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ESPRESSO Data Flow in operations: results of commissioning activities

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ABSTRACT

ESPRESSO, the next generation ESO VLT high-resolution ultra-stable spectrograph, after the successful Preliminary Acceptance Europe held at the integration site of the Observatory of Geneva, has been re-integrated at Paranal and started its commissioning activities at the end of 2017. One critical aspect for ESPRESSO future operations, compared with other instruments currently running at ESO, is the way it will be operated which poses several constraints on its data flow. ESPRESSO has been conceived and developed as a “truly science-grade products generating machine” thanks to its fixed format and long-term stability. In addition to the Data Reduction Software (DRS), a Data Analysis Software (DAS), developed within the standard ESO Data Flow System, will be provided to the users – a novelty for the instruments at Paranal. Moreover, ESPRESSO will be fed either by the light of any of the UTs or by the incoherently combined light of up to four UTs, a feature which required a re-thinking of the current Paranal data handling injection schema. In this paper, after describing the main challenges and peculiarities of the ESPRESSO data flow system listed above, we will present the results of the first commissioning activities and the lessons learned to handle data produced by an instrument with such ambitious scientific requirements.

Keywords: data flow, data reduction, data analysis, quality control, calibrations, VLT

1. ESPRESSO AT VLT

On the night of 27 November 2017, ESPRESSO, the Echelle SPectrograph for Rocky Exoplanet and Stable Spectroscopic Observations, has successfully achieved first light on ESO's Very Large Telescope at the Paranal Observatory. ESPRESSO is a third-generation, fiber-fed, high-resolution, ultra-stable echelle spectrograph considered the successor of the ESO HARPS spectrograph installed at La Silla Observatory capable to achieve a precision, never reached before, of just a few centimeters per second in radial velocity measurements. The second unique characteristic is that it could be fed by the light of any of UT's as well as by the incoherently combined light of all four UT's together thus making ESPRESSO a spectrograph installed at the largest optical telescope in terms of collecting area in the world. This opens new insights in several field of astronomy where high resolution, efficiency and precision is required and will allow exploiting the two main scientific drivers for ESPRESSO:

- finding and characterizing less massive exo-planets and their atmospheres;
- search for possible variability of the fundamental constants of physics.

A detailed description of the instrument, the consortium of institutes and countries involved in its design and constructions and the main milestones reached in the course of last years has been extensively presented in several papers (see for example¹); interested reader could refer to those and references therein. Here we would like just recall that ESPRESSO successfully passed PAE (Preliminary Acceptance Europe) at the Observatory of Geneva in August 2017 where integration of the whole instrument took place.

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The PAE provided in-depth verification of the single devices, all sub-systems and the instrument as a whole. The full DFS set-up at integration site allows gathering a huge amount of calibrated data that proved and confirmed expectations both in terms of achievable precision and spectral resolution. Eventually the consortium received green light of ESO for shipping the instrument at VLT Observatory where re-integration in the Coudé Combined Laboratory (CCL) started as soon as first mechanical parts arrived.

Before the spectrograph re-assembly, also the installations of the Coudé Trains, the optical paths that relay the light from the four telescopes to the CCL, took place. Each of them hosts nine different large optical elements of superb quality, installed inside tunnels covering a distance of about 60 m capable to deliver the light at the entrance of the spectrograph with minimum aberrations and maximum efficiency. The first Coudé Train on UT4 was completed in September 2016 and on 25 September 2016, for the first time, the light of a star observed from the UT4 telescope reached the CCL. Successive measurements on the gathered first light images confirmed that all the required performance were met thus assessing the validity of the selected technological solutions. In forthcoming months all the other three UTs were equipped with their own Coudé Trains optics and after the very positive on-sky test verifications, final ESPRESSO installation in CCL could start.

After final re-assembly and installation verification, everything was ready to start the commissioning activities. ESPRESSO in this respect was quite peculiar since it required on-sky configuration and testing on each of the UTs respectively (the so-called *single-UT* mode) and on all four altogether (the so-called *multi-UT* mode), essentially repeating the “first light” for five times! The very first light was achieved on the night of 27th November 2017 on UT1 showing immediately the unique capabilities of ESPRESSO already with the first obtained spectra. On the night of 3rd February 2018 also the 4-UT mode started real on-sky testing with the first historic astronomical observation where light from all four UTs fed the spectrograph making the VLT the largest optical existing telescope in terms of collecting area.

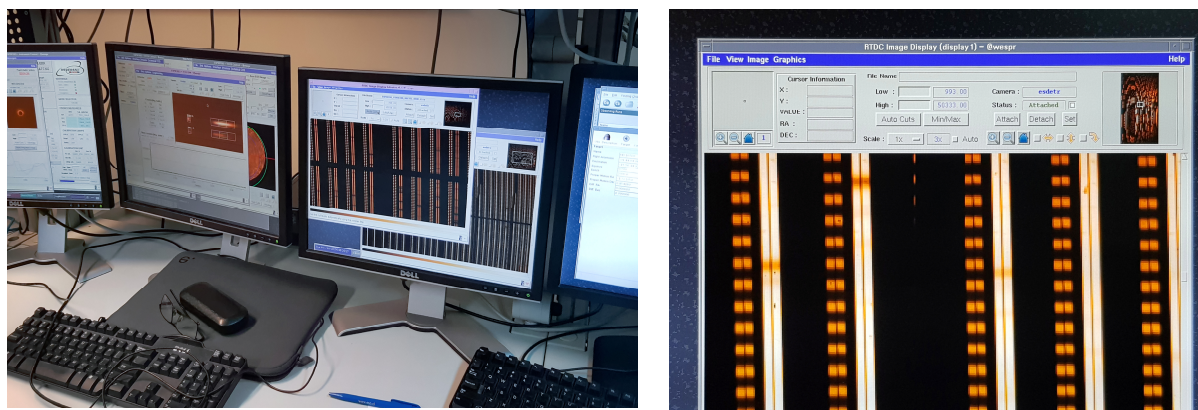


Figure 1. Left: first data obtained during the first light on November 2017; right: first spectrum achieved combining light with all four unit telescopes.

After the successful final commissioning held beginning of May, ESO took the decision to deliver ESPRESSO to astronomical community starting from October 2018.

The main aim of this paper is to present the operational constraints and challenges of ESPRESSO instrument for future routine scientific observations as emerged also from the ESPRESSO first commissioning activities. It is worth to recall that ESPRESSO will be offered both in visitor and in service observing modes with the peculiarity, due to its distributed nature, to be able to operate with any of the UT's in a seamless way also as a “replacement” of any other instrument that could become temporary unavailable. Moreover, the observational strategies for exo-planets characterization and the use of all the UT's simultaneously, even though limited to specific observing programmes, impose stringent requirements for current Paranal operations scheme. In section 2 we will present how the standard Paranal schema has been therefore adapted to cope with these requirements, in section 3 we will illustrate some key operational aspects, whereas in section 4 we will present how the overall system behaves “in practice” with the first real on-sky commissioning observations.

2. ESPRESSO DATA FLOW AND ITS FINAL DEPLOYMENT

In order to cope with the challenging scientific requirements and thanks to its fixed spectral format and long-term stability, ESPRESSO has been conceived starting from the preliminary design phases as “truly science-grade products generating machine”. To this purpose, in addition to the standard Data Reduction Software (DRS) package, a dedicated ESPRESSO Data Analysis Software (DAS) package has been developed² with the aim to extract scientific information as soon as reduced data are available. Figure 2 shows ESPRESSO DFS packages as installed and deployed in Paranal.

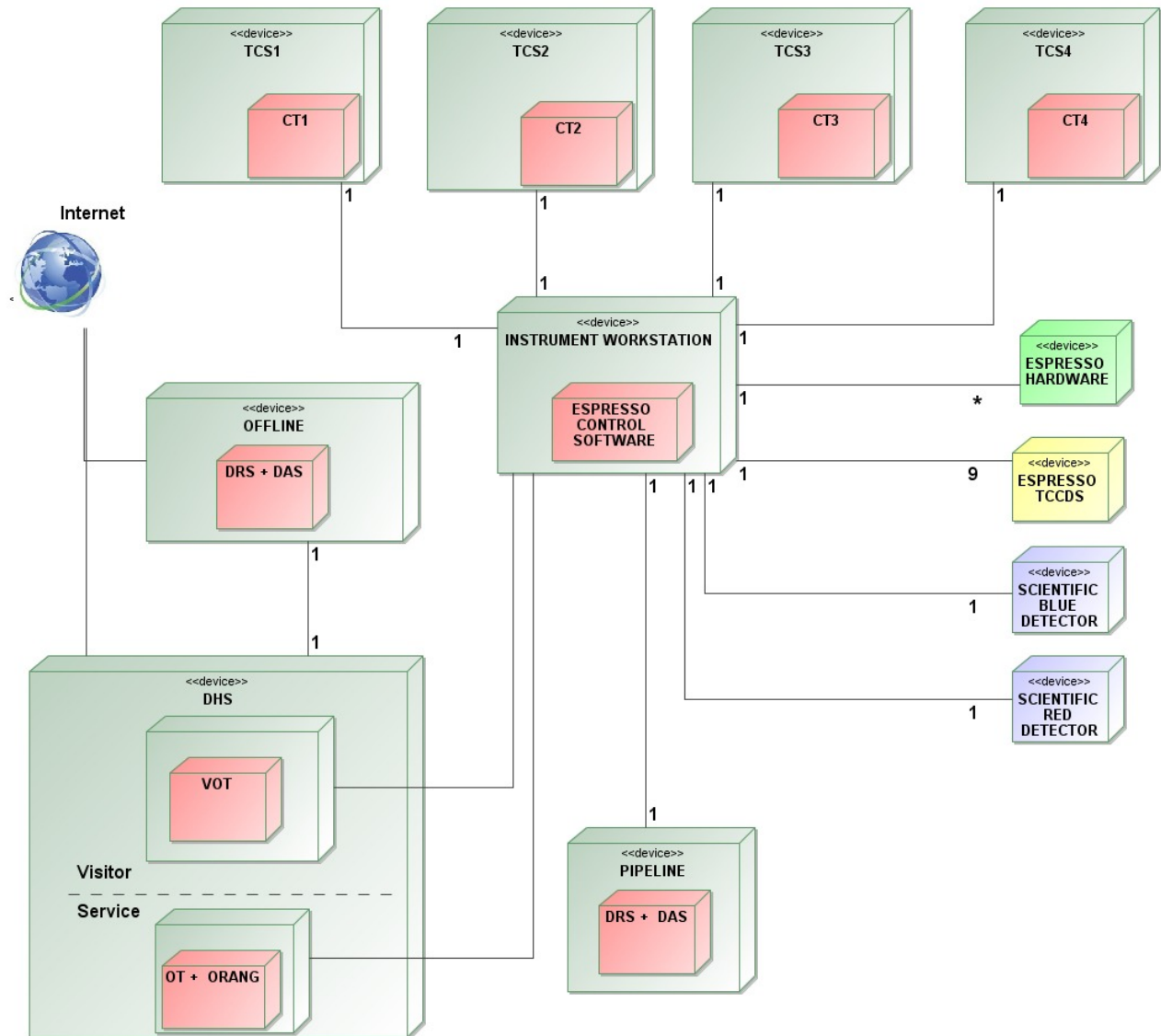


Figure 2: ESPRESSO final DFS deployment at Paranal. CT = Coudé Train, other acronyms are described in the text.

The flexibility to use ESPRESSO from any of the 4 UTs comes at a cost. From the operational and the DFS point of view the standard Paranal scheme had to be updated, to allow operations of ESPRESSO from all the four UTs control stations. Normally each UT has its own pipeline, data handling (DHS) and offline workstations, and these are shared by all instruments installed at that telescope. In the case of ESPRESSO it has been decided to use dedicated workstations, so to have only one instance of the pipeline running, and to have data confined only to the dedicated computers and not spread over various workstations. Therefore, differently than the other systems in Paranal, ESPRESSO uses its own

pipeline, offline and DHS workstations. The DHS computer is used for data handling in all observing modes and for observation management when operating in 4UT mode, while in 1UT mode the corresponding UT DHS workstation is used for ESPRESSO observations management. The figure 3 (courtesy of Carlos Guirao) describes the ESPRESSO DFS: the instrument workstation communicates with the required UT DHS (1UT mode) or with the ESPRESSO DHS (4UT). The on-line archive system and the data transfer tasks are run from the ESPRESSO DHS workstation.

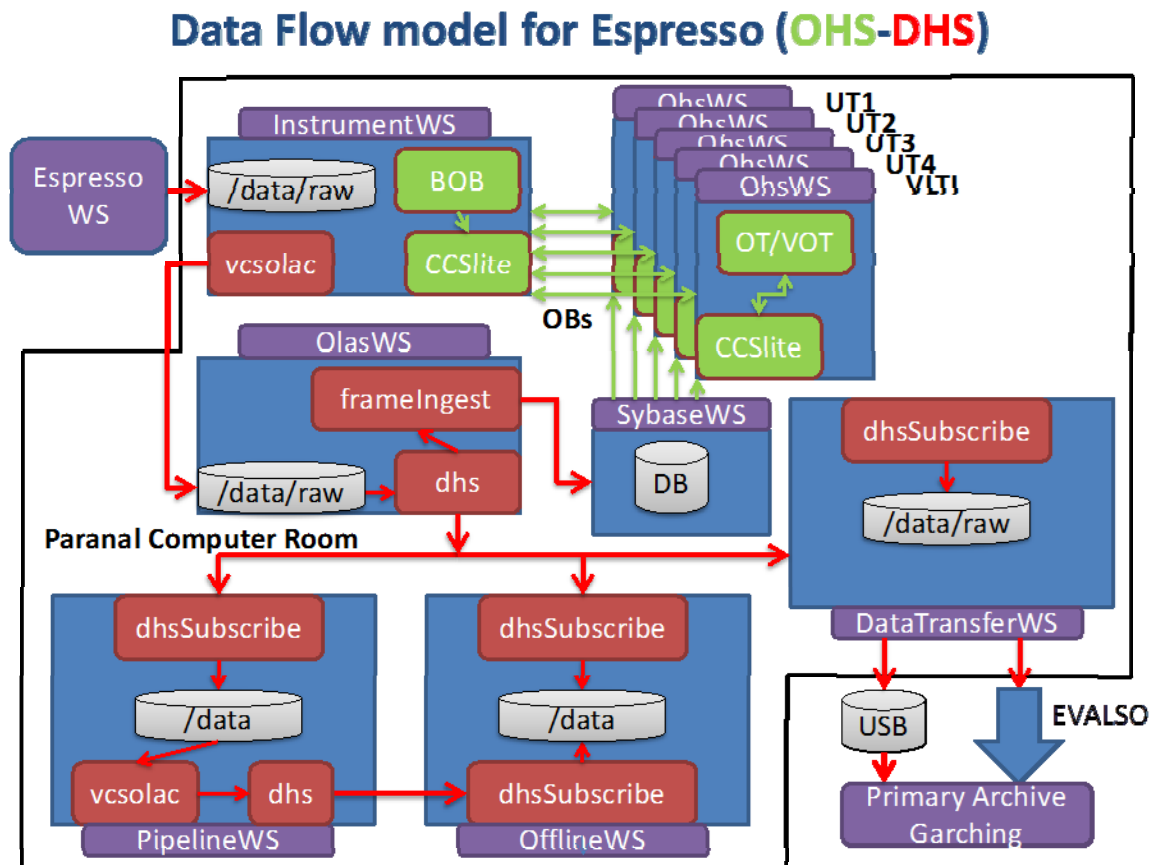


Figure 3: schematic of ESPRESSO DFS deployment.

Data reduction pipelines are used by Paranal (and La Silla) operations as quick-look tools to do a real-time coarse assessment of the quality of calibrations and science observations. Pipelines are implemented in C using the ESO Common Pipeline Library, and the corresponding recipes are executed via the ESO recipe executor (*esorex*) or via *ESOReflex*³. When the data arrive at ESO Garching (generally within one hour), a more thorough data processing and evaluation is performed by the Quality Control (QC) group. Here, the pipeline is used to automatically process raw calibration frames into master calibrations, generate quality control parameters to monitor the instrument and detector performance in order, and to assess, the quality of the calibrations and science observations. Pipelines are also used to produce the processed data available through the ESO archive, and are made available to the science community to enable scientists do their own data reduction. For the latter use case, ESO distributes the *ESOReflex* environment. *ESOReflex* is an interactive data reduction system allowing to run data reduction recipes in a defined sequence, called workflow. In addition it is capable to organize the data, plot intermediate and final products offering an easy, simple and intuitive interactive user interface and customize the data reduction parameters and cascade.

At Paranal pipelines and in particular the ESPRESSO one run unsupervised within the DFS where a fully automatic reduction of the acquired calibrations and/or observations is performed in a few minutes. Coupled to the pipeline there are moreover two tools running in parallel, the Data Organizer (DO) and the Reduction Block Scheduler (RBS). The DO continuously pools a predefined directory to search for incoming new raw data. It allows to automatically classify them

using a few relevant keywords from the raw data FITS header, associate the appropriate data reduction recipe and the relevant required input static and master calibrations contained in a fixed data area, defines the products filename prefix in a unique way, and eventually may also use appropriate data reduction parameters. All this information is contained in an ASCII file, the Reduction Block (RB). Optionally the DO may also use master calibrations created within a user defined time, usually set to one day, instead than the ones taken by the local calibration database area, to allow reduction with recent master calibrations. The rules to control the creation of RBs are the Organization Classification and Association (OCA) rules, defined in a dedicated ASCII file.

The RBS schedules and controls the reduction of RBs. It is possible to run multiple RBs at the same time, and in case of pipeline with parallelized code, it is also possible to run a recipe using multi threads.

3. ESPRESSO OPERATIONS

A critical component of the ESPRESSO DFS is represented by its control software, whose major responsibility is eventually to produce the final scientific image with proper header information suitable to be processed (automatically) by the DRS and DAS as described in section 2. The ESPRESSO control software architecture follows the required architecture for the VLT instruments and it is described in great detail in⁵. Here we would like just to emphasize that ESPRESSO operations follow the typical standard VLT operations for an astronomical observation. During the observing run, the Observation Block (OB) to be executed is loaded on the Observation Handling (OH) workstation and then sent to the BOB (Broker for Observation Block) tool on the IWS. BOB reads the contents of the OB and executes one by one the templates specified in there. Each template consists in general of a sequence of commands determining completely a scientific exposure. It allows presetting the telescope, to setup the instrument and detector so that the required scientific observation could be properly performed. The typical sequence of commands sent by science observation templates to execute an exposure is:

- SETUP (one or more)
- START (exposure)
- WAIT (till exposure is finished).

As a result of an exposure, the data produced by the two scientific detectors, all the information coming from instrument hardware subsystems, exposure meter data and instantaneous and integrated images are merged in a single multi-HDU FITS file which is in turn transferred to the on-line archive and data handling workstation.

For ESPRESSO operations particularly critical are the acquisition and field stabilization phases. During the acquisition phase, after telescope presetting, a correction is necessary in order to center the object on the fibre entrance. This is a quite standard operation also in other instruments, but in ESPRESSO it is particularly demanding since in the case of 4 UT mode the overall time to perform it must be minimized as much as possible. In ESPRESSO this has been achieved by fully automatizing the procedure. A carefully designed and tested algorithm is able to find automatically the most luminous object in the field (which usually coincides with the object under interest due to the small instrument field-of-view), computes the required correction and send it to the telescope. Before continuing with the next phase the user can confirm the proper object centering by looking at the on-the-fly images produced by two TCCDs which show the field and pupil respectively, repeat the whole procedure or switch to manual mode. Careful tests performed during the commissioning periods in different environmental conditions (various seeing values, different airmasses, varying meteorological conditions) showed the validity of the whole procedure limiting the manual mode to only a few cases of very crowded field or diffuse objects. Figure 4, left panel, shows the ESPRESSO operational GUI where three tabs could be noticed. The first one, named “*Pointing*”, is automatically activated at the acquisition phase. The red cross shows the result of the automatic finding algorithm which should coincide with the object to be centered in normal conditions. The panel allows to change the exposure time and the neutral density filter position, however a guess for both quantities is automatically derived from the object magnitude that a user is requested to provide. Parameters have been tuned and in standard Paranal conditions basically no, or very little, intervention is eventually required by the operator. This is particularly important in 4-UT mode where any manual intervention could result in time losses since it needs to be potentially repeated on each of the unit telescopes separately.

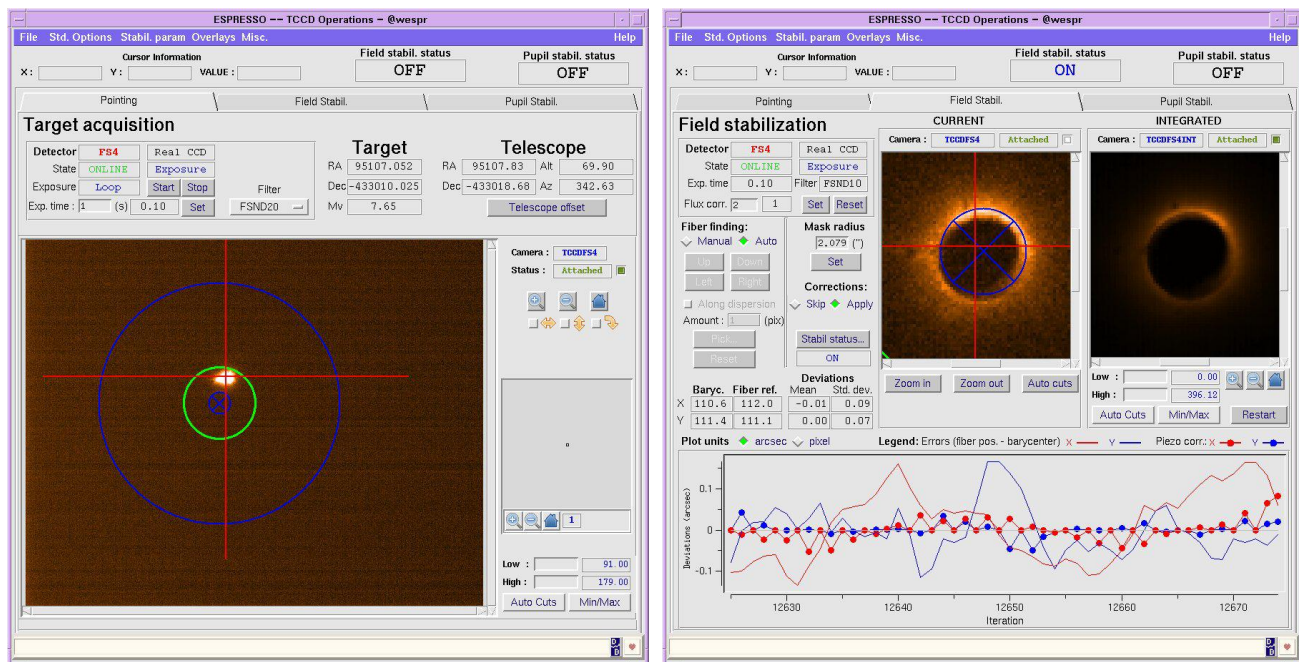


Figure 4: ESPRESSO operational GUI with tab activated for the pointing phase (left) and stabilization phase (right); see text for a detailed description.

Crucial to assess the stringent scientific requirements in terms of radial velocity precision and flux maximization is the “stabilization” phase. The purpose of the (field) stabilization is to maintain the object centered on the fiber during the whole duration of the scientific exposure. The TCCD(s), one per front end, acquires the image in a continuous loop up to 7 Hz; two auxiliary software processes, in real-time, analyze the obtained image and command the low-level piezo tip-tilt devices such to try to keep the object well centered on the fiber. Figure 4, right panel, shows the same operator GUI of the left panel, but this time with the stabilization tab activated. Two images can be seen: the instantaneous one, which displays the image as soon as it is acquired (max frequency around 7 Hz) and the integrated image. The integrated image is the sum of the images obtained during a scientific exposure and it is used both to visually check the quality of the stabilization and to re-compute continuously the fiber center for optimal star positioning. Also for the stabilization phase, based on the provided magnitude, most of the values are pre-computed thus minimizing any operator intervention. The GUI offers all the tools (for algorithm parameter settings, exposure time adjustment and manual selection of the fiber position) to allow manual corrections in case the pre-computed one fails.

Besides the stabilization itself, which controls and monitors the proper injection of the light in the fiber bundle, the signal-to-noise ratio of the ongoing scientific exposure is also continuously monitored by the ESPRESSO exposure time meter (EM). In ESPRESSO, the EM is actually a small spectrograph in itself and a dedicated process continuously computes the counts in three spectra channels from images obtained by a separate TCCD. Figure 5 shows the GUI that has been implemented and it is used to help the operator to monitor ESPRESSO performance during a scientific exposure. As for the stabilization case also here all the parameters are pre-computed thus minimizing any operator intervention.

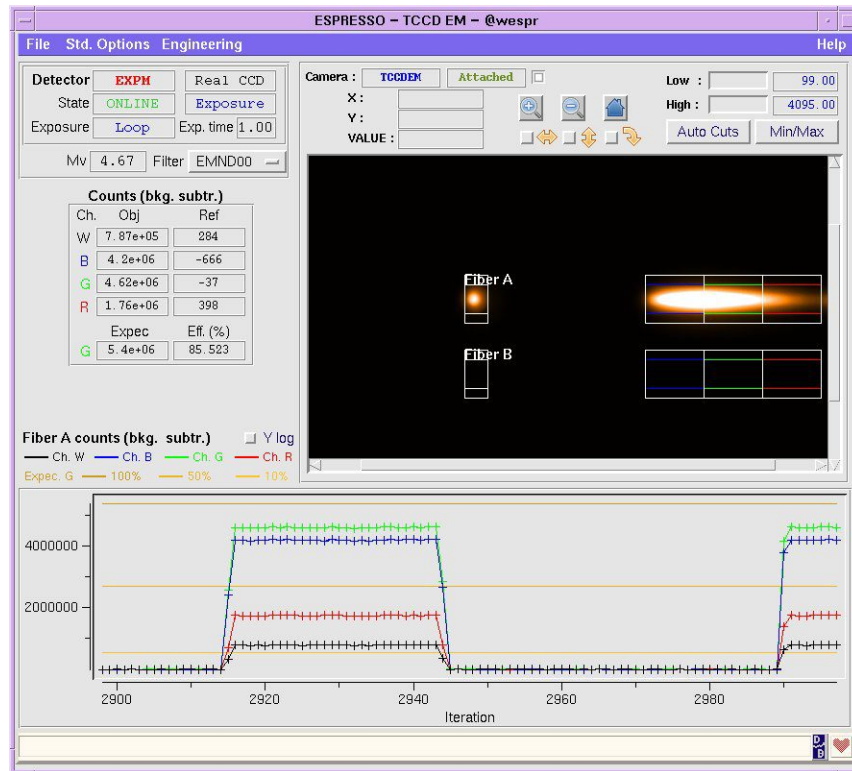


Figure 5: ESPRESSO exposure meter; the image displays the produced spectrum, the overlays (boxes) show the channels where counts are computed, the graph shows in real-time how the counts varies in the three channels.

4. ESPRESSO “SCIENCE” SOFTWARE IN A NUTSHELL

As described in section 2, key components of the DFS are represented by the DRS and DAS. The following two sections show the first encouraging results obtained during the commissioning activities, which essentially assess the validity and maturity of both libraries in terms of performance and produced scientific outputs.

4.1 Data Reduction Software: challenges and commissioning results

The ESPRESSO Data Reduction Library (DRL) and its reduction cascade have been thoroughly described in ². Here we would like just to recall that it is developed within the standard ESO pipeline environment and makes use of the Common Pipeline Library (CPL). The top-level part of the ESPRESSO DRL is made of a set of CPL recipes, which are intended to be self-consistent software pieces able to fully process the raw data type assigned to them. The ESPRESSO DRL will comprise a total of 11 calibration recipes and one science recipe, which can be associated to raw data types. It is worth to emphasize that all ESPRESSO configurations (actually, instrument modes) will produce data that are sufficiently similar so that the global reduction chain is always the same (i.e. we are always dealing with high-resolution echelle spectra produced by a fiber-fed instrument). All the DRL recipes are therefore the same for all instrument configurations (same algorithms), and the mode-specific information that is required to properly process frames are passed to the recipes through a static FITS configuration tables as part of the set of input frames (SoF). This strategy is chosen to avoid duplicating recipes with the big advantage that the ESPRESSO pipeline is able to reduce data from other fiber-fed echelle spectrographs like HARPS, once the proper configuration files are provided.

During the four periods of commissioning from November 2017 to May 2018, ESPRESSO data reduction has been tested in the real observing conditions. The pipeline is fully automatic, reducing the acquired data on-the-fly with the latest available calibrations. Thanks to a functionality put in place by ESO, the so-called virtual-products, each science image can be reduced using the wavelength calibration taken few hours or even minutes before. This is necessary to get the ultra-high radial velocity (RV) precision, as it is the case for ESPRESSO. The pipeline performs the cross-correlation and provides the user information on the RV of the observed object as soon as the data is reduced. An example of a single one-dimensional (S1D) spectrum obtained immediately after the observation and its zoom into spectral lines is shown on Figure 6.

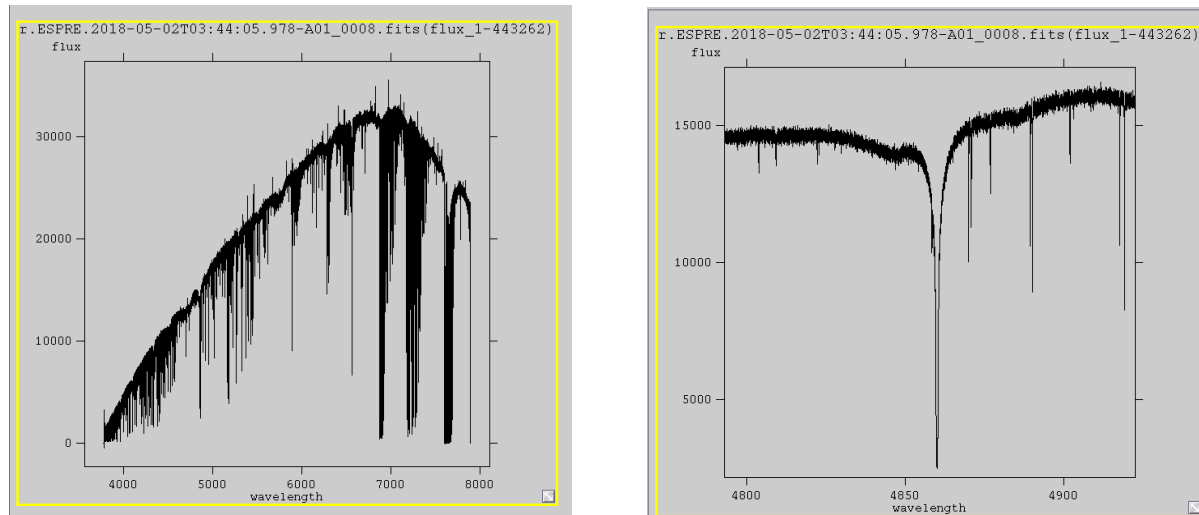


Figure 6. Left: S1D produced by the ESPRESSO DRS and right, a zoom of the same spectrum.

In order to obtain the already mentioned high precision RV measures, a very accurate wavelength calibration is mandatory. ESPRESSO has different options to perform the wavelength calibration. The use of a ThAr lamp spectrum is known and has been used successfully for many years on different spectrographs, e.g. on HARPS. Newer methods are the ones based on the processing of a Fabry Perot (FP) or a Laser Frequency Comb (LFC) spectra. The advantage of these two methods is their regularity in flux and across the wavelengths. Figure 7 shows one order of the LFC spectrum where the regular spacing and the almost constant flux level could be easily noticed.

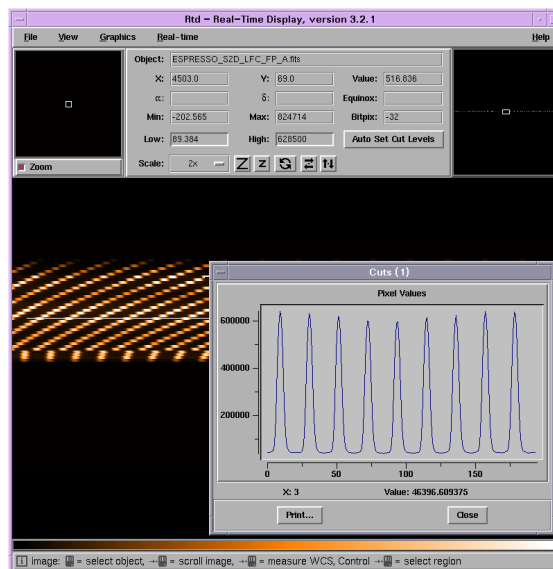


Figure 7: single two-dimensional (S2D) spectrum extracted from the LFC exposure with one order shown by cuts.

An example of the final product obtained by the DRS is shown instead in Figure 8. It represents (top panel) the cross correlation function (CCF) of a RV standard close to the Moon. The blue line is the CCF of the star spectrum and the RV dip corresponding to the Moon RV is clearly visible. The orange line is the CCF of the star spectrum after subtraction of the sky spectrum. Bottom panel show instead the CCF of the sky spectrum alone.

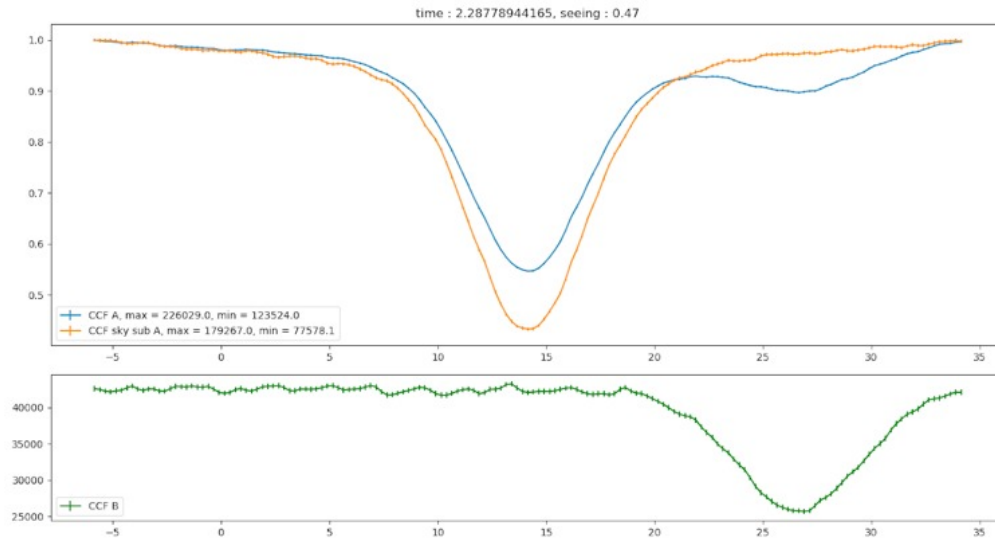


Figure 8: the cross correlation function (CCF) of a RV standard close to the Moon. See text for description.

4.2 Data Analysis Software: challenges and commissioning results

The ESPRESSO DAS comprises a total of 13 recipes. It is split into four branches: one for the analysis of QSO spectra and three for the analysis of star spectra. Some of the recipes are common to more branches while others are specific to the treated spectra (see Table 1). Each DAS branch is managed by a dedicated Reflex workflow. All the recipes are available off-line at the telescope on a dedicated workstation and the users have the possibility to install the whole package also on his/her computer.

The first two recipes, *espda_coadd_spec* and *espda_mask_spec*, provide tools to prepare the DAS output for the subsequent analysis. Different exposures from the same target can be combined into a single spectrum and selectively masked to avoid problematic regions (e.g. telluric bands). The co-addition is a lossless procedure: while a re-binned spectrum is produced by merging information from different exposures into a new wavelength grid, the original pixels are still preserved in a combined table which is propagated throughout the analysis.

The QSO branch contains recipes to detect, identify, and fit the absorption lines, while estimating at the same time the level of the unabsorbed continuum (including both the non-thermal component and the QSO emission lines). After a list of absorption lines has been created by *espda_create_linelist* by finding the most prominent minima in the flux spectrum, a blind fit of the lines is performed by *espda_fit_line* to determine the continuum. Different algorithms are used for the regions redwards and bluewards from the Lyman- α emission; the latter region is commonly referred as "Lyman- α forest", and is characterized by a large number of frequently blended absorption features. The stability of the line removal/continuum fitting procedure in the Lyman- α forest is ensured by modeling in advance the effective opacity that is expected and revising the estimation as the lines are incrementally fitted from the strongest to the weakest ones. Related absorption lines, produced by different ions at the same redshift, are identified by *espda_iden_syst* and fitted by *espda_fit_line* with multiple Voigt profiles. Proper constraints between the relevant line parameters (redshift, column density, thermal and turbulent broadening) are automatically set by the recipe, but can be adjusted by the user through a

graphical user interface. Depending on the user's choice, the procedure can automatically add line components until a good fit has been achieved, chi-squared-wise.

Operation	Branch	Name
Co-addition of spectra	star, quasar	<i>espda_coadd_spec</i>
Creation of a spectral mask	star, quasar	<i>espda_mask_spec</i>
Creation of a list of absorption lines	star ^a , quasar	<i>espda_create_linelist</i>
Continuum fitting of a 1D spectrum	quasar	<i>espda_fit_qsocont</i>
Identification of the absorption systems	quasar	<i>espda_iden_syst</i>
Voigt-profile fitting of absorption lines	star ^a , quasar	<i>espda_fit_line</i>
Measurement of the EW of spectral lines	star	<i>espda_compu_eqwidth</i>
Computation of the stellar parameters	star	<i>espda_compu_starpar</i>
Continuum fitting of single orders	star	<i>espda_fit_starcont</i>
Comparison with a synthetic spectrum	star	<i>espda_synth_spec</i>
Computation of the radial velocity using a synth. spec.	star	<i>espda_rv_synth</i>
Computation of the radial velocity	star	<i>espda_compu_radvel</i>
Computation of the stellar activity indexes	star	<i>espda_compu_rhk</i>

Table 1. List of recipes; ^a at present, these two recipes are implemented only in the QSO branch

An absorption system detected and fitted on the spectrum of quasar HE0515–4414 (observed during the Commissioning 1b run) is shown in Figure 9. The figure gives an example of the Reflex provided functionality, which allows to plot and interact with the recipe products, adjusting the recipe parameters and in case repeating the execution. A similar interface is available for all recipes of the QSO branch.

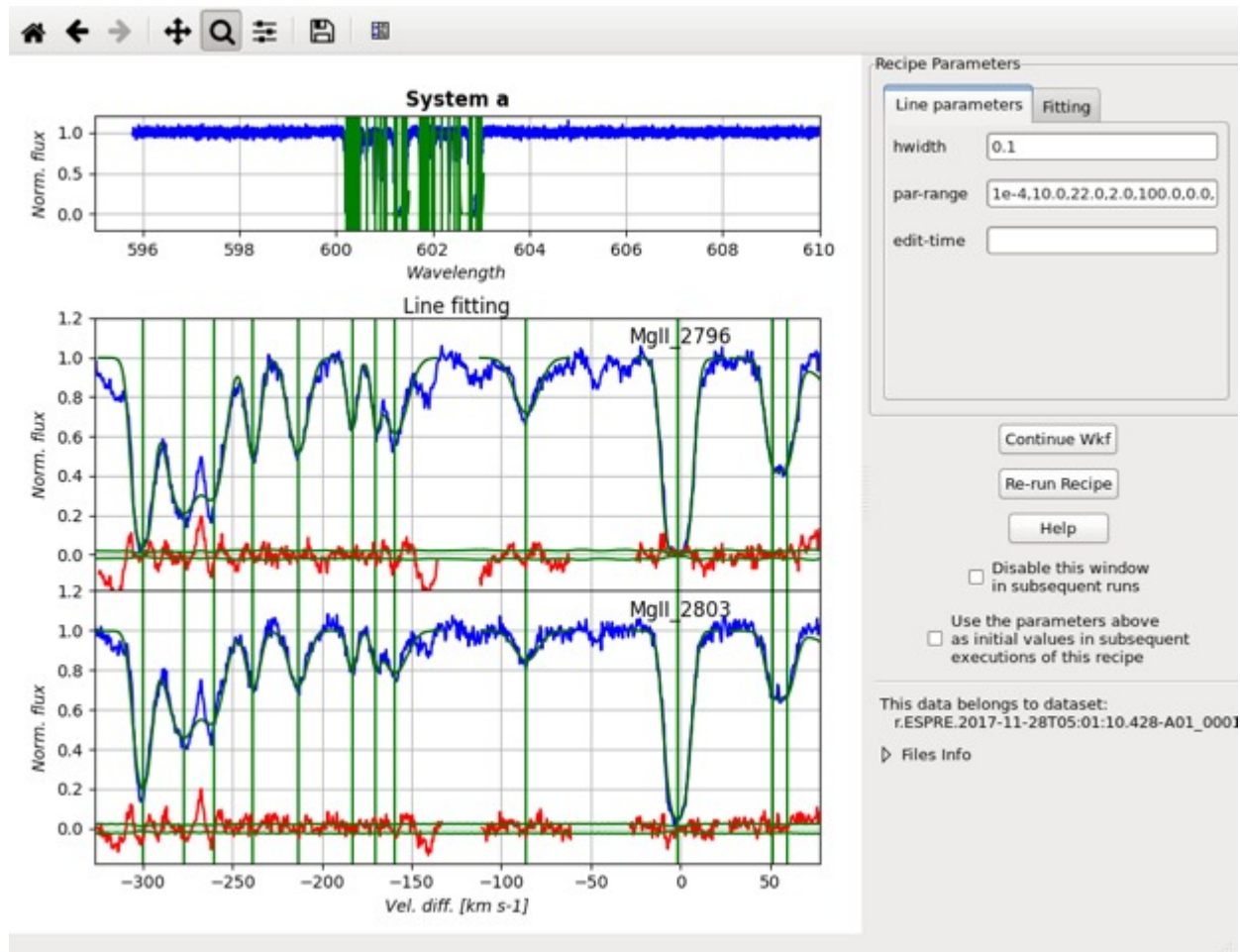


Figure 9: A MgII absorption system fitted with the ESPRESSO DAS. Blue: normalized spectrum; green: best-fit composite Voigt profile; red: residuals.

The first star branch (STAR I) contains instead recipes to measure the equivalent widths of the absorption lines and determine other stellar parameters like the effective temperature and the metallicity of the observed star. The corresponding Reflex workflow does not contain interactive modules but allows for a seamless execution of the procedures. The equivalent widths are computed by the recipe *espdacompu_eqwidth* by fitting multiple Gaussian profiles to a list of detected absorption lines, normalized to a local continuum. Another recipe, *espdacomputarpar*, uses the line list to compute the effective temperatures and the iron abundance. The recipe is meant to be used on solar type stars.

The second star branch (STAR II) contains recipes to fit the star continuum and to compare the observed spectrum with the synthetic spectrum. The continuum is fitted order by order by the recipe *espdafitstarcont* with a polynomial function. A catalogue of synthetic spectra⁶ produced by the ASSET code⁸ using Kurucz model atmospheres⁷ is provided, covering effective temperatures from 3,500 to 7,000 K, surface gravitational accelerations values from 10 to 10⁵ cm s⁻², iron-over-hydrogen abundances from 10⁻⁵ to 10^{0.5} (relative to the Sun). The recipe *espdasynthspec* compares the observed spectrum with one synthetic spectrum interpolated within the catalogue for a given set of stellar and broadening parameters. The next recipe, *espdarvsynth*, performs the cross-correlation of the observed 1D normalized, merged stellar spectrum with the interpolated synthetic spectrum. A plot produced by Reflex from the output of this recipe is shown in Figure 10. The radial velocity computed by the second star branch is significantly less precise than the one computed by the DRS (depending on the stellar rotation and signal-to-noise of the spectrum, the precision can be below

1 km s⁻¹), but can be applied to any stellar spectrum, including giant, subgiant, and dwarf stars, both metal-poor and metal-rich.

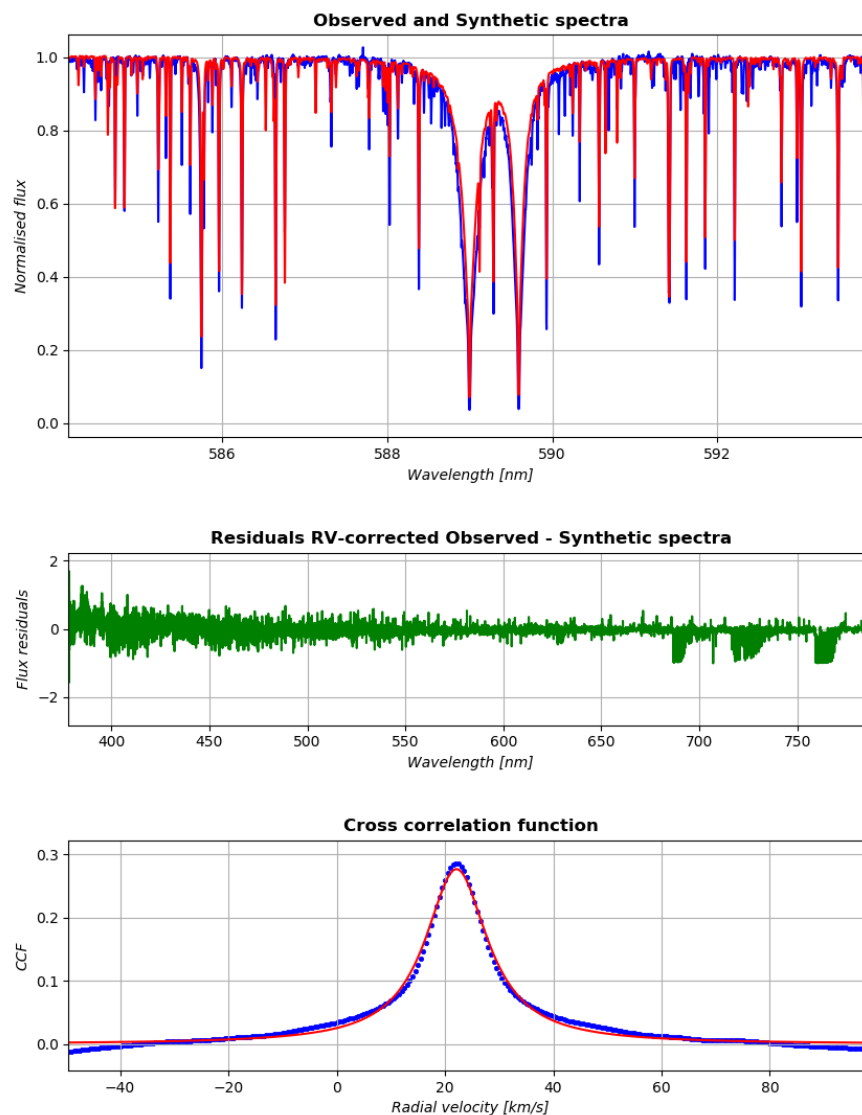


Figure 10. Top: plot of the output produced by the recipe *espda_rv_synth* for ESPRESSO data of the RV standard star HD 35854; blue: the observed normalized merged spectrum corrected for RV compared with the synthetic spectrum (red). Center: Observed - synthetic flux residuals. Bottom: cross-correlation function fitted with a Lorentzian function plus a polynomial of order 1.

The radial velocity algorithm implemented in the DRS, achieving a sub-m s⁻¹ precision, is also included in the DAS as a part of the third star branch (STAR III, recipe *espda_compu_radvel*), to provide the user the possibility to apply it off-line at the end of the data reduction process run at the telescope. The third star branch also contains the recipe *espda_compu_rhk*, to compute the Ca II H&K activity index, S-index on the Mt Wilson scale and log(R'HK).

The four DAS workflows were installed and tested on the off-line machine at Paranal and are currently being used to analyze the reduced products from Commissioning 1 and 2 periods.

5. CONCLUSIONS

ESPRESSO, the next generation ESO VLT high-resolution ultra-stable spectrograph, is ready for operations. After the very successful commissioning periods where instrument performance have been assessed and validated ESO gave green light for starting routine observations from October 2018 in single UT mode. 4 UT mode will be offered in 2019 after a final science verification phase. In this paper we have presented the overall ESPRESSO DFS, its challenges and peculiarities describing how it has been adapted to fit the current data flow schema in Paranal. Careful requirements analysis conducted in early instrument design phases allowed us moreover to develop an almost automatic and very flexible operational schema that could be seamlessly used both for one and 4 UT cases. This will ease operations at the telescope, minimizing the overall overheads and maximize the produced scientific outputs.

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