hwidth	0.1	[0.025, 10]	Half width for line grouping [nm].
par-range	[1.0e - 4, 10.0, 17.0, 2.0, 50.0, 0.0, 0.0]	None	Range of line parameters (redshift maximum variation, min column density, max column density, min thermal line width, max thermal line width, min turbulent line width, max turbulent line width)
edit-file	VOID	None	Name of the file with instructions to edit the line parameters.
add	0	None	Wavelengths of additional, manually-selected lines.
fit-flag	TRUE	[TRUE, FALSE]	Flag to fit the lines.
iter-max	1	[1, 1000]	Maximum number of iterations.
grp-sel	0	[0, number of groups]	Group of lines selected for fitting, 0 meaning all groups.
model-resol	140,000	[10 ³ , 10 ⁶]	Resolution of the instrument model.

9.7 espda_compu_eqwidth

The recipe espda_compu_eqwidth computes the equivalent widths for a list of absorption lines.

9.7.1 Input

Type	TAG	short description	n
dap	FSPEC_PRE	Full spectrum	0 or 1
dap	RSPEC_PRE	Rebinned spectrum	0 or 1
ref	LINE	Line list	0 or 1

9.7.2 Output

default recipe file name	PRO.CATG	short description
LINE_EQWIDTH.fits	LINE_EQWIDTH	List of detected lines with computed equivalent widths

9.7.3 Quality control

name	frames	description
QC.DET.NLINE	LINE_EQWIDTH.fits	Number of detected lines
QC.FIT.NLINE	LINE_EQWIDTH.fits	Number of fitted lines

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9.7.4 Parameters

alias	default	range	description
space	0.3	[0.1,5]	Width of the local spectral region for each side of the line [nm]
ew_min	2.0	[0., 400.]	Minimum accepted value for a line EW to be saved in the products [mÅ]
cont_rejt	-1	[0.5, 1.]	Rejection threshold for the continuum determination. The default value depends on the signal-to-noise ratio
cont_iter	5	[1,20]	Number of iteration to fit the continuum
det_line_thres	0.02	[0.0,0.5]	Normalized threshold for line acceptance in line identification
det_line_smwidth	4	[1,50]	Number of pixels in the boxcar to be averaged to fit the continuum; useful to deal with noisy spectra
fit_ngauss_width	0.5	[0.1, 2.5]	Initial guess for the parameter related with the width of the Gaussians [mÅ]
det_line_resol	0.01	[0.001,0.1]	Minimum accepted separation between two lines used for the multigaussian fit. Also used to identify the lines to be measured [nm]

9.8 espda_compu_starpar

The recipe espda_compu_starpar estimates the effective temperature and [Fe/H] for solar-type star spectrum.

9.8.1 Input

Type	TAG	short description	n
dap	LINE_EQWIDTH	List of lines with computed equivalent widths	1
ref	LINE_RATIO_CALIB	Table with line ratio calibration coefficients	1
ref	LINE_FEH_CALIB	Table with [Fe/H] calibration coefficients	1

9.8.2 Output

default recipe file name	PRO.CATG	short description
RSPEC_STARPAR.fits	RSPEC_STARPAR	Rebinned spectrum with computed parameters in the header

9.8.3 Quality control

name	frames	description
DAS.TEFF	RSPEC_STARPAR.fits	Computed effective temperature [K]
DAS.TEFF.ERROR	RSPEC_STARPAR.fits	Error obtained from the standard deviation of all line ratios used
DAS.TEFF.NCALIB	RSPEC_STARPAR.fits	Number of line ratios used to determine T_{eff}
DAS.TEFF.NCALIBIND	RSPEC_STARPAR.fits	Number of independent line ratios used to determine T_{eff}
DAS.FEH	RSPEC_STARPAR.fits	Computed value of metallicity [Fe/H]
DAS.FEH.ERROR	RSPEC_STARPAR.fits	Error obtained from the standard deviation of all line ratios used
DAS.NLIN.FEH	RSPEC_STARPAR.fits	Number of lines used to determine [Fe/H]

9.8.4 Parameters

None

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9.9 espda_fit_starcont

The recipe `espda_fit_starcont` fits the stellar continuum of 2D spectra order by order

9.9.1 Input

Type	TAG	short description	n
dap	FSPEC_ORIG	Original full spectrum	1

9.9.2 Output

default recipe file name	PRO.CATG	short description
NORD_SPEC.fits	NORD_SPEC	Order spectrum continuum normalized
NMERG_SPEC.fits	NMERG_SPEC	Rebinned spectrum continuum normalized

9.9.3 Quality control

name	frames	description
DAS.QC.STARCONT.MEAN.MFLUX	NMERG_SPEC.fits	mean flux of the rebinned, merged, observed spectrum
DAS.QC.STARCONT.MEAN.MFLUXERR	NMERG_SPEC.fits	mean flux error of the rebinned, merged, observed spectrum
DAS.QC.STARCONT.MEAN.MSNR	NMERG_SPEC.fits	mean signal to noise of the rebinned, merged, observed spectrum

9.9.4 Parameters

alias	default	range	description
ord-lrejt	0.5	[0.0, 1.5]	Multiplication factor to determine the low rejection threshold
ord-hrejt	2.0	[1.5, 3.0]	Multiplication factor to determine the high rejection threshold
ord-niter	5	[1, 10]	Number of iteration to fit the continuum
ord-ford410	0	[0, 9]	Order of the fitting function for wavelengths < 410 nm
ord-ford450	1	[0, 9]	Order of the fitting function for wavelengths < 450 nm
ord-ford510	2	[0, 9]	Order of the fitting function for wavelengths < 510 nm
ord-ford800	3	[0, 9]	Order of the fitting function for wavelengths < 800 nm
flux-kappa	3	[3, 5]	Number of sigma for clipping for rebinning. If equal to -1 the clipping is not carried out
flux-velstep	0.5	[0.3, 100]	Step of velocity binning [km s ⁻¹]

9.10 espda_synth_spec

The recipe `espda_synth_spec` interpolates three synthetic spectra within a grid and compare them with the observed spectrum.

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9.10.1 Input

Type	TAG	short description	n
dap	NMERG_SPEC	Rebinned spectrum continuum normalized	1
ref	SYNTH_SPEC	Synthetic spectra library	-

9.10.2 Output

default recipe file name	PRO.CATG	short description
SMERG_SPEC.fits	SMERG_SPEC	Rebinned spectrum continuum normalized with additional columns with the best fit synthetic spectrum

9.10.3 Quality control

name	frames	description
DAS.QC.SYNTH.TEFF	SMERG_SPEC.fits	T_{eff} of the selected, interpolated synthetic spectrum
DAS.QC.SYNTH.LOGG	SMERG_SPEC.fits	$\log g$ of the selected, interpolated synthetic spectrum
DAS.QC.SYNTH.FEH	SMERG_SPEC.fits	[Fe/H] of the selected, interpolated synthetic spectrum
DAS.QC.SYNTH.VINS	SMERG_SPEC.fits	V_{ins} of the selected, interpolated synthetic spectrum
DAS.QC.SYNTH.VROT	SMERG_SPEC.fits	V_{rot} of the selected, interpolated synthetic spectrum
DAS.QC.SYNTH.VMAC	SMERG_SPEC.fits	V_{mac} of the selected, interpolated synthetic spectrum
DAS.QC.SYNTH.MODEL1	SMERG_SPEC.fits	Model 1 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MODEL2	SMERG_SPEC.fits	Model 2 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MODEL3	SMERG_SPEC.fits	Model 3 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MODEL4	SMERG_SPEC.fits	Model 4 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MODEL5	SMERG_SPEC.fits	Model 5 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MODEL6	SMERG_SPEC.fits	Model 6 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MODEL7	SMERG_SPEC.fits	Model 7 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MODEL8	SMERG_SPEC.fits	Model 8 of the selected cube within the grid of synthetic spectra
DAS.QC.SYNTH.MEAN.MFLUX.W680	SMERG_SPEC.fits	mean flux of the rebinned, merged, observed spectrum for wavelength below 680 nm
DAS.QC.SYNTH.MEAN.FSYNTH.W680	SMERG_SPEC.fits	mean flux of the selected synthetic spectrum for wavelength below 680 nm
DAS.QC.SYNTH.MEAN.RESID.W680	SMERG_SPEC.fits	mean value of the residuals observed spectrum minus synthetic spectrum for wavelength below 680 nm
DAS.QC.SYNTH.STDEV.RESID.W680	SMERG_SPEC.fits	standard deviation of the residuals observed spectrum minus synthetic spectrum for wavelength below 680 nm

9.10.4 Parameters

alias	default	range	description
synth-teff	5777	[3500., 7000.]	stellar effective temperature [K]
synth-logg	4.438	[1.0, 5.0]	Stellar surface gravity $\log [\text{cm s}^{-2}]$
synth-feh	0.0	[-5.0, +0.5]	Stellar metallicity [Fe/H]
synth-vins	2.14, 1.58, 4.28	[0., 15.]	Instrumental broadening for the HR, UHR and MR mode, respectively $[\text{km s}^{-1}]$
synth-vrot	1.6	[0., 300.]	Stellar rotational velocity $[\text{km s}^{-1}]$
synth-vmac	3.2	[0., 10.]	Stellar macroturbulent velocity $[\text{km s}^{-1}]$

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9.11 espda_rv_synth

The recipe `espda_rv_synth` computes the radial velocity for a stellar spectrum from the cross-correlation with a synthetic spectrum.

9.11.1 Input

Type	TAG	short description	n
dap	SMERG_SPEC	Rebinned spectrum continuum normalized with additional columns with the selected synthetic spectrum	1 -

9.11.2 Output

default recipe file name	PRO.CATG	short description
RMERG_SPEC.fits	RMERG_SPEC	Table with the rebinned spectrum continuum normalized, the selected synthetic spectrum and the computed parameters in the header
CCF_SPEC.fits	CCF_SPEC	Cross-correlation function

9.11.3 Quality control

name	frames	description
DAS.QC.RVSYNTH.RVCCF	RMERG_SPEC.fits	RV from the fit to the full CCF [km s^{-1}]
DAS.QC.RVSYNTH.RVECCF	RMERG_SPEC.fits	error of RV from the fit to the full CCF [km s^{-1}]
DAS.QC.RVSYNTH.RVCORE	RMERG_SPEC.fits	RV from the fit to the core of the CCF [km s^{-1}]
DAS.QC.RVSYNTH.RVECORE	RMERG_SPEC.fits	error of RV from the fit to the core of the CCF [km s^{-1}]
DAS.QC.RVSYNTH.RVFINAL	RMERG_SPEC.fits	finally adopted RV [km s^{-1}]
DAS.QC.RVSYNTH.RVEFINAL	RMERG_SPEC.fits	error of the finally adopted RV [km s^{-1}]
DAS.QC.RVSYNTH.MEAN.MFLUX.W680	RMERG_SPEC.fits	mean flux of the rebinned, merged, observed spectrum for wavelength below 680 nm
DAS.QC.RVSYNTH.MEAN.FSYNTH.W680	RMERG_SPEC.fits	mean flux of the selected synthetic spectrum for wavelength below 680 nm
DAS.QC.RVSYNTH.MEAN.RESIC.W680	RMERG_SPEC.fits	mean value of the residuals observed spectrum minus synthetic spectrum for wavelength below 680 nm
DAS.QC.RVSYNTH.STDEV.RESIC.W680	RMERG_SPEC.fits	standard deviation of the residuals observed spectrum minus synthetic spectrum for wavelength below 680 nm

9.11.4 Parameters

alias	default	range	description
ccf-cen	0.	[-850., 850.]	Guess radial velocity [km s^{-1}]
ccf-win	350.	[10., 1000.]	CCF window width [km s^{-1}]
ccf-fitg	FALSE	[TRUE, FALSE]	flag to use a Gaussian to fit the CCF (TRUE) or use a Lorentzian (FALSE)
ccf-frv	FALSE	[TRUE, FALSE]	flag to use the RV derived from the CCF fit (TRUE) or from the CCF core fit (FALSE)
syn-fct	1	[0.01, 1000]	adjusted multiplication factor for the synthetic spectrum

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9.12 espda_compu_radvel

The recipe `espda_compu_radvel` compute the radial velocity for a stellar spectrum by cross-correlating it with a mask of the specific stellar type.

9.12.1 Input

Type	TAG	short description	n
drp	S2D_BLAZE	Spectrum in the [extracted pixel,spectral order] space	1
drp	BLAZE	Blaze function	1
ref	MASK_LUT	Mask Look up table	1
ref	MASK_TABLE	Line mask tables for specific stellar types	11
ref	FLUX_TEMPLATE	Flux distribution as a function of wavelengths for different stellar types	1

9.12.2 Output

default recipe file name	PRO.CATG	short description
ESPRESSO_CCF	CCF	Cross-correlation function

9.12.3 Quality control

name	frames	description
ESO RV START	ESPRESSO_CCF	Coordinate at reference pixel
ESO RV STEP	ESPRESSO_CCF	Coordinate increment per pixel
QC ORDER _m COSMIC NB2	ESPRESSO_CCF	Additional cosmics found in each order
QC ORDER _m FLUX CORR	ESPRESSO_CCF	flux correction for the order m
QC FLUX CORR MIN	ESPRESSO_CCF	min of flux correction
QC FLUX CORR MAX	ESPRESSO_CCF	max of flux correction
QC SCIRED FLUX CORR CHECK	ESPRESSO_CCF	flux correction QC
QC CCF RV	ESPRESSO_CCF	radial velocity [km s ⁻¹]
QC CCF RV ERROR	ESPRESSO_CCF	error on Radial velocity [km s ⁻¹]
QC CCF FWHM	ESPRESSO_CCF	CCF FWHM [km s ⁻¹]
QC CCF FWHM ERROR	ESPRESSO_CCF	CCF FWHM error [km s ⁻¹]
QC CCF CONTRAST	ESPRESSO_CCF	CCF contrast
QC CCF CONTRAST ERROR	ESPRESSO_CCF	CCF contrast error
QC CCF CONTINUUM	ESPRESSO_CCF	CCF continuum level [e-]
QC CCF MASK	ESPRESSO_CCF	CCF mask used
QC CCF FLUX ASYMMETRY	ESPRESSO_CCF	CCF asymmetry (km s ⁻¹)
QC CCF FLUX ASYMMETRY ERROR	ESPRESSO_CCF	CCF asymmetry error (km s ⁻¹)
QC CCF BIS SPAN	ESPRESSO_CCF	CCF bisector span (km s ⁻¹)
QC CCF BIS SPAN ERROR	ESPRESSO_CCF	CCF bisector span error (km s ⁻¹)
QC COMPU RADVEL CHECK	ESPRESSO_CCF	overall compu_radvel check

9.12.4 Parameters

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alias	default	range	description
rv_step			RV step [km s^{-1}]
rv_center			CCF center [km s^{-1}]
rv_range			in km s^{-1} of half window in which CCF is computed [km s^{-1}]
mask_table_id			Correlation mask type [F9, G2, ...]
mask_width			Width of mask holes [km s^{-1}]
flux_correction_type			Flux correction type [AUTO/NONE/sp_type]

9.13 espda_compu_rhk

The recipe espda_compu_rhk computes the activity indexes R'HK from a stellar spectrum

9.13.1 Input

Type	TAG	short description	n
drp	S1D	One-dim. merged spectrum	1

9.13.2 Output

default recipe file name	PRO.CATG	short description
S1D_RHK_analyzed.fits	RHK_FLUX	One-dim. merged spectrum with updated keywords reporting the indexes values

9.13.3 Quality control

name	frames	description
QC.RHK.CAII_BV	S1D_RHK_analyzed	B-V colour of the star
QC.RHK.CAII_S_RAW	S1D_RHK_analyzed	
QC.RHK.CAII_SMW	S1D_RHK_analyzed	
QC.RHK.CAII_SERR	S1D_RHK_analyzed	
QC.RHK.CAII_RHK	S1D_RHK_analyzed	
QC.RHK.CAII_RHK_ERR	S1D_RHK_analyzed	
QC.RHK.CAII_PROT	S1D_RHK_analyzed	
QC.RHK.CAII_PROT_ERR	S1D_RHK_analyzed	
QC.RHK.CAII_AGE	S1D_RHK_analyzed	
QC.RHK.CAII_AGE_ERR	S1D_RHK_analyzed	

9.13.4 Parameters

alias	default	range	description
bv	0.82		B-V colour of the star
rv	9999.		Star's RV
ca_alpha	1.044		Calcium index alpha

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ca_beta	0.031		Calcium index beta
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10 Algorithms and recipe details

In this section we describe the main algorithms implemented in the ESPRESSO DAS recipes. Relevant data analysis parameters are typed in **bold** face. For convenience we omit the common prefix **espda** for the recipe.

10.0.1 Coaddition of spectra (coadd_spec)

This recipe is used to combine different observations of the same object, in order to maximize the SNR. Input spectra are obtained from the DR pipeline as multiextension FITS frames. The recipe works with spectra whose orders have not been merged (S2D). These spectra are concatenated into a single spectrum (FSPEC_PRE) in which all pixels keep their wavelength and the information on the order and spectrum of origin. In this way, the subsequent recipes can access the original information extracted by the DRS avoiding the issues related to rebinning (e.g. correlation between noise values in adjacent pixels). For inspectional and plotting use, the recipe gives in output also a coadded, rebinned one-dimensional spectrum (RSPEC_PRE), if **rebin-flag** is TRUE. The recipe can work also with 1D merged spectra; in this case the output product will be a coadded, rebinned spectrum. The wavelength are expressed either in vacuum or in air, depending on the value of parameter **air-flag** (FALSE by default).

Coaddition is performed with a “drizzle”-like procedure:

- The wavelength grid of the rebinned spectrum is defined, with a wavelength range defined by **wavel-max/wavel-min** and a velocity step defined by **vel-step**.
- For each pixel of the rebinned grid, a list of “contributors” is determined (i.e., pixels of the original spectra that overlap the given pixel).
- The flux densities of the contributors is averaged, using as weights both the measured errors and the amount of overlap between original and final pixels.

Stellar spectra are corrected for radial velocity to the rest frame (only in workflow STAR I). The radial velocity is copied from keyword CCF RV if present, the user can also modify the radial velocity value changing the parameter **rv**.

If **equal-flag** is TRUE, input spectra are equalized to the same flux level before coaddition or concatenation, to prevent incorrect weighting of flux values that could be due to slit losses and/or incorrect flux calibration. By default, the first input spectrum is adopted as a reference (parameter **equal-ref**). Equalization is performed by rescaling the flux in each order to the average flux of the reference spectrum. Optionally, the recipe can eliminate the pixels with deviating flux values via kappa-sigma clipping (parameter **kappa**).

In the case of quasar spectra, the instrumental profile (currently modeled as a Gaussian) is interpolated at each wavelength of FSPEC_PRE and RSPEC_PRE, to be used in line fitting (see Section 10.0.6). Information about the instrument resolution (from parameter **model-resol**) is also saved in the spectral tables.

10.0.2 Masking of spectra (mask_spec)

This recipe is used interactively to create a mask of selected spectral regions, and to apply it to a spectrum. Masks are useful to restrict the analysis to a subset of the available wavelength coverage. The recipe allows the

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user to interactively create a mask. In the output spectrum the masked wavelengths are deleted.

The limits of the masked regions may be passed to the recipe also through the parameter **mask-limit** as a series of pairs of wavelength values separated by a dash, then separated by commas (e.g. 400-410,560-570, ...). The frame to be masked is designed by the parameter **mask-exp**, with 0 meaning that the mask has to be applied to all frames.

10.0.3 Detection of absorption lines (create_linelist)

This recipe is used to create a list of absorption lines. The position of line peaks is determined by looking for local minima in the flux density spectrum and evaluating them by prominence. The procedure works as follows:

- The spectrum is smoothed to mask features below a given scale (expressed as a velocity). This is done to avoid interpreting as lines the pixel-to-pixel fluctuations in the flux density due to noise.
- The smoothed spectrum is scanned to detect local minima.
- The flux density value at each minimum is evaluated against the value at the two adjacent local maxima. If the difference between minimum and maximum values in either direction is above a given threshold, the minimum is considered prominent enough to be a line. The threshold is defined by parameter **accept** as a multiple of the local error in flux density (i.e. the average of errors at the two adjacent maxima).

Such procedure is repeated for different values of smoothing velocity between **vel-step-min** and **vel-step-max**, to detect lines of different strength. Lines detected at subsequent repetition are considered only once.

In both the stellar and quasar case the user can add interactively lines that have not been detected automatically, by clicking on the interactive plot (the information is passed by the parameter **add**, which is automatically set by Reflex and is not meant to be modified by the user).

10.0.4 Continuum level estimate in quasar spectra (fit_qsocont)

This recipe fits the continuum component of a quasar spectrum and normalizes the flux to the fitted continuum. We call “continuum” the convolution of the non-thermal component of the spectrum (usually approximated by a power law) and the strong, Doppler-widened emission lines.

The fit of the region longwards of the quasar HI Lyman- α emission is quite straightforward: only sparse absorption lines are found due to ionic transitions of chemical elements heavier than He, and the continuum is easily interpolated between the lines. In this case, a C-spline fit of the flux (with velocity sampling defined by **vel-sampl-red**) is adopted as continuum and all lines are fitted simultaneously.

The region shortwards of the Lyman- α emission, on the other hand, is affected by a large number of absorption lines (increasing with redshift) mainly due to the HI Lyman- α transition. They arise in the intervening matter along the line of sight and are a trace of the fluctuations of the IGM density. These lines are called, in general, Lyman- α forest. The transmitted flux in the Lyman- α forest is reduced by a factor depending on redshift and on the effective IGM optical depth, τ_{eff} , which is computed by integrating the convolution between the column

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density distribution and the curve of growth between 0 and a given maximum column density $N_{\text{lim}}(\text{HI})$:

$$\tau_{\text{eff}}(N_{\text{lim}}) := \frac{\int_0^{N_{\text{lim}}} N^{-\gamma} G(N) dN}{\int_0^{\infty} N^{-\gamma} G(N) dN}, \quad (1)$$

where γ is the power law index of the column density distribution and the curve of growth is approximated as

$$G(N) = \begin{cases} 0, & N \geq N_{\text{max}} \\ N, & N \leq 10^{14} \\ (10^{14}/14 \ln 10) \ln N, & 10^{14} \leq N \leq 10^{18} \\ (9/7)10^5 \sqrt{N}, & 10^{18} \leq N \leq N_{\text{max}} \end{cases} \quad (2)$$

with N_{max} the maximum column density measured for an HI Lyman- α transition (a user-defined value).

In this case, the continuum estimation procedure works as follows:

- The spectrum of flux density is multiplied by a corrective factor C , to take into account the effective optical depth:
$$C := e^{\alpha(1+z)^\beta \tau_{\text{eff}}}. \quad (3)$$
- The corrected flux density is smoothed with a C-spline function (velocity sampling defined by **vel-sampl-blue**), to determine a guess continuum.
- The strongest absorption line is fitted with respect to the guess continuum using a Voigt profile. The adopted resolution is defined by **model-resol**, while the ranges of Voigt parameters are defined by **par-range** (see Section 9.6). The column density N of the fitted line is taken as a new value of N_{lim} , to update the estimation of τ_{eff} and C .
- The fitted line is removed by dividing the observed density flux by the fitted profile. The guess continuum is then updated on the spectrum with the line removed. To avoid division by zero in the case of saturated lines, the region where the fitted profile is below a given fraction **peak-thres** of the local continuum are masked.
- The previous steps are iterated adding one line at a time and updating the guess continuum, until all lines are fitted or a maximum number of iteration **iter-max-temp** is reached. At each iteration, N_{lim} is estimated as the median of the number distribution of column densities for the fitted lines. Lines that are closer than **hwidth** nm are grouped and fitted together.

It is worth noting that as the iterations go on the estimation of τ_{eff} relies less on the initial theoretical assumptions and more on the actual distribution of column densities observed along the line of sight. This helps the initial guess continuum converge towards the true unabsorbed level of emission. The residual contribution to C due to lines below the detection threshold is used to enhance the flux once all lines are fitted, taking into account the effect of diffuse absorption which otherwise would go undetected.

The described procedure is run on the rebinned spectrum (RSPEC) and is not applied to the spectrum as a whole, but to individual chunks of size defined by **vel-sampl-blue** and **vel-sampl-red**. Only the result of the last iteration is applied to the full spectrum (containing all the original pixels of all the orders of all the exposures, FSPEC) and validated with a χ^2 test. The continuum measured in each chunk is then merged and saved in RSPEC_CONT and FSPEC_CONT.

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The algorithm is more effective when the signal-to-noise ratio of the spectrum is high (>30). In case of local failure, the automatically-computed continuum can be corrected by hand by the user, by clicking on the interactive plot (the information is passed by the parameter **spline-knots**, which is automatically set by Reflex and is not meant to be modified by the user).

10.0.5 Identification of line systems (**iden_syst**)

This recipe identifies detected absorption lines with known atomic or ionic transitions and groups them into absorption systems. An absorption system is formed by a group of absorption lines, corresponding to different atomic transitions observed more or less at the same redshift.

Two execution stages are foreseen for this recipe, the identification and the refinement stage.

- In the *identification* stage, the recipe identifies the absorption systems by looking for redshift coincidences. The approach is similar to the one described in [14]:
 - The list of redshifts is computed by dividing the wavelengths of the lines detected in the spectrum by a list of the laboratory wavelengths of the most commonly observed transitions in quasar spectra (e.g. NV 1239, 1243; SiII 1260, 1304, 1526; OI 1302; CII 1334; SiIV 1393, 1402; CIV 1548, 1551; FeII 2344, 2382, 2586, 2600; MgII 2796, 2803; CaII 3935, 3970; NaI 5891, 5897 Å). Only lines with peak lower than a fraction **peak-tresh** of the local continuum are considered.
 - If two or more coincident redshifts are found, a candidate system is defined and the average redshift is computed. The minimum number of lines to define a system is set by parameter **grp-num**, while the maximum accepted difference in redshift between lines of the same group is determined by **start-dz**.
 - Candidate systems are then checked against a set of selection rules and are either rejected or confirmed. Selection rules will be of two kinds: existence rules, which cause the candidate system to be rejected when violated (e.g. presence of a sufficient number of lines, presence of the Lyman- α line if in the wavelength range, etc.), and acceptance rules, which cause a single line to be rejected when violated (e.g. consistency between the two members of a doublet, etc.).
- In the *refinement* stage, the recipe adds new transitions to the confirmed systems. A larger reference list of laboratory wavelengths for ionic transitions is used at this stage, to identify (in principle) all remaining lines. The recipe checks the regions of the spectrum where lines are expected to be, given the redshift of the input absorption systems, and if lines are found in these regions (within a velocity difference **add-dv**) they are added to the systems and checked again for consistency.

In Reflex, a Python actor is used to plot the results and to let the user confirm or reject the newly added line by visual inspection.

10.0.6 Voigt profile fitting of absorption systems (**fit_line**)

This recipe fits a set of quasar absorption lines with multiple Voigt profiles. Absorption lines are grouped into absorption systems (groups of lines due to different ions but at the same redshift) and are modeled together with any other line or system that may occur in the wavelength range used for fitting.

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The Voigt function V is the convolution of a Gaussian profile and a Lorentzian profile. The Gaussian profile describes the Doppler broadening in the medium where the line is produced, while the Lorentzian profile is a combination of the natural width of the line and the effect of particle collisions in the medium. In the case of an absorption line, the optical depth produced by transition at frequency ν_0 is

$$\tau_\nu = N \frac{\sqrt{\pi} e^2}{m_e c} \frac{f}{\Delta\nu_b} V(a, u),$$

$$a \equiv \frac{\Gamma}{4\pi\Delta\nu_b}, u \equiv \frac{\nu - \nu_0}{\Delta\nu_b}$$

where N is the column density of the medium, e is the electron charge, m_e is the electron mass, c is the speed of light, f is the oscillator strength of the transition, Γ is the transition damping constant, and $\Delta\nu_b$ is the Doppler broadening due to thermal velocities and turbulence in the medium. The Voigt function is defined as follows:

$$V(a, u) \equiv \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{\exp(-y^2)}{a^2 + (u - y)^2} dy. \quad (4)$$

Except for special values of a and u , an analytical solution of this integral does not exist in literature. A suitable way to assess this problem has been described in [29], where the following representation of the Voigt function as a single proper integral with a damped sine integrand is adopted:

$$V(a, u) = \exp(a^2) \operatorname{erfc}(a) \exp(-u^2) \cos(2au) + \frac{2}{\sqrt{\pi}} \int_0^u \exp[-(u^2 - y^2)] \sin[2a(u - y)] dy. \quad (5)$$

The computation of this proper integral can be carried out by the standard GSL routine for numerical integration, *gsl_integration*. The term $\exp(a^2) \operatorname{erfc}(a)$ may be subject to an overflow/underflow limitation when a is large (order of 10). In this case, one can use the following approximation, accurate to the 16th decimal digit up to $a = 200$ with $n = 7$ [29]:

$$\exp(a^2) \operatorname{erfc}(a) \approx \frac{1}{\sqrt{\pi}a} \sum_{i=0}^n \frac{(-1)^i (2i)!}{i! (2a)^{2i}}. \quad (6)$$

The integral representation above can be also used to tabulate the Voigt function on a grid of (a, u) values. The tabulated values can be used to interpolate (through the bilinear interpolation formulae) the function at any value of a and u , significantly reducing the computation time.

The actual fitting of spectral lines is a minimization procedure in a multidimensional space. Each line is defined by four parameters: the redshift z , the column density N , the thermal Doppler broadening b , and the turbulence broadening b_{tur} . We have

$$z \equiv \frac{\nu_0 - \nu_{\text{obs}}}{\nu_{\text{obs}}}, b \equiv \sqrt{\frac{2kT}{m}}, b^2 + b_{\text{tur}}^2 = c^2 \left(\frac{\Delta\nu_b}{\nu_0} \right)^2. \quad (7)$$

where ν_{obs} is the observed central frequency of the line, k is the Boltzmann constant, T is the medium temperature, and m is the mass of the particles. The observed line profile I_ν is the convolution between the intrinsic profile and the instrumental profile $\Phi_{\delta\nu}$; if the continuum level is $I_{\nu,0}$, we have

$$I_\nu(\mathbf{x}) = \Phi_{\delta\nu} \otimes I_{\nu,0} \exp[-\tau_\nu(\mathbf{x})], \quad \mathbf{x} \equiv (z, N, b, b_{\text{tur}}). \quad (8)$$

For L lines, \mathbf{x} is a vector in a space with up to $4L$ dimensions. If some of the line parameters are constrained, the number of dimensions decreases to $M = 4L - C$, where C is the number of constraints. Two kinds of constraints are allowed:

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1. parameters which are kept fixed at a given value;
2. parameters which are common to two or more lines (common parameters are allowed to vary, but they are always kept equal to each other).
3. thermal Doppler parameters of ions of different elements linked to be at the same temperature (Doppler parameters vary with the square root of the ratio of the element masses, see Eq. 7).

The function to be minimized is the reduced chi-square function $\chi^2(\mathbf{x})$ defined as follows:

$$\chi^2(\mathbf{x}) \equiv \frac{1}{R - M - 1} \sum_{r=1}^R \frac{[I_r(\mathbf{x}) - F_r]^2}{E_r}, \quad (9)$$

where R is the number of data points along a wavelength grid, F_r and E_r are the flux and flux error values at these points, and I_r is the line profile computed at the same points.

The reduced chi-square is minimized using the standard GSL tool for multidimensional minimization, *gsl_multimin*. The routine proceeds from a guess choice of parameters \mathbf{x}_0 using a Levenberg-Marquardt algorithm to find the “downhill” direction from \mathbf{x}_0 in the parameter space (other algorithms will be also tested for speed and robustness). In practice, a vector $\mathbf{x}_{M,0}$ suitable for minimization is extracted from \mathbf{x}_0 according to the adopted constraints. Components of \mathbf{x}_0 with a constraint of the first kind are not included in $\mathbf{x}_{M,0}$; components of \mathbf{x}_0 with a mutual constraint of the second kind are included as a single component in $\mathbf{x}_{M,0}$. When the downhill direction is found, $\mathbf{x}_{M,0}$ is updated into $\mathbf{x}_{M,1}$ and its component are used to update the original vector \mathbf{x}_0 into \mathbf{x}_1 . Components of \mathbf{x}_0 with a constraint of the first kind are copied as they are into \mathbf{x}_1 ; all components of \mathbf{x}_0 with a mutual constraint of the second kind are replaced in \mathbf{x}_1 by the corresponding value from $\mathbf{x}_{M,1}$. The procedure is iterated until a given threshold for the reduced chi-square is reached and the final value \mathbf{x}_n is taken as best-fit solution for the line profiles.

Lines are grouped and fitted together if they are sufficiently close to each other (the half width of the maximum separation is set by parameter **hwidth**) or if they share one or more common parameters. Only the spectral regions around lines are used to compute the reduced χ^2 . The Voigt parameters are fitted within a range defined by **par-range**, an comma-separated array of seven values corresponding respectively to the maximum allowed redshift variation Δz and the minimum/maximum values of $\log N$, b , and b_{tur} respectively. The instrumental profile is modeled as a Gaussian with FWHM defined from the nominal resolution (parameter **model-resol**).

The user is allowed to put constraints on these parameters, through a Python actor. The information is passed through a file pointed by the parameter **edit-time**, which is automatically set by Reflex and is not meant to be modified by the user. The user may also add components to improve the quality of the fit by clicking on the interactive plot. Also in this case, the information is passed by a parameter (**add**) which is also not meant to be modified by the user).

Optionally, the recipe can iteratively fit an absorption system by automatically adding components where they are needed to minimize the reduced χ^2 . The number of iterations is defined by **iter-max** and corresponds to the maximum number of added components (by default, this parameter is set to 0, meaning that no component is automatically added). If the recipe is unable to decrease the reduced χ^2 by adding new components, it provides in output the solution with the lowest reduced χ^2 obtained during the iterations.

Optionally, line fitting can be disabled (by setting **fit-flag** to FALSE). In this case, the profile obtained with the guess values of Voigt parameters is issued in output.

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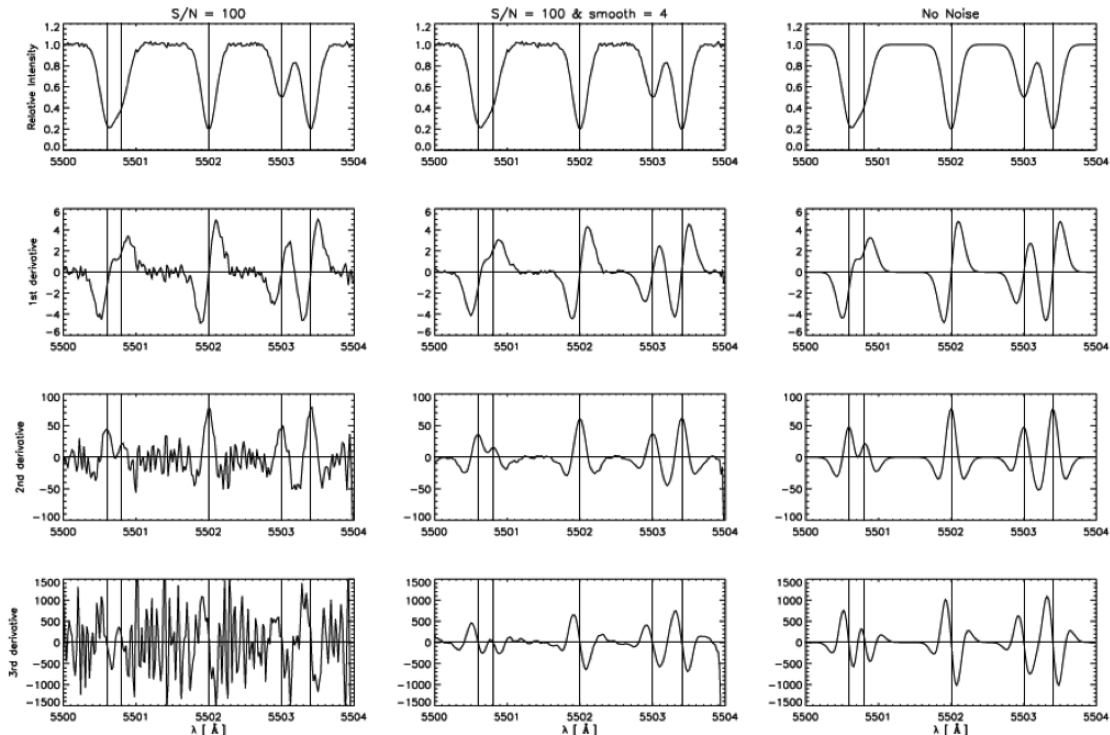


Figure 10.0.0: A simulated normalized spectral region and the respective 1st, 2nd, and 3rd derivatives. In the right panel it is easily seen that the local maxima of the 2nd derivative, which can be found using the zeros of the 3rd derivatives, estimate the center of the lines of the simulated spectrum very well. Note that using this we can see extremely blended lines that do not present zeros on the 1st derivative. The left and middle panels show how a smoothing of the flux is useful for eliminating the noise when computing the derivatives (adapted from [22]).

When all groups of lines have been fitted, the output parameters are used to compute an overall best-fit profile for the whole spectrum. A Voigt-fitted spectrum and a line list with best-fit parameters are produced.

The line fitting procedure is quite robust in the presence of one or a few pixels affected by CRHs or bad pixels, due to the significant number of pixels sampling the line profile (in a single frame, or even better in the case of the coaddition of several frames). Based on previous experience, results of Voigt profile fitting are robust for spectra with signal-to-noise ratio larger than ~ 10 .

10.0.7 Computation of the line equivalent width in stellar spectra (compu_eqwidth)

This recipe computes the equivalent widths of the absorption lines defined in an input list (LINE_STARP). The position of the line peak or peaks in the spectrum is determined using some mathematical properties of the derivatives of a function. It is well known that the zeros of the derivative of a function give us the local minima and maxima. The zeros of the 2nd derivative give us the inflection points, i.e. the points where the function changes its concavity. The local maxima of the 2nd derivative will give us the center of the absorption lines directly. The best way to find these maxima is to use the zeros of the 3rd derivative of the function. This can be seen in the right panel of Figure 10.0.0. It is clear that the maxima of the second derivative give us a good

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estimation of the position of the lines in the original spectra even for cases of strong blended lines (e.g. 5500.6 Å and 5500.8 Å in Figure 10.0.0). To determine the peak or peaks to fit the spectral line, it is necessary to obtain the first three numerical derivatives of the surroundings of the line profile.

Noise can be a problem, especially when determining numerical derivatives, where the noise propagates very fast (left panel of Figure 10.0.0). To overcome this problem, we make use of a numerical smoothing applied to the arrays of the derivatives with a boxcar average of a given width eliminating some of the noise. The use of such a smoothing parameter is illustrated in the middle panel of Figure 10.0.0. The smooth result of an array of values is described by the expression

$$R_i := \begin{cases} \frac{1}{w} \sum_{j=0}^{w-1} A_{i+j-w/2}, & i = \frac{w-1}{2}, N - \frac{w-1}{2} \\ A_i, & \text{otherwise} \end{cases} \quad (10)$$

where A is the array to be smoothed, w the width of the boxcar to be averaged, N the number of array elements, and R the resulting smoothed array. Even using this numerical trick, if the noise is high the procedure may identify more lines than actually present. To overcome this possible problem, we have introduced another parameter, which is linked to the spectral resolution, it determines the minimal distance between consecutive lines. A typical value for this parameter is 0.1 Å.

The procedure to compute the equivalent widths works as follows:

- The lines in the list are detected in the spectrum with the derivative technique. Only lines with a peak stronger than **det-line-thres** (in normalized units) are accepted.
- The local continuum is determined at each line position considering a wavelength interval with half width set by **space**. The continuum is fit iteratively (with a maximum number of iteration **cont-iter**). In each iteration, the points within a boxcar of width **det-line-smwidth** are fit to a 2nd order polynomial and normalized accordingly. The points with a value lower than **cont-rejt** are rejected.
- Each line is fit with a multiple Gaussian with a width set by **fit-ngauss-width** and a minimum separation between the different components of **det-line-resol**. The list of equivalent widths obtained from the fit and larger than a minimum threshold (set by **ew-min**) are then copied in table LINE_EQWIDTH.

10.0.8 Computation of the effective temperature and metallicity from stellar spectra (compu_starpur)

This recipe estimates the effective temperature and iron abundances for solar type stars using the equivalent widths computed by the previous recipe and comparing them with two static calibrations tables: LINE_RATIO_CALIB and LINE_FEH_CALIB.

The algorithm for this recipe is based on the works: [23], [24], and [25]. In those works, a very-high quality sample of high-resolution HARPS spectra was used to derive calibrations for line-ratios to estimate the effective temperature, T_{eff} . Similarly, to derive [Fe/H] a calibration was derived in combination with the T_{eff} derived by the line-ratios, using selected iron lines.

For T_{eff} , specific constraints were applied to the line-ratios to be good thermometers:

- line ratios should be composed of lines close together in the wavelength domain. We adopted a separation ≤ 70 Åas in [27]. This condition aims at eliminating possible errors coming from the continuum determination in the measurement of the equivalent widths for these lines;

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- lines in the ratio should have an excitation potential difference greater than at least 3 eV. In this way, we are compiling line ratios that are more sensitive to effective temperature variations. This is true because the equivalent width of the lines with higher excitation change faster with temperature than the ones from lower excitation potential lines (Gray 1994).

For the [Fe/H] estimation, the selected lines have to be independent on “secondary” parameters such as $\log g$ and microturbulence. We kept only the dependence on the abundance of iron (which we want to estimate) and the natural dependence on T_{eff} (which we can remove once we estimate T_{eff} from the line-ratio calibration). Therefore the constraints were the following:

- only Fe I lines were selected. Other elements were not consider for obvious reasons. Lines due to ionized iron (Fe II) were also removed given their sensitivity to the surface gravity;
- strong lines ($> 75 \text{ m\AA}$) are removed due to their strong dependence on microturbulence.

The latest calibrations presented [25] are those currently used in this recipe. These new calibrations allowed to expand the parameter range to sub-giant and giant FGK stars. They consist of 322 line equivalent width ratios and 100 Fe I lines that can be used to compute T_{eff} and [Fe/H], respectively. The stellar parameter limits of applicability of these calibrations (in the current recipe) are T_{eff} : [4500, 6500] K, $\log g$: [2.5, 4.9] dex and [Fe/H] : [−0.8, 0.5] dex. These calibrations provide in general a standard deviation of 74 K for T_{eff} and of 0.07 dex for [Fe/H].

The recipe takes the equivalent width measurements from the previous recipe, then it compiles the line-ratios that can be computed from the available measurements. For each computed line-ratio a T_{eff} is estimated. In the optimal case, we obtain 322 individual estimations of T_{eff} , and 100 estimations of [Fe/H] for each analysed spectrum. The final values are obtained by computing a weighted average of the individual estimations. The uncertainty on the final values are obtained after considering the standard deviation and the number of line-ratios used to compute the weighted average.

10.0.9 Determination of the stellar continuum (fit_starcont)

This recipe computes the continuum order by order in a stellar spectrum by fitting a polynomial function of order n to the spectrum and produces the merged 1D normalized spectrum with a velocity binning **flux-velstep**. The recipe uses as input the table with concatenated fluxes with wavelengths corrected to barycentric reference, i.e. the output of the recipe `espa_coadd_spec`.

The recipe initiates a loop over spectral orders, from blue to red, performing the same operations to a given order for all different input spectra of the same target. The performed steps are the following:

- The fluxes and errors of each order are initially normalized by the median (or the mean if the median is zero), to operate with small numbers.
- A initial rejection of all points with negative flux values and a fit of the continuum is performed with:
 - a zero-order polynomial (constant level) for wavelength below 540 nm;

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- a first-order polynomial (linear function) for wavelengths above 540 nm.
- Then, a loop is initiated that iterates for $n = \text{ord-niter}$ (default 5) times and performs the polynomial fit of order n , and masks the deviating points of a given spectral order. By default, a different polynomial order is used depending on the wavelengths of the given spectral orders. An increasing polynomial order is adopted for longer wavelengths mainly because for solar-type stars, the number of stellar lines typically increases for shorter wavelengths and the signal-to-noise ratio decreases for shorter wavelengths. We adopt by default the following:
 - Order number = 0 for wavelengths shorter than 410 nm
 - Order number = 1 for wavelengths shorter than 450 nm
 - Order number = 2 for wavelengths shorter than 510 nm
 - Order number = 3 for wavelengths shorter than 800 nm
- In each iteration, the unmasked stellar flux points are fitted and the standard deviation of the normalized unmasked flux points (flux divided by the continuum fit) is derived.
- After each iteration, the continuum and the fluxes are evaluated and the condition for rejection to mask a given point i is applied if:
 - $\text{flux}[i]/\text{cont}[i] > 1.0 + \text{cstd} * \text{hrej}$
 - $\text{flux}[i]/\text{cont}[i] < 1.0 - \text{cstd} * \text{lrej}$

where $\text{flux}[i]$ and $\text{cont}[i]$ are the flux and continuum values of pixel i , cstd is the constant standard deviation of the normalized fluxes and **ord-hrej** and **ord-lrej** are the high and low rejection parameters, respectively.
- The outliers in flux points are determined using the higher and lower rejection parameters and these masked points are excluded in the next iteration. This process is repeated until convergence and/or maximum number of iterations.
- Finally, using fitting function coefficients, the continuum function is created for all wavelength (masked and unmasked) points.

10.0.10 Identification of the synthetic spectrum closer to the observed one (**synth_spec**)

This recipe compares the observed 1D stellar spectrum normalized to the continuum with one synthetic spectrum interpolated from a grid of synthetic spectra for a given set of stellar parameters (effective temperature, **synth-teff**, and surface gravity, **synth-logg**) and metallicity, **synth-FeH**, and broadening parameters (instrumental broadening **synth-vins**, stellar rotational velocity, **synth-vrot**, and macroturbulent velocity, **synth-vmac**).

The whole grid of synthetic spectra [15], computed with the ASSET code [] using Kurucz model atmospheres [28], [20], will cover T_{eff} values from 3,500 to 7,000 K, $\log(g)$ values from 1 to 5 dex and $[\text{Fe}/\text{H}]$ values from -5 to +0.5 dex.

The recipe works as follows:

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- First, a search for the near eight synthetic spectra is done, i.e. the corners of a cube in the parameter space (T_{eff} , $\log g$, $[\text{Fe}/\text{H}]$), for the input set of stellar parameters. Then, an interpolated synthetic spectrum is created using a tri-linear interpolation procedure;
- the flux points of the synthetic spectrum are then interpolated over the wavelength array of the observed spectrum using a cubic spline function;
- the resulting normalized flux points of the synthetic spectrum, with the wavelengths already in logarithmic scale, are first convolved with a macroturbulent Gaussian profile (of width **synth-vmac**), then with the rotational profile (**synth-vrot**) and finally with the instrumental Gaussian profile (**synth-vins**).

10.0.11 Computation of the radial velocity from the comparison with a synthetic spectrum (rv_synth)

This recipe derives the radial velocity of the star by cross-correlating the observed 1D stellar spectrum normalized to the continuum with a synthetic spectrum already interpolated and convolved, which is the output of the recipe `espdasynth_spec`.

The user can decide whether to fit the cross-correlation function (CCF) with a Gaussian or with a Lorentzian function setting the parameter **ccf-fitg** to TRUE or FALSE (default), respectively. There is the choice also to derive the radial velocity (RV) from the fit of the whole CCF curve or from the fit of the CCF core only with the parameter **ccf-frv** sets to TRUE or FALSE (default), respectively.

The recipe follows these steps:

- Both the synthetic and the observed spectra are normalized to the stellar continuum flux, and therefore the continuum level should be at 1. Thus, before performing the cross-correlation, 1 is subtracted from the normalized fluxes of the observed and synthetic 1D spectra;
- wavelengths $\lambda < 675$ nm are selected for the computation of the CCF;
- the CCF is computed with a loop over all pixel/RV values;
- the CCF is fitted with a second-order polynomial plus a Lorentzian (or a Gaussian) function, and the centroid and its error in radial velocity is obtained;
- then, the fit of the three closer points to the maximum value of the CCF are fitted using a second-order polynomial (a parabola) and the centroid and its error in radial velocity is derived for the core of the CCF;
- the final adopted RV depends on the choice of the user, the default is the RV estimated from the fit of the core of the CCF.

10.0.12 Computation of the radial velocity with the CCF method (compu_radvel)

The ESPRESSO DAS implements a cross-correlation module that computes the cross-correlation function (CCF) of a S2D spectrum with respect to a binary template (mask) of a given spectral type. The radial velocity (RV) is then obtained from a Gaussian fit to the CCF. This is the technique that has been successfully used on the ELODIE, CORALIE, HARPS, SOPHIE and HARPS-N spectrographs. One of its main advantages

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is that CCFs can be computed in an automatic way with only a few line masks at hand. Line masks are simply numerical mask consisting of 1 and 0 value-zones, with the non-zero zones corresponding to the theoretical positions and widths of the stellar absorption lines at zero velocity, and can be created for various spectral types. The main steps of the algorithm are:

- Compare the global flux distribution in the S2D spectrum to a static flux template that approximately corresponds to the spectral type of the star. The S2D flux is scaled accordingly to match the flux distribution of the template. In this way, spectra of any given star are always brought to the same flux distribution, which ensures that variable atmospheric conditions will not induce systematic effects in the CCF computation.
- Shift the wavelength scale of the S2D spectrum to the Solar System barycenter using the barycentric correction.
- Define a uniform radial velocity grid (with step **rv_step** and half-range **rv_range**), approximately centered on the radial velocity of the star (specified by **rv_center**).
- For a given RV value in the grid v , shift the line mask (whose width is defined by **mask_width**) by the corresponding Doppler shift, project the line mask onto the S2D spectrum using a specified line width (about one pixel), and sum the S2D flux that goes through the so-defined mask "holes":

$$\text{CCF}(v) = \sum_l \sum_{x,o} p_{l,x,o}(v) f_{x,o} \quad (11)$$

where $f_{x,o}$ is the value of the 2D spectrum for the order o at the pixel location x and $p_{l,x,o}$ is the fraction of the l th line of the template which falls into the pixel (x, o) at the velocity v . The flux from partial pixels is computed via simple linear interpolation. The sum is actually a weighted sum, using line depths as weights to optimally extract the Doppler information. During this process, the S2D spectrum is locally blaze-corrected to remove any continuum slope around spectral lines. This produces one point of the CCF.

- Loop over all RV values.
- Fit a Gaussian profile to the CCF to derive RV, FWHM and contrast (see Figure 10.0.0).

Note that, by construction, CCFs are simply co-added spectral lines in velocity space, weighted by their depth and continuum flux. As such they can be considered as a "master" spectral line for the star. Uncertainties on the CCF data points are obtained by propagation of S2D error maps through the cross-correlation stage, which is a simple additive process (fluxes from many spectral lines are co-added). Finally, an estimate of the radial velocity uncertainty is obtained by converting CCF flux errors into RV errors using the measured CCF derivative, as described in the appendix of [17].

10.0.13 Computation of the activity indexes (compu_rhk)

This recipe computes the Ca II H&K activity index, on the Mt Wilson scale as $\log(R'HK)$ as defined in [18] and [21]. The main steps of the algorithm are:

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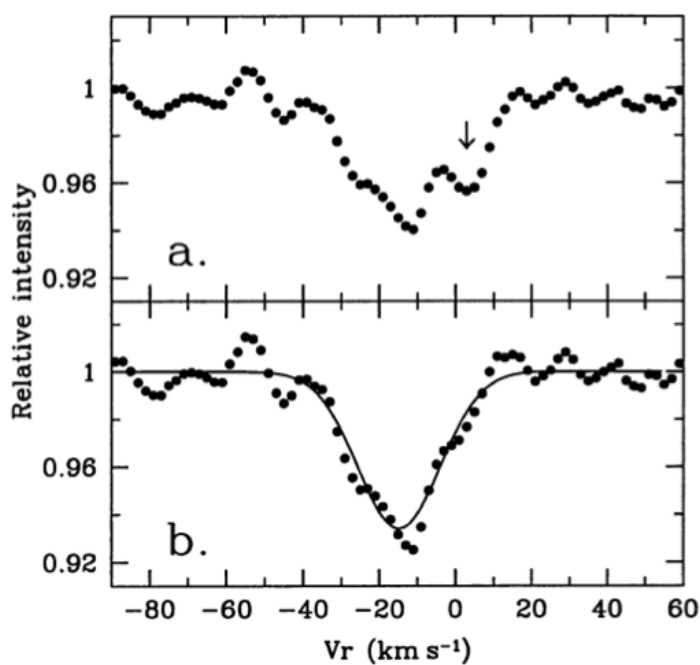


Figure 10.0.0: *a) CCF of a faint star contaminated by the CCF of the solar spectrum (indicated by the arrow). b) Same CCF after the subtraction of the CCF of the sky. The solid line is the Gaussian fit to the observed points. Adapted from [16].*

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- Measure integrated fluxes and errors in the four Mt Wilson passbands: H, K, R and V
- Compute the R'HK activity index
- Compute estimates of stellar rotation period and age from R'HK index

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11 Installation

ESO pipelines can be installed via several methods, depending on your OS, most of which facilitate easy installation, upgrade and removal. Please see the "ESO Data Reduction Pipelines and Workflow Systems" page (<https://www.eso.org/pipelines>).

This chapter gives generic instructions on how to obtain, build and install the ESPRESSO Data Analysis Software. Even if this chapter is kept as up-to-date as much as possible, it may not be fully applicable to a particular release. This might especially happen for patch releases. One is therefore advised to read the installation instructions delivered with the ESPRESSO DAS distribution kit. These release-specific instructions can be found in the file `README` located in the top-level directory of the unpacked ESPRESSO DAS source tree. The supported platforms are listed in Section 11.1. It is recommended reading through Section 11.2.2 before starting the installation.

A bundled version of the ESPRESSO DAS with all the required tools and an installer script is available from www.eso.org/pipelines, for users who are not familiar with the installation of software packages.

11.1 Supported platforms

The utilisation of the GNU build tools should allow to build and install the ESPRESSO DAS on a variety of UNIX platforms, but it has only been verified on the VLT target platforms:

- Linux (glibc 2.1 or later),
- Mac,

using the GNU C compiler (version 3.2 or newer). Gasgano is installed by the `install_pipeline` script and is supported provided the user has a proper installation of the Java Development Kit (version 1.6.0 or newer) and has set the `JAVA_HOME` environment variable properly during the kit installation. It is not sufficient to have the Java Realtime Environment to have successfully installed the `libgasganoapl.*` libraries needed to properly interface Gasgano with the installed `sinfoni` recipes. We recommend the user to look carefully at the log produced during installation and possible warnings.

11.2 Building the ESPRESSO DAS

This section shows how to obtain, build and install the ESPRESSO DAS from the official source distribution.

11.2.1 Requirements

To compile and install the ESPRESSO DAS one needs:

- the GNU C compiler (version 3.2 or later),
- the GNU `gzip` data compression program,

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- a version of the `tar` file-archiving program, and,
- the GNU `make` utility.

An installation of the Common Pipeline library (CPL) must also be available on the system. Currently the CPL version 7.2.2 or newer is required. The CPL distribution can be obtained from www.eso.org/cpl.

In order to run the ESPRESSO DAS recipes a front-end application is also required. Currently there are two such applications available, a command-line tool called *EsoRex* and the Java based data file organizer, *Gasgano*, which provides an intuitive graphical user interface (see Section 5.2, page 16). At least one of them must be installed. The *EsoRex* and *Gasgano* packages are available at www.eso.org/cpl and www.eso.org/gasgano respectively.

For installation instructions of any of the additional packages mentioned before please refer to the documentation of these packages.

11.2.2 Compiling and installing the ESPRESSO DAS

The ESPRESSO DAS distribution kit 1.4.0 contains:

espda-pipeline-manual-1.4.0.pdf	The ESPRESSO DAS manual
install_pipeline	Install script
cfitsio3450.tar.gz	CFITSIO 3450
cpl-7.2.2.tar.gz	CPL 7.2.2
esorex-3.13.10.tar.gz	esorex 3.13.10
gasgano-2.4.8.tar.gz	GASGANO 2.4.8
espda-kit-1.4.0.tar.gz	ESPRESSO DAS 1.4.0

Here is a description of the installation procedure:

1. Change directory to where you want to retrieve the ESPRESSO DAS recipes 1.4.0 package. It can be any directory of your choice but not:

```
$HOME/gasgano
$HOME/.esorex
```

2. Download from the ESO ftp server, www.eso.org/pipelines, the latest release of the ESPRESSO DAS distribution.
3. Verify the checksum value of the tar file with the `cksum` command.
4. Unpack using the following command:
`tar -xvf espda-kit-1.4.0.tar`

Note that the size of the installed software (including *Gasgano*) together with the static calibration data is about 27Mb.

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5. Install: after moving to the top installation directory,

cd espda-kit-1.4.0

it is possible to perform a simple installation using the available installer script (*recommended*):

./install_pipeline

Note: on recent Mac OS in order to properly install the kit it may be useful to set the following environment variable:

```
export JAVA_HOME=/System/Library/Frameworks/JavaVM.framework/
```

(beware: the execution may take a few minutes on Linux and several minutes on SunOS).

By default the script will install the ESPRESSO DAS recipes, *Gasgano*, *EsoRex*, all the necessary libraries, and the static calibration tables, into a directory tree rooted at `$HOME`. A different path may be specified as soon as the script is run.

The only exception to all this is the *Gasgano* tool, that will always be installed under the directory `$HOME/gasgano`. Note that the installer will move an existing `$HOME/gasgano` directory to `$HOME/gasgano.old` before the new *Gasgano* version is installed.

Important: the installation script would ensure that any existing *Gasgano* and *EsoRex* setup would be inherited into the newly installed configuration files (avoiding in this way any conflict with other installed instrument pipelines).

Alternatively, it is possible to perform a manual installation (*experienced users only*): the `README` file located in the top installation directory contains more detailed information about a step-by-step installation.

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12 Abbreviations and acronyms

CCF	Cross-Correlation Function
CPL	Common Pipeline Library
DAS	Data Analysis Software
DFS	Data Flow System department
DRS	Data Reduction System
ESO	European Southern Observatory
ESOREX	ESO-Recipe Execution tool
ESPRESSO	Echelle SPectrograph for Rocky Exoplanets and Stable Spectroscopic Observations
FITS	Flexible Image Transport System
GUI	Graphical User Interface
OB	Observation Block
QC	Quality Control
RON	Read Out Noise
SNR	Signal-to-Noise Ratio
SDD	Software Development Division
SOF	Set Of Frames
UT	Unit Telescope
VLT	Very Large Telescope