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ABSTRACT

The current E-ELT instrumentation plan foresees a High Resolution Spectrograph conventionally indicated as HIRES whose Phase A study has started in 2016. An international consortium (stemmed from the existing "HIRES initiative") is conducting a preliminary study of a modular E-ELT instrument able to provide high-resolution spectroscopy ($R \sim 100,000$) in a wide wavelength range (0.37-2.5 μm). For the aims of data treatment (which encompasses both the reduction and the analysis procedures) an end-to-end approach has been adopted, to directly extract scientific information from the observations with a coherent set of interactive, properly-validated software modules. This approach is favoured by the specific science objectives of the instrument, which pose unprecedented requirements in terms of measurement precision and accuracy. In this paper we present the architecture envisioned for the HIRES science software, building on the lessons learned in the development of the data analysis software for the ESPRESSO ultra-stable spectrograph for the VLT.

Keywords: data flow, data reduction, data analysis, ESO E-ELT, high-resolution spectroscopy, instrument pipeline, science machine

1. INTRODUCTION: HIRES IN A NUTSHELL

Since 2008, several design options for the first generation of instruments to be installed at the European Extremely Large Telescope (E-ELT) have been envisioned under the auspices of ESO. Among them, two high-resolution spectrographs for the optical and near-infrared bands (named respectively CODEX[1] and SIMPLE[2]) were originally proposed; following the recommendation of the E-ELT Science Working Group, the two projects merged in early 2013 into the so-called "HIRES initiative", E-ELT HIRES being the provisional name of the instrument.[3] The new project was formalized in 2015 when the HIRES initiative, after a successful answer to an ESO Request for Information, was appointed to conduct the Phase A of the instrument development, starting from 2016. A new consortium was created, including the original countries involved in the HIRES initiative (Chile, Denmark, France, Germany, Italy, Portugal, Spain, Sweden, Switzerland, and United Kingdom) and two additional countries (Brazil and Poland), under the PI-ship of A. Marconi (INAF–Italy).

A detailed description of HIRES is the subject of Ref. 4. Here we recall the main features of the instrument, as described in a white book (discussing its scientific aims) and in a blue book (detailing the technical concept). The wide range of science cases HIRES is meant to address can be summarized as follow:

- The detection and characterization of the atmospheres of extrasolar planets; the high-resolution spectral mapping of Solar System objects; the study of protoplanetary and proto-stellar disks;
- The determination of chemical composition and atmospheric parameters of stars beyond the immediate neighborhood of the Sun; the extension of galactic archaeology to the Local Group and beyond;

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- The observation of the intergalactic medium (IGM) as a way to study cosmic reionization and nucleosynthesis by the first population-III stars; the study of stellar and AGN feedback in wide range of galaxy masses, morphology and redshift through IGM tomography;
- The study of extragalactic transients (e.g. gamma-ray bursts);
- Contributions to fundamental physics by direct observation of the Universe accelerated expansion (the so-called Sandage test[5,6]) and by constraining a possible variations of the fine-structure constant and of the electron-to-proton mass ratio.

To achieve such ambitious goals, the instrument is designed to be extremely versatile and to combine high-resolution and high-sensitivity with an exceptional thermo-mecanical stability, to push the limits of wavelength accuracy already set by VLT ESPRESSO.[7] Here are the main specifications:

- Spectral resolution in the range $50,000 \lesssim R \lesssim 100,000$, with a ultra-high resolution mode at $R \approx 200,000$;
- Simultaneous wavelength coverage in the range $0.37\,\mu\mathrm{m} \lesssim \lambda \lesssim 2.5\,\mu\mathrm{m}$;
- Multiplexing capability up to 5-10 objects within a field of view of a few arcmin, with spectral resolution in the range $10,000 \lesssim R \lesssim 50,000$;
- wavelength accuracy (and overall stability over one night) of the order of $10\,\mathrm{cm\,s^{-1}}$ (goal: $2\,\mathrm{cm\,s^{-1}}$ for the Sandage test, maintained over a timescale of some decades);
- sky subtraction accuracy within 1%.

These combined requirements can only be met adopting a modular architecture, in which a few spectrographic units are combined into a single instrument and effectively share the same telescope focus. A possible conceptual layout for HIRES is shown in Fig. 1

Both the architecture of the instrument and the range of science case poses an unprecedented challenge to the treatment of observational data and raises the bar for software versatility and reliability. In this paper, we give an overall description of the HIRES subsystems involved in data treatment (including tools for both reduction and scientific analysis: see Sec. 2) and present its modularity as a way to cope with the instrument complexity. We also discuss the concept of pixel conservation (Sec. 3) as a way to achieve a reliable treatment of the errors in the analysis and consequently validate the results of fitting procedures. In the conclusion (Sec. 4) we discuss possible applications of the software beyond the specific scope of the instrument.

2. DATA TREATMENT WITHIN THE HIRES DATA FLOW SYSTEM

The HIRES Data Flow Systems (DFS) is a collection of software subsystems developed as an integral part of the larger E-ELT DFS to prepare, schedule, and execute the observation, and to store and process the acquired data. The main subsystems of the HIRES DFS are:

- The Observation Preparation Software (OPS), which assists the user in creating the observing blocks, and is equipped with a dedicated Exposure Time Calculator (ETC);
- The Instrument Control Software (ICS), which complements the telescope control software and operates the instrument during the calibration and observation procedures, according to the specifications in the observing blocks;
- The Data Reduction Software (DRS), which removes the instrumental signature from the raw data and calibrates the output spectra in wavelength and flux;
- The Data Analysis Software (DAS), which processes the reduced spectra to automatically extract meaningful information (e.g. stellar parameters, continuum-normalized spectra, lists of identified absorption lines, etc.).

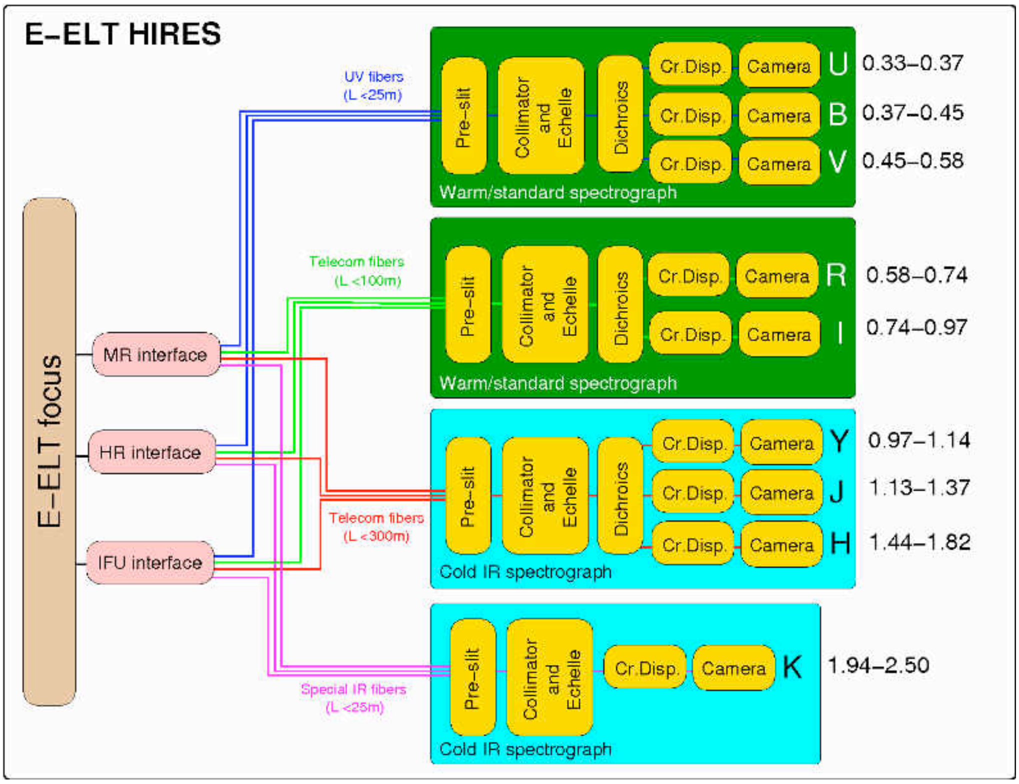

Figure 1. A possible architecture for the HIRES instrument, here split into four spectrographic units with nine detectors, optimized to different optical and near-infrared bands.

The availability of dedicated software tools for both reduction and analysis, treated as separate though tightly connected parts of the same conceptual pipeline, follows the approach already adopted for ESPRESSO,[8–10] which is strongly favored by the subtlety of the instrument science cases. With respect to ESPRESSO, the HIRES data treatment pipeline must be able to handle the enhanced capability of the instrument, including its greater precision in wavelength calibration and its extended wavelength range, reaching the near-infrared bands where the atmospheric transmittance is low and the sky emission requires careful modeling. Similarly to their ESPRESSO counterparts, the DRS and DAS for HIRES will be made up of stand-alone modules (*recipes*) performing separate operations, to be executed either individually or in cascade through both command-line and graphical user interfaces provided by ESO. A breakdown of the foreseen operations (which correspond one-to-one with DRS or DAS recipes) is given in Fig. 2. The code is meant to be available for both online and offline operations on a dedicated workstations in the E-ELT control room on Cerro Armazones, and will be publicly released for download to the scientific community.

2.1 Data reduction

The DRS design is aimed to be highly modular (to comply with the complex architecture of the instrument) yet to avoid any unnecessary overlaps among its parts. This result is achieved by a two-layer model, in which the algorithms are clearly decoupled from the configuration tools needed to apply them to the raw data. The final goal is to process data from different spectrographic units using the exact same algorithms, properly fed with the relevant configuration parameters (e.g. theoretical model of the spectrograph, CCD geometry parameters, etc.) formatted into a static FITS table. Each recipe is therefore dependent on a small number of setup parameters, controlling only the algorithmic details of the operation (e.g. thresholds for kappa-sigma clipping, specific choices

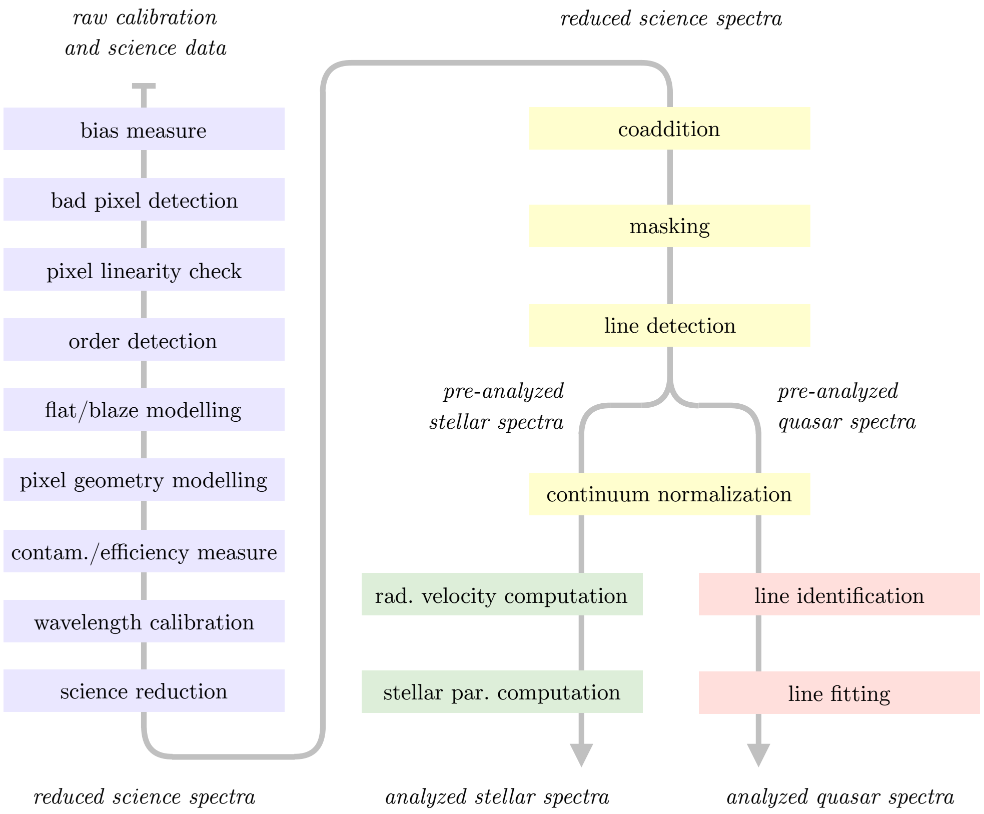

Figure 2. Preliminary scheme of the HIRES data treatment pipeline. Data reduction modules are on the left (light blue), data analysis modules are on the right (light yellow: shared modules; light green: stellar modules; light red: quasar modules). Two branches for the analysis of stellar and quasar spectra have been delineated so far.

for pixel averaging, etc.). The effectiveness of the two-layer model is to be tested and appreciated in advance on HARPS,[11] HARPS-N,[12] and ESPRESSO data; the reduction software for HARPS-N and ESPRESSO already share a significant number of algorithmic solutions (see e.g. Ref. 13).

The foreseen reduction chain is straightforward (left part of Fig. 2). Operations are meant to be performed automatically with minimal supervision from the end user: the execution of each recipe is triggered by a specific kind of raw calibration data (e.g. bias, dark, and flat frames, etc.) or raw science data (i.e. target exposures), and depends on the products of the uphill recipes, feeding the downhill ones. A core concept in data reduction is the conservation of pixels throughout the chain (see Sec. 3). Ideally, the final reduced spectra can be mapped pixel-by-pixel to the original raw science data and possess the same information content, only cleaned from the instrumental signature and complemented with information to calibrate the wavelength and the flux in each pixel. Interactive tools (such those provided by the ESO Reflex environment[14]) are available for the end user inspect the results and tweak the recipe setup parameters.

Wavelength calibration is arguably the most delicate step of data reduction, given the accuracy and precision required by the HIRES science cases. A set of laser frequency combs (LFCs)[*] optimized to the wavelength range of the different spectrographic units is envisioned as a primary wavelength reference for the instrument. Thanks to the HIRES architecture, it can be provided as a simultaneous reference, appearing next to the spectrum of the science target on the detector. In addition to being an optimal wavelength calibrator, the LFC also provides

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[*] A LFC is a pattern of narrow, equally spaced emission lines generated by a mode locked laser, which overcomes the limitations of lamp spectra (line blending, uneven spacing).[15,16]

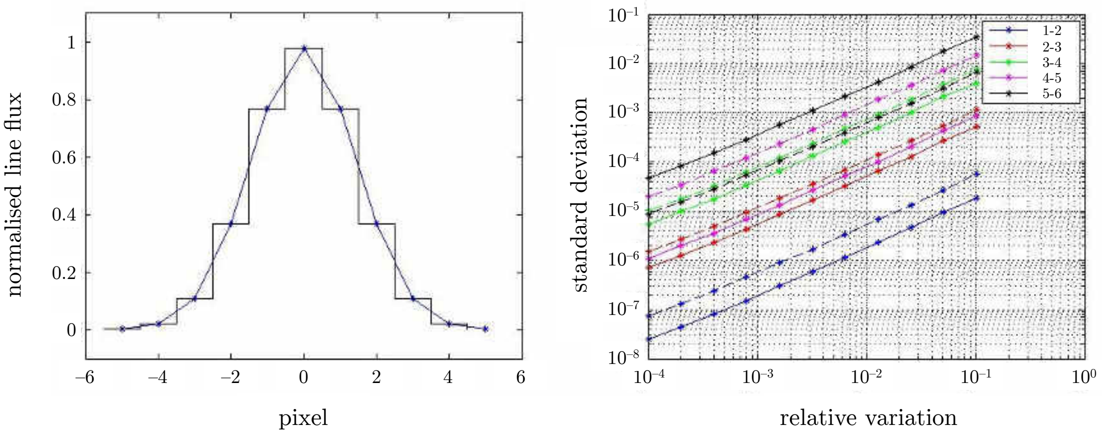

Figure 3. Effect of pixel size variation on the centroid of a simulated LFC line. *Left panel:* the simulated line (black), defined on 11 detector pixels, with its Gaussian parametrization (blue). *Right panel:* Standard deviation of the fitted centroid computed over 10,000 realizations of the LFC line, as a function of the relative variation in pixel size. The different colors denote which pixels were affected (variation was modeled by shifting the boundary between two adjacent pixels, so that the size of one pixel is increased, and the size of the other is decreased by the same amount). When the tail pixels are affected (1-2), the centroid is better defined than when the central pixels are affected (5-6). Results obtained with flat-field global corrections (dashed lines) are generally better, except for the central pixel case. [Excerpt from the ESPRESSO data reduction library documentation.]

a way to monitor the detector characteristics, most importantly the local variation in size and sensitivity of the detector pixel grid. Tests on data simulated for ESPRESSO show that the LFC is able to detect and correct for relative variations in pixel size of the order of $\sim 10^{-4}$, whose effect is unrecoverable by flat fielding alone and could account for a systematic error in wavelength calibration of $10\,\mathrm{m\,s^{-1}}$ or more[17] (see Fig. 3).

Subtraction of the sky background is also a delicate operation, particularly in the J, H, and K bands of the near infrared, crowded by typically bright, frequently blended sky emission lines. A well-known approach to background modeling is the so-called Kelson technique,[18] which exploits the spatial extension of the sky lines as they appear on the non-rebinned raw spectra to effectively oversample their profile. The Kelson technique has been successfully applied, for example, to VLT X-shooter near-infrared data[19] within a pixel-conserving reduction model (see Sec. 3); the greater resolution of HIRES will allow for an even more precise sky line modeling and subtraction. Optical and near-infrared bands from I redwards are also affected by telluric absorption, which in the J and K bands reduces the atmospheric transmittance to zero. This effect is routinely corrected for by extracting the spectrum of telluric absorption from high-SNR observation of standard stars; telluric correction is not always effective, though, and leaves strong residuals especially in the regions with lower transmittance. An alternative technique under consideration for HIRES uses the fact that telluric lines appear shifted on different exposures of the same science target, when the exposures are referred to the barycentric coordinate frame of the Solar System: as a result, different exposures can be used to recover the lost information in line-affected wavelength windows. Such technique is expected to be effective in less-crowded regions and will benefit from the high resolving power of HIRES.

2.2 Data analysis

Compared to the DRS, the DAS is relatively independent on the instrument architecture, as it handles reduced data only. Its design is primarily driven by the instrument foremost science cases, which mostly depend on the analysis of stellar and quasar spectra. The goal is to provide the end user with science-grade data products obtained through purposely designed, specifically validated algorithms. As for the DRS, the DAS recipes are meant to be executed automatically, with an additional degree of freedom in their arrangement, which can be adapted by the end users to meet their specific requirements. The latter feature is essential to the data analysis, which typically involves several iterations through the same operations.[10]

The DAS chain is more complex than the reduction chain, and may be split into multiple branches focusing on individual science cases. A preliminary layout has been developed by similarity with the ESPRESSO data analysis software, and consist of two main branches, for the analysis of stellar and quasar spectra respectively, with a set of operations common to both branches (right panel of Fig. 2). Though depicted as an arrow passing through the recipes, the chain is not necessarily linear in its execution: existing steps can be generally skipped or swapped, and additional steps may be added at a later time to comply with emerging demands. Here is a prospective list of the operations, by no means exhaustive:

- For the stellar branch: computation of high-precision radial velocities; estimation of stellar parameters (equivalent width, effective temperature, metallicity) and activity indeces.
- For the quasar branch: detection and identification of the absorption systems; Voigt-profile fitting of the absorption lines; determination of the continuum level by line fitting and removal.

The algorithms involved in these operations are adapted from the data analysis software for ESPRESSO, considering the increased capabilities of HIRES and the increased requirements set by its science cases.

Pixel conservation, further discussed in Sec. 3, is essential to correctly estimate the errors on flux and consequently to allow a proper validation of the line-and-continuum fitting procedure with common best-fit estimators (like the χ^2 test).[10] Pixel conservation is enforced in the DAS by a proper handling of the reduced spectra coming from the DRS (possibly including several exposures for a given science target), which are reformatted both as a coadded spectrum (rebinned to a wavelength grid of choice) and as a combined spectrum (including all the original pixel with their own wavelength, without any rebinning). Further details about the coaddition procedure, as it is implemented in the ESPRESSO data analysis software, can be found in Ref. 10.

3. PIXEL CONSERVATION AS A GENERAL APPROACH TO DATA TREATMENT

A core idea behind the treatment of HIRES data is that the information propagated throughout the chain must be susceptible to be traced back at any moment to the original pixels of the detector. In practice, this means that all operations needed to remove the instrumental signature must be done on a pixel basis (maintaining the same grid from the beginning to the end) and be completely reversible; conversely, operations that combine information from different pixels (e.g. averaging or rebinning) should be limited to the extraction of information and should never be combined with each other. The reason is that the latter ones are essentially disruptive in nature, interfering with a correct propagation of the errors, and induce biased results if scientific measurements are performed on their downhill products. The benefit of pixel conservation has already been demonstrated in the reduction and analysis of VLT UVES high-SNR quasar spectra, by comparing the results produced by the standard ESO pipeline[20] with those obtained with a custom pipeline, specifically designed to test the correct propagation of the errors.[21]

To formalize a conservative approach to pixel propagation, let us consider a set of several raw science exposures R_i, possibly taken at different epochs. Each exposure generates an images that can be represented as a set of pixel readouts s_p (in ADU). We define reduced spectrum S a set of points $(\lambda_p, I_p, \sigma^2(I_p))$ defined on the same pixel grid, with λ_p the calibrated wavelength (in nm), I_p the calibrated flux density (in J m^{-2} s^{-1} nm^{-1}) and $\sigma^2(I_p)$ its variance (in J m^{-2} s^{-1} nm^{-1}). It is worth noting there is no reason for counting pixels from different raw observations separately, as long as the one-to-one correspondence between points of R_i and S is preserved; the reduced spectrum contains as many pixels as the whole set of i exposures, as counted by the subscript p.

From a theoretical point of view, the reduction procedure consists in finding a map between R_i and S, or more specifically a function $m_{i,p}$ such that

$$I_p = m_{i,p}(s_p), \tag{1}$$

because λ_p only depend on the position of the pixel in the detector, given the instrument optical layout, and is univocally determined by wavelength calibration. The subscript i in $m_{i,p}$ indicates that the function could be

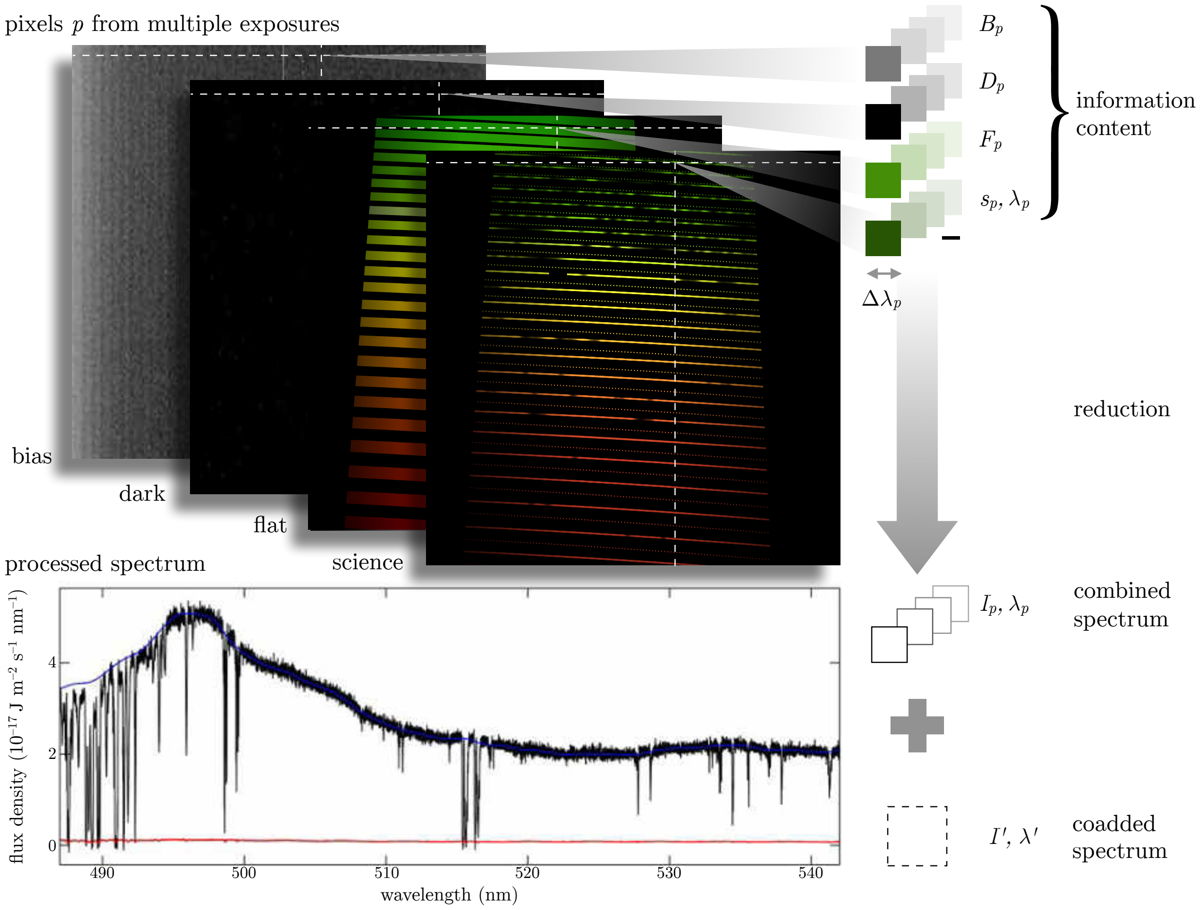

Figure 4. Scheme of the pixel conservation approach as implemented by the HIRES data treatment. Pixels from raw calibration and science frames are collected; one science exposure with its main associated calibrations is shown in the upper left panel. The information content of a given pixel is completely described by the readouts of the master bias, master dark, master flat, and science frames (B_p, D_p, F_p, and s_p, respectively; here p counts over all pixels of all exposures, possibly taken at different epochs) and by its wavelength and size (λ_p and $\Delta\lambda_p$, respectively), as determined by wavelength calibration (the simultaneous wavelength reference provided by the LFC can be seen in each orders of the science frame echellogram as an array of dots). The reduction procedure computes the flux density I_p for all the original pixels in a reversible way: the result is a combined spectrum which retains the whole information content of the original exposures. The analysis procedure may mix the contributions from different pixels (e.g. to produce a coadded spectrum rebinned into a wavelength grid of choice), but the combined spectrum is passed along throughout the chain and is used whenever the original information is required. In the lower left panel, a processed quasar spectrum is shown. The black and red lines are the flux density and its variance, rebinned to a fixed-velocity step of 1.6 km s^{-1}, while the blue curve is the estimated level of continuum emission, validated on the combined spectrum (results obtained by the data analysis software for ESPRESSO[10] on test UVES data).

different for different exposures. The map in Eq. (1) does not introduce any correlation other than the correlation already present among the detector readouts, due both to the instrumental point spread function (which blurs the incoming signal at a scale much larger than the pixel size) and to possible defects of the detector (such as blooming). If the errors on pixel readouts are reliable, then the propagated variance of I_p, $\sigma^2(I_p)$, can be safely used for statistical purposes (e.g. to estimate the goodness of fit of a given model).

In practice, a general closed-form expression for $m_{i,p}$ can be very complicated. A rough formulation for the HIRES case, not including treatment of the detector bad pixels, can be put as follows:

$$m_{i,p}(s_p) := \left[\frac{s_p - B_{i,p} - D_{i,p}}{F_{i,p}/f_i(\lambda_p)} - b_i(\lambda_p)\right] \frac{G}{A\Delta\lambda_p T_i \eta(\lambda_p) r(\lambda_p)}, \tag{2}$$

where

- $B_{i,p}$, $D_{i,p}$, and $F_{i,p}$ are pixel readouts from an average bias image, a bias-subtracted dark image, and a bias- and dark-subtracted flat image associated with the exposure i, expressed in ADU; the dark image must be taken with the same integration time of the exposure i);
- f_i is a model for a flat image (not taking into account pixel-to-pixel variations in the detector response), while b_i is a model of the background (including sky emission and scattered light); both models should be computed from calibrations associated to the exposure i and expressed in ADU;.
- G is the detector gain (in e ADU^{-1}), A is the collecting area of the telescope (in m^{-2}), $\Delta\lambda_p$ is the pixel size (in nm), and T_i is the integration time of exposure i;
- η and r are the overall efficiency of the system (telescope and instrument together) and the flux response curve of the instrument (in e m^{2}J^{-1});

With these definitions, the dimensionless variance on the photon counts that can be inferred from s_p is

$$\sigma^2 := \left(s_p - B_{i,p} - D_{i,p} + R^2\right) G = \left[A\Delta\lambda_p T_i \eta(\lambda_p) r(\lambda_p) m_{i,p}(s_p) + b_i(\lambda_p) G\right] F_{i,p}/f_i(\lambda_p) + R^2 G \tag{3}$$

with R the detector readout noise. $\sigma^2(I_p)$ can be computed from σ^2 by standard error propagation, using Eqs. (2) and (3). The described approach is reversible as it does not disruptively mix readouts from different pixels. We can abstract the information associated to a given pixel as a tuple $P := (s_p, \lambda_p, \Delta\lambda_p, B_p, D_p, F_p)$[†] which is propagated as a whole through the data treatment chain and can be used to reconstruct at any time the spectrum S, provided the system parameters and the functions η, r, d_i, f_i, and b_i are known. A more complete formalization includes the variances of the different quantities as elements of the tuple.

Pixel conservation needs to be broken in many circumstances, both in reduction (e.g. to compute the functions d_i, f_i, and b_i, which require a smoothing of the detector readouts over several pixels) and in analysis (e.g. to model the spectral continuum as a B-spline on a number of knots extracted from the original flux spectrum). If the computed quantities are to be propagated along the chain, it is important to sample them back to the original grid of pixels, and to add them to the pixel information tuple (together with their variance). A rebinned spectrum S' should never be substituted from its non-rebinned counterpart S, to avoid an irrecoverable loss of information. Even when multiple spectra with the same pixel grid are weighted-average into a single spectrum, the operation generally disrupts the error statistics.[10] This justifies the approach to coaddition described in Sec. 2.2. An overall depiction of the pixel conservation through the DRS and DAS is given in Fig. 4.

4. CONCLUSION

The software tools for data reduction and analysis envisioned as a part of the Data Flow System for HIRES build on the expertise gained with HARPS-N and ESPRESSO, and aim to formalize a novel approach to data treatment in which the original information from the detector pixels is conserved throughout the processing

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[†] The i subscripts have been dropped for clarity, given that p already counts over all exposures.

chain. This is the only approach that guarantees a correct treatment of the errors in the analysis, and is strongly called for by the extremely demanding science cases envisioned for the instrument.

The relevance of such approach motivates its extension beyond the immediate scope of the instruments. ESO has recently developed a High-level Data Reduction Library[22] (HDRL), which provides advanced standardized solutions to data reduction operations, and would be a preferred framework to generalize the algorithms envisioned for HIRES. The HDRL would be naturally complemented by a High-level Data Analysis Library (HDAL) based on the tools developed for ESPRESSO and proposed for HIRES. A possibility to be studied within the context of the HIRES DRS and DAS development is to adapt both the HDRL and HDAL to the cloud computing paradigm, enforcing a Software-as-a-Service model (SaaS) which would ease code maintenance by effectively eliminating portability issues. Another possibility favored by the non-linear structure of the HIRES DAS is to make it available through a Science Gateway, with the additional possibility of customizing the analysis chain to cope with different science cases. The demand for validated analysis software in the emerging era of precision spectroscopy strongly pushes the conception of data treatment software in this direction.

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