

Quality Control of VLT-UVES data

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ABSTRACT

UVES is the UV-Visual high-resolution echelle spectrograph mounted at the 8.2m Kueyen (UT2) telescope of the ESO Very Large Telescope. Its data products are pipeline-processed and quality checked by the Data Flow Operations Group (often known as QC Garching). Calibration data are processed to create calibration products and to extract Quality Control (QC) parameters. These parameters provide instrument health checks and monitor instrument performance. Typical UVES QC parameters are: bias level, read-out-noise, dark current of the three CCD detectors used in the instrument, *rms* of dispersion, resolving power, CCD pixel-to-pixel gain structure, instrument efficiency. The measured data are fed into a database, compared to earlier data, trended over time and published on the web (http://www.eso.org/qc/index_uves.html). The QC system has evolved with time and proven to be extremely useful. Some examples are given which highlight the impact of careful QC on instrument performance.

Keywords: Quality control, UVES, trend analysis, data reduction pipelines, instrument performance

1 THE VLT ECHELLE SPECTROGRAPH UVES

UVES, the ESO UV-Visual Echelle Spectrograph, is attached to the Nasmyth B focus of the 8.2m UT2/Kueyen telescope which is part of the Very Large Telescope (VLT) of the European Southern Observatory (ESO) situated on Cerro Paranal. It is operational since April 1, 2000. It is extensively described by Dekker et al. (2000).

UVES is a two-arm (UV-visual and visual-nearIR) echelle spectrograph with optical components optimized for the respective wavelength range. The UVES echelle gratings provide a resolving power of up to $R = 80,000$ in the blue, and $R = 110,000$ in the red arm. The telescope beam can be split with dichroic mirrors so that both arms can collect light simultaneously. The blue arm has an EEV 2Kx4K CCD windowed to 2Kx3K; the red arm comes with an array of 2 CCDs (one EEV, and one MIT-LL optimized for near-IR use, with 2Kx4K pixels each). The dichroic modes are used frequently. Then a single exposure (sky or calibration) produces 22 million pixels.

The image of a star on the slit can be split using the image slicer (Dekker et al. 2002). For highest radial velocity precision, UVES has also a mode with an iodine absorption cell in the beam.

UVES will soon become part of the larger FLAMES multiobject spectral facility which provides a fiber connection from the fiber positioner OzPoz to UVES. In this fiber mode, UVES can observe up to 8 objects simultaneously in the red arm.

Like the other VLT instruments, UVES is operated in two ways, namely in Visitor Mode (VM) which is the traditional observing mode with the astronomer on site, and in Service Mode (SM) where observations are executed by the local staff whenever local conditions match the user specifications. Service Mode observations currently account for about half of all UVES science observations. An important difference between SM and VM is that SM programmes have only standard instrument setups. The reward for this restriction are quality-checked master calibration data and pipeline-reduced science data which are delivered at the end of the programme run.

Initially UVES shared the available time at Kueyen with FORS2. Since July 2001, when FORS2 was moved, it is the only instrument at that telescope. In Period 68 (October 2001 - March 2002), it has produced a total of about 35,000 frames, 16,800 of which (48 %) are calibration frames, and 8500 (24 %) are science frames (the rest is acquisition and test data). This amounts to roughly 500 GB of raw data.

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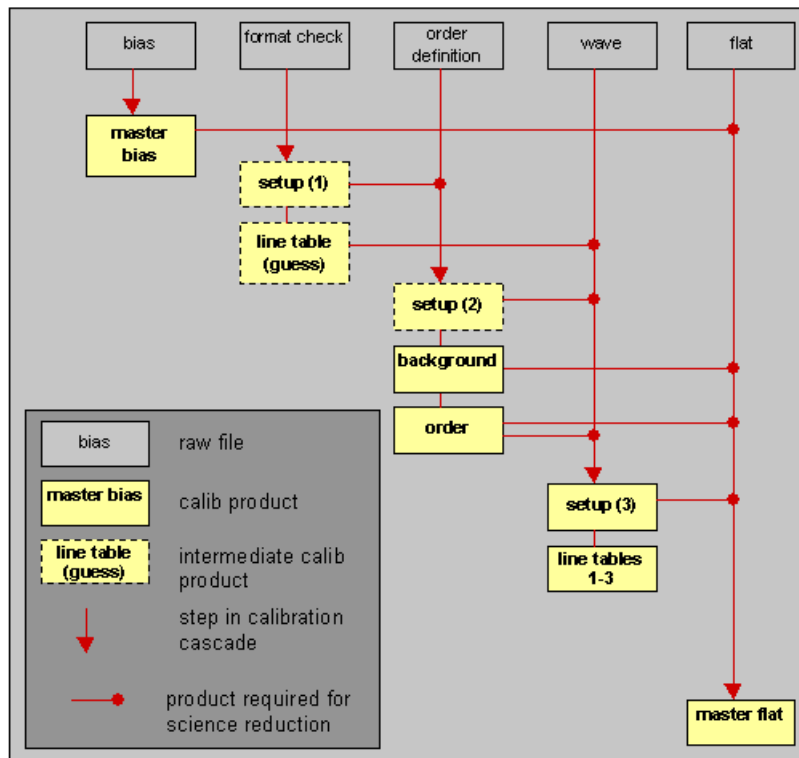


Figure 1. The UVES calibration cascade. Raw frames (grey) are processed into calibration products (bold) which may afterwards be recycled into updated versions or be re-used for other calibration products. All bold solid boxes represent a calibration product which is needed for science reduction. Find more details under http://www.eso.org/qc/UVES/pipeline/cal_scheme.html

2 UVES PIPELINE

As for the data from all VLT instruments, the UVES calibration and science data are processed by a pipeline. The UVES pipeline is MIDAS-based (Ballester et al. 2000) and comes in three instances:

- quick-look: available on the mountain
- off-line: run by the Data Flow Operations Group at Garching headquarters
- home: exported to users.

The pipelines are identical in all cases, the difference comes from operations. On the mountain, data are processed in real-time, using standard calibration solutions. The goal is to provide quality checks, and to provide a quick-look impression of the data. The Data Flow Operations Group (DFO) at Garching headquarters uses the pipeline off-line, to process all calibration data taken in standard modes (see Hanuschik et al. 2002) into master calibration data. These are quality-checked and archived. These solutions are used to reduce the SM science data. The quality of the pipeline products is almost science grade².

To process a complete set of calibrations, the UVES pipeline first makes a comparison between technical calibrations (FORMATCHECK and ORDER-DEFINITION frames) and the UVES physical model. This gives a first-guess solution about the spectral format in X and Y direction. The final dispersion solution is achieved with the WAVE arc lamp calibration frame. Detector signatures are removed using the master BIAS frame. The pixel-to-pixel response, as well as fringing (in the red), slit function and blaze function, is removed using master FLAT frames. Instrument response is recorded with a flux STANDARD star frame.

² For a more detailed overview of the UVES pipeline and its recipes, check out <http://www.eso.org/qc/UVES/pipeline/>.

These calibrations have to be processed in the proper order in order to give the best possible results. This order defines the UVES *calibration cascade* (see Figure 1). For a specific instrument setting, there are 13 calibration files (biases and flats come as sets of 5 raw frames, the others as single frames).

3 QUALITY CONTROL AND TRENDING

The proper association and the proper processing sequence of calibration data are already aspects of Quality Control. Association of outdated frames (spanning time intervals too long to be likely stable) would significantly reduce the quality of the products since they don't properly describe the instrument signature.

In a more general sense, Quality Control (QC) deals with

- the quality of the raw data,
- the quality of the products and of the product creation process,
- the performance of the instrument component involved.

Fundamental for UVES Quality Control is the use of the pipeline. The UVES pipeline has built-in QC procedures which allow to derive condensed QC information, the so-called QC1 parameters. These are stored in the FITS headers of the product files (and in a log file) and extracted into a database. Other such parameters have been implemented in post-pipeline procedures.

This set of parameters provides in-depth, up-to-date and continuous knowledge about the instrument status. The investigation of this set of parameters, plotted e.g. over time, is the **trending**. Trending exhibits long-term behaviour features such as aging and stability of instrument components. Equally important are short-term sudden changes indicative of problems.

The implementation of the UVES QC process follows the general guidelines presented elsewhere (Hanuschik et al. 2002). Table 1 shows the Quality Control items and instrument components presently monitored.

Table 1. UVES Quality Control items

Component	Item
detector	bias level, read noise, dark current; fringing; linearity
gratings	stability of spectral format; resolving power, precision of dispersion solution
slit	slit noise
lamps, filters	FF lamp stability, filter throughput
all components	efficiency

4 UVES TRENDING RESULTS

4.1 QC web interface

As part of the QC service provided by the Data Flow Operations Group in Garching, there is extensive web documentation about Quality Control, pipeline usage and Service Mode data. It is accessible under <http://www.eso.org/qc/>. The UVES QC information (parameters, plots, documentation) can be retrieved from <http://www.eso.org/qc/UVES/qc/qc1.html>. Most of the results described in the following sections can be found under that URL in more detail.

4.2 Detector characteristics: Bias, Dark

From the beginning, all existing BIAS frames, and the deep DARK exposures, from all three detectors have been evaluated for the most fundamental detector properties:

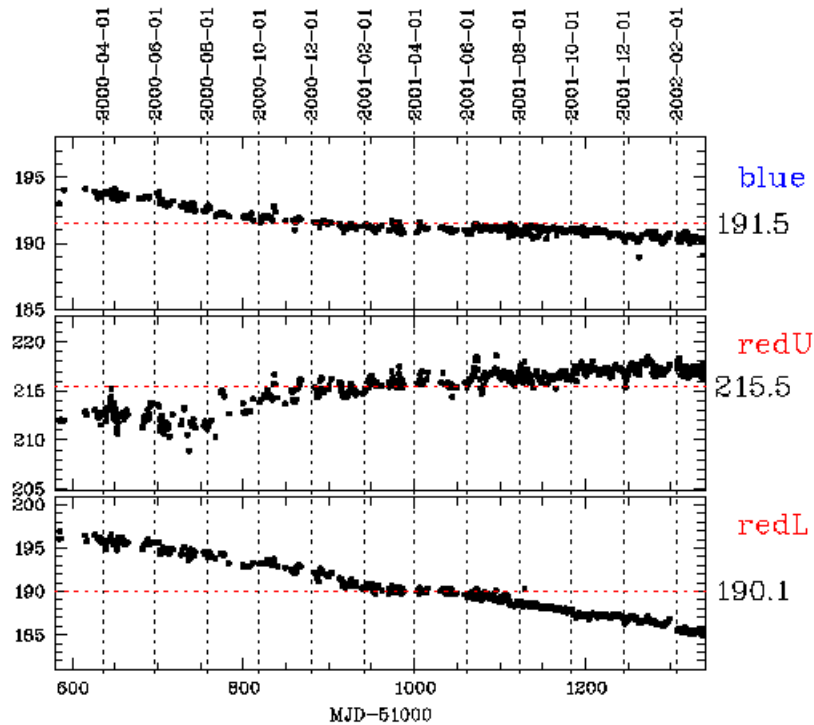


Figure 2. The first two years of UVES bias values. The mean bias value for each of the three CCDs is plotted for the range 2000-02 up to 2002-02 (unbinned values only). The short-term scatter for the red upper CCD is due to variations in the ambient temperature of the CCD electronics which is unregulated. The long-term trends are aging effects. "redU" means "red upper CCD" (MIT-LL); "redL" = red lower = EEV.

- average bias level
- read noise (raw and master)
- structure
- dark current.

The monitoring of these parameters checks the health of the detectors. They are described under "bias" and "dark current" of the UVES QC link <http://www.eso.org/qc/UVES/qc/qc1.html>.

The mean bias level is very stable for the blue and the red EEV CCDs ("redL" stands for "red lower") while it is modulated by the ambient, unregulated temperature in case of the red MIT-LL CCD ("redU" for "red upper"). The long-term trend shows a change rate of about 1-2 ADU per 100 days. Figure 2 shows these trends over the past 2 years.

The read noise is monitored in the master bias frames. It checks the overall stability of the CCDs, as well as the proper working of the master creation process. Master bias frames are stacks from typically five input frames. Stacking should reduce the read noise of a raw frame by a factor of about $\sqrt{5}$. This is routinely checked. Figure 3 shows that the RON indeed has been very stable over two years.

4.3 Wavelength calibration

Each arc lamp exposure is used by the pipeline to measure QC parameters from the arc lamp emission lines. The most important QC1 parameters are:

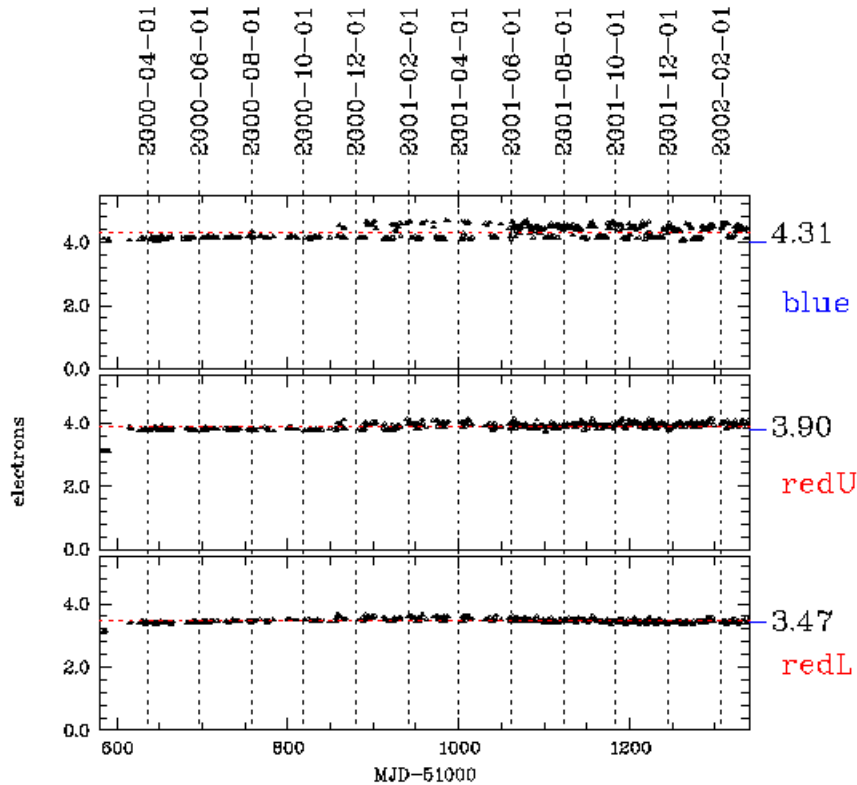


Figure 3. Read noise (in electrons) of the three CCDs, same range in time as Figure 2. The measured RON values for the blue CCD scatter due to some imperfection of the measuring algorithm. The RON values are remarkably stable over two years and are very close to the laboratory values (indicated by a short bar close to the mean values). "redU" is the MIT-LL CCD, "redL" the EEV. All values are for readout speed 225 kpixels/sec.

- resolving power $R = \lambda/\Delta\lambda$, and
- standard deviation of the dispersion solution, σ .

Others are e.g. minimum and maximum wavelength, and the number of lines selected, N_{sel} . They are described under "resolution" and "dispersion" of the UVES QC link <http://www.eso.org/qc/UVES/qc/qc1.html>.

Resolving power R is evaluated as median over a Gaussian fit to all selected lines. Typically 300-1000 lines are selected per CCD. This parameter is compared to model predictions based on commissioning data, to ensure that actual values can always be assessed in the context of nominal performance. Figure 4 shows the record of daily health check measurements which check for the stability of the highest possible resolving power (about 92,000 in the blue; 115,000 and 94,000 in the red, values referring to the EEV and MIT-LL CCD, resp., at 2 px sampling). Any problem with the proper focussing or alignment of the camera e.g. due to earthquakes would show up here.

The proper slope of resolving power with increasing slit width, as compared to laboratory data, is also monitored in Figure 4 (right). Here *all* available wavelength calibration data are used.

Dispersion solution. The quality of the dispersion solution is measured by the standard deviation of the difference between the found and the fitted position. Figure 5 shows the typical performance for the daily health check calibrations which are taken at highest useful (2 px sampling) resolution. The *rms* scatter for these data is about 2-4 mÅ. The slope of this parameter with slit width is linear for the most widely used slit widths (less than 2 arcs, rightmost part of Figure 5).

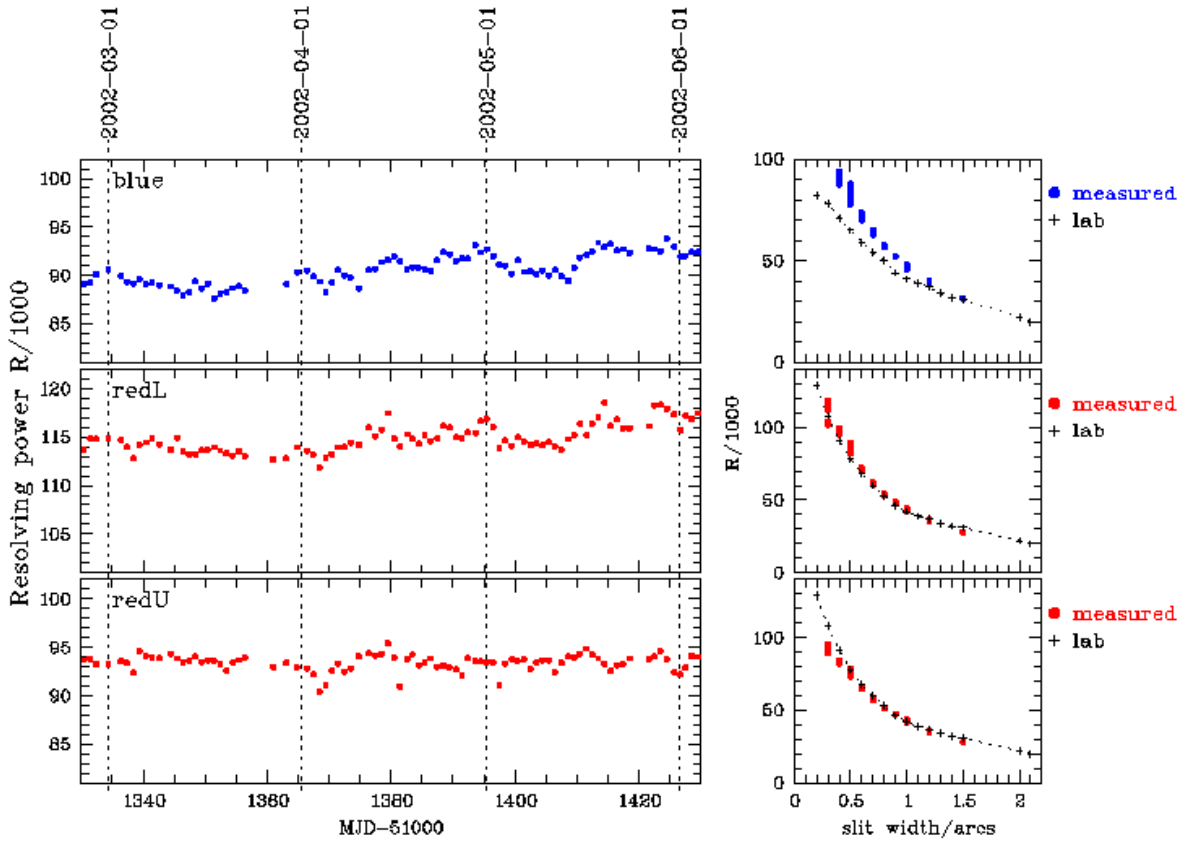


Figure 4. Resolution trending. **Left:** Trending plot for the two daily resolution checks, which monitor the blue and the red camera. These data are taken with the slit set to 0.4 (blue camera) and 0.3 arcs (red), respectively, which corresponds to highest possible resolving power at 2 px sampling. "redU" is the MIT-LL CCD, "redL" the EEV. **Right:** Complete resolution checks. All available resolving power data, including those from the left figure, are plotted over slit width. These diagrams check for the proper performance of the UVES resolution for the slit widths used for science spectra. The data are compared to model predictions based on commissioning data.

4.4 Spectral format

Differential shifts of the spectral format can be caused by thermal and pressure drifts, and by sudden non-thermal effects like earthquakes. By design, UVES is not pressurized or temperature-stabilized. Shifts in cross-dispersion (Y) direction mainly affect the UVES pipeline since the proper shift has to be found automatically. Technical calibrations (format check and order definition frames) are used by the pipeline to adjust an initial guess of the spectral format, based on the physical model (see Figure 1). The final determination of the spectral format is based on the wavelength calibration frames. The grating positions are monitored under "grating shifts" of the UVES QC link.

Since the temperature slope of the grating shifts is linear and can be measured easily, a compensation for the thermal drifts has been implemented in the instrumental software. Figure 6 shows a comparison between grating positions before (left) and after (right) this compensation has been established. Data are shown for two of the four gratings. This figure also shows the impact of a major earthquake which occurred on May 12, 2000. It gave the blue gratings a bounce shifting the spectral format by more than 10 pixels. Meanwhile health check calibrations for the spectral format are measured daily in order to allow maintenance staff to react quickly.

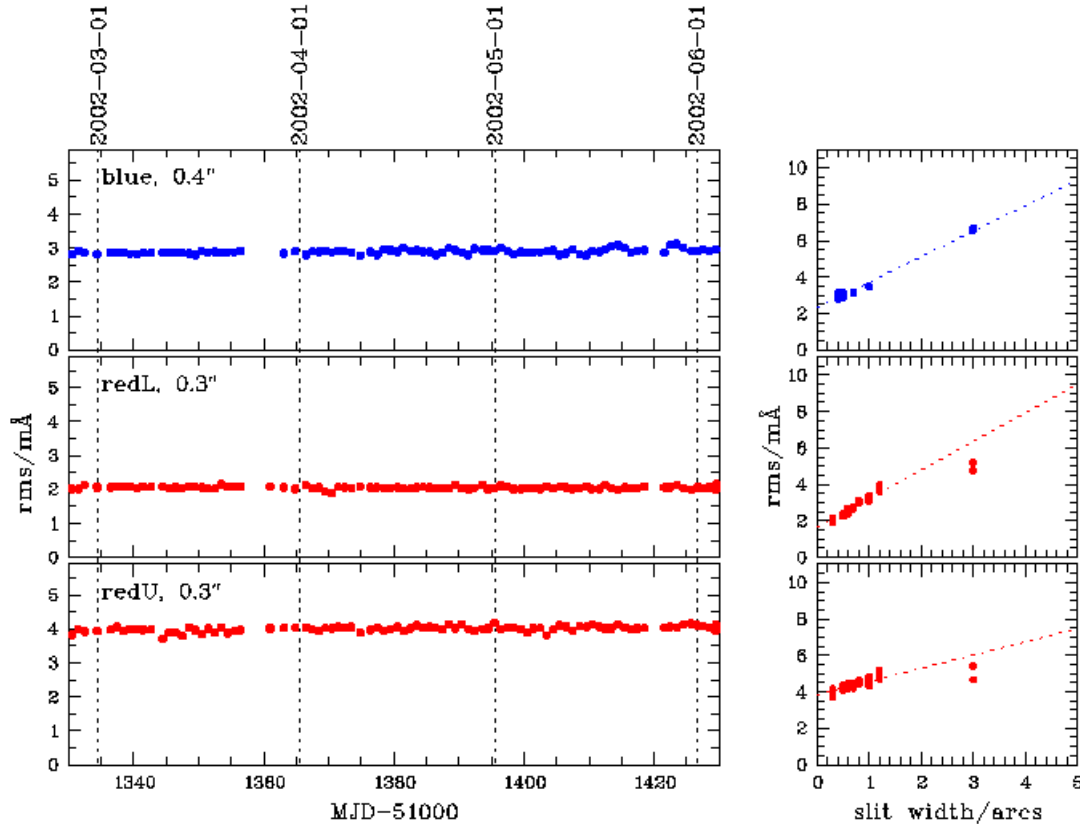


Figure 5. Dispersion solution. Shown is the residual *rms* (fitted minus measured positions) of all identified arc lamp emission lines. **Left:** Daily health checks, measured for all three CCDs (blue: setting 437 nm at 0.4 arcs slit width; red: setting 580 nm at 0.3 arcs slit width). Typical rms values for the dispersion solution are 2-4 mÅ. "redU" is the MIT-LL CCD, "redL" the EEV. **Right:** All rms values plotted vs. slit width. The most frequently used slits below 2 arcs follow a linear law. All data are unbinned.

4.5 Flat fielding

Lamp-illuminated flat field frames are exposed regularly. They are used to measure the QC parameters fixed-pattern noise, slit function, and lamp efficiency. More details are described under "FF structure" of the UVES QC link <http://www.eso.org/qc/UVES/qc/qc1.html>.

Small-scale structure. The small-scale structure of the flat field exposures is relevant for the signal-to-noise characteristics of the extracted science spectra. The pixel-to-pixel gain variations (so-called fixed-pattern noise) are registered by the flat field so that they cancel out on the flattened science data. The price to pay is some residual photon noise in the master flats. To monitor these two components of small-scale structure and distinguish them, the following strategy is applied:

Master flats are typically created from stacks of five input raw frames. A difference frame, $diff_{21}$, is created from two such raw frames which are identical apart from statistical noise. The *rms* in a small subwindow (typically 100x100 px²) of the difference frame measures the photon noise of a raw frame, σ_{ph} :

$$\sigma_{21} = \sigma_{ph} * \sqrt{2} .$$

In a second step, a single raw frame is copied. It is shifted by 1 pixel in dispersion direction, and subtracted from itself. In this derivative frame, the *rms* in a small subwindow is

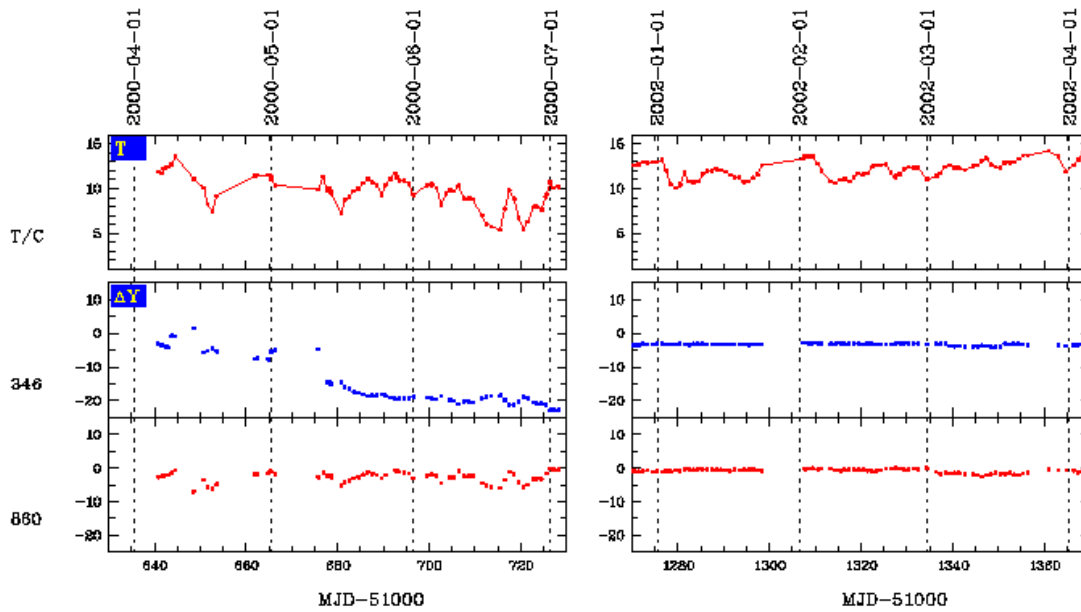


Figure 6. Daily health checks for the grating positions. Two extracts from the health check data stream are shown here, both with the grating temperature plotted on top of the Y position of the blue grating #2 and the red grating #4. **Left:** Data from 2000-4...2000-07. No temperature compensation was available, and a major earthquake in May gave the blue grating table a bounce by -10 px which was detected on the trending plot. **Right:** In 2002, the gratings have their Y (and also X) position thermally controlled and show a very smooth trend.

$$\sigma_{\text{deriv}} = \sqrt{2} * \sqrt{\sigma_{\text{ph}}^2 + \sigma_{\text{fp}}^2},$$

where σ_{fp} is the fixed-pattern fluctuation which is by definition a fixed property per pixel, but is now randomized by the shift. Photon noise and fixed-pattern structure can then be derived by combining both equations.³ An additional noise source is read noise which can be neglected in this context.

The ideal flat field would have $\sigma_{\text{ph}} \ll \sigma_{\text{fp}}$ everywhere. By creating master flat frames (which have, with 5 input frames, their photon noise reduced by $\sqrt{5}$), this condition can be met for a large part of the frame. Therefore the quality of the flat field frames can be monitored by trending the two noise parameters. Flat frames in the photon-noise regime should obviously not be used for science reduction, at least not if S/N is critical.

Figure 7 shows the trending of the measured sigma values vs. exposure level. Broken lines indicate the expected scaling laws which are linear in case of fixed-pattern noise, and square-root for random photon noise. The measured numbers nicely follow these scaling laws⁴.

The right-hand part of Figure 7 shows a sketch of the scaling laws, including the read-noise component which is otherwise neglected here. The turnover from photon noise (3) into the fixed-pattern domain (4) is around 1600 ADU for all three UVES CCDs. This means all pixels with flux larger than about that value are in the fixed-pattern domain. The amplitude of the fixed-pattern structure is about 0.7% (rms) for all three CCDs.

³ The reason for taking small subwindows is to avoid any residual large-scale gradient in both the derivative and the difference frames.

⁴ Since usually exposure times for the flat field exposures are fixed, the curves are not continuously populated. Broader coverage is mainly caused by lamp aging. Clustering is caused by certain standard setups (e.g. the bluest setup with 346 nm central wavelength causes the group around 4000 ADU in the uppermost box).

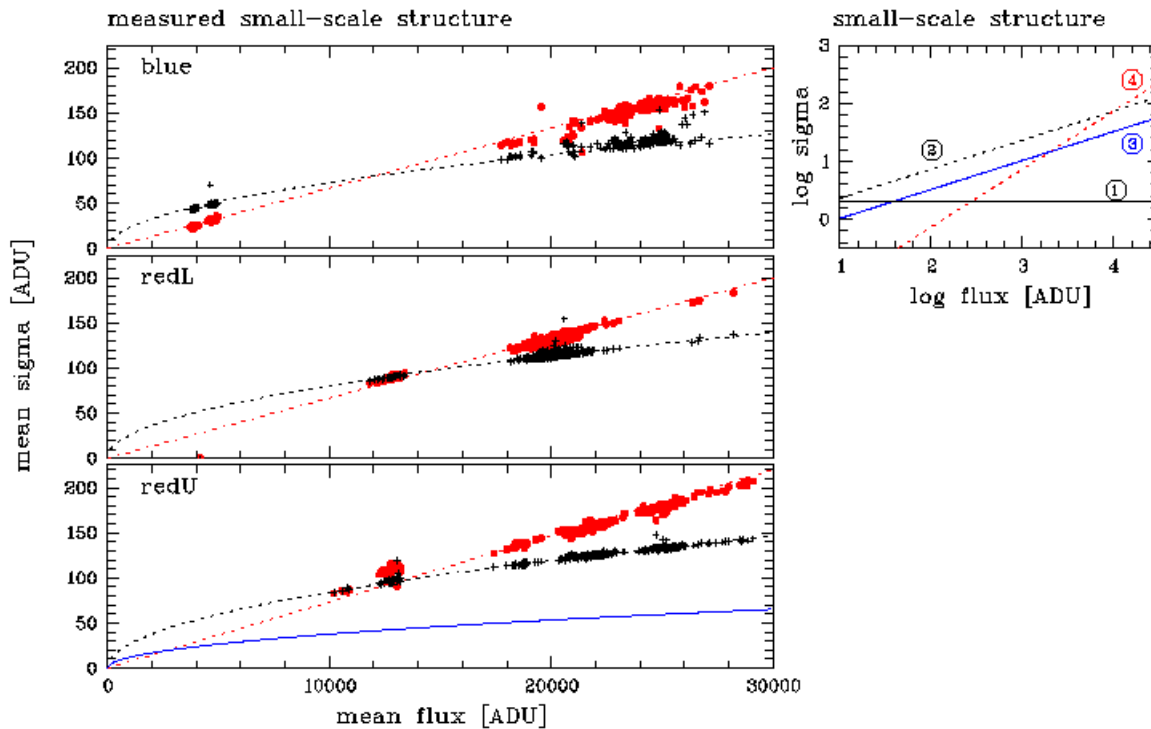


Figure 7. Trending of small-scale properties of UVES flats. **Left:** the two main components (photon noise and fixed-pattern structure) are plotted vs. the mean flux level measured in master flats, for all three CCDs ("redU" is the MIT-LL CCD, "redL" the EEV). These parameters follow a square-root law (statistical shot noise) and a linear law, resp. These laws, scaled to the observed sigma values, are plotted as broken lines. The solid line is the residual photon noise for a master flat. **Right:** Schematic sketch of the scaling laws in a log-log diagram; 1 - read noise; 2 - photon noise (single raw frame); 3 - photon noise (master flat); 4 - fixed-pattern structure.

Fringing. The extreme red setting (central wavelength 860 nm) has additional structure on a larger spatial scale and is therefore not included in Figure 7. This component is due to two effects: CCD surface structure (especially strong in the red lower CCD), and fringing. The surface structure has fixed-pattern properties, i.e. is stable with time. There are also strong fringes showing up which again are stable, at least relative to the spectral format.

4.6 Efficiency measurements

The overall efficiency of UVES is measured routinely from both flat field data and standard star measurements. These calibrations cover different aspects of instrument efficiency. The lamp data can be obtained anytime during daytime, but are affected by intrinsic instability of the light source. They are used primarily to detect sudden problems with filter vignetting etc. The standard star data can be obtained in a limited time window only, and suffer from instabilities of the atmospheric conditions. They are primarily useful for long-term performance monitoring and spectral efficiency curves.

Flat field lamps. From the daily stream of flat field calibrations, efficiency data for frequently used setups are monitored. Main QC item is the exposure level as function of time. Soon after being established, this trending feature helped to detect a significant degrading of the flat field exposure levels in July 2001 (Figure 8). Visual inspection of the blue order separation filter (CuSO₄, a hygroscopic crystal) proved its degrading due to humidity. It has been replaced in November 2001, with a significant increase in blue efficiency.

Standard stars. Flux standard stars are measured in evening and morning twilight whenever possible. They are processed by the pipeline to monitor the efficiency of the entire system [telescope + instrument + detector] (Figure 9). The scatter around the mean values is partly due to variations in night quality. The trending is extremely useful to get indications about problems with the instrument efficiency.

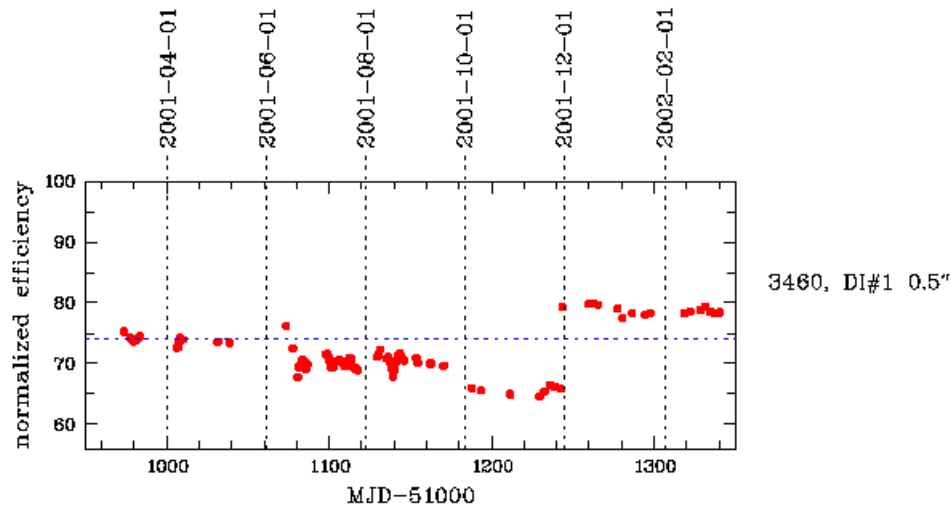


Figure 8. Filter degradation, detected by trending. The record of mean flat-field exposure levels shows a degrading in efficiency around July 2001 for the blue settings. One of them (central wavelength 346 nm, dichroic #1, 0.5" slit width) is shown here. The broken line marks the reference level for trending. The filter replacement took place by the end of November 2001.

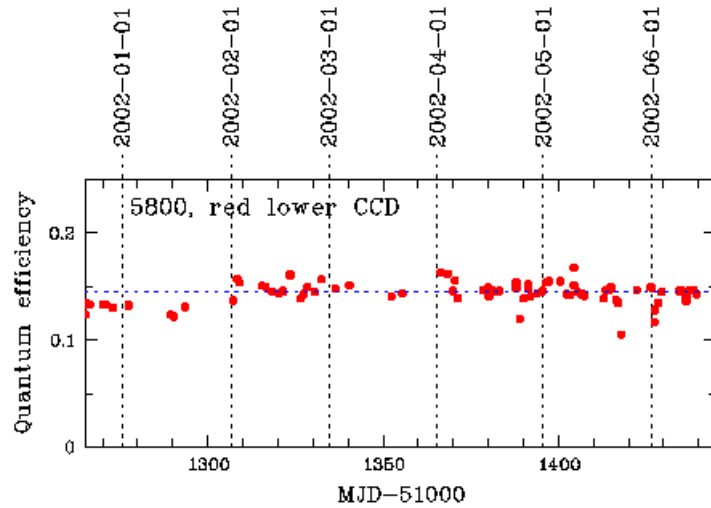


Figure 9. Trending of system efficiency. We show data for a selected setting (580 nm central wavelength, red lower CCD = MIT-LL). This trending plot is used to watch the health of the system telescope + instrument + detector. The increase in efficiency in February 2002 has been caused by the recoating of the UT2 primary mirror.

The data points are collected at the blaze wavelength of each echelle order by the pipeline. If one carefully selects the high-quality data (from nights known from other instruments to be photometric, from pointings at low airmass etc.), this yields the chromatic efficiency curve shown in Figure 10. This curve is derived and checked regularly. A description can be found under "efficiency" of the UVES QC link (www.eso.org/qc/UVES/qc/qc1.html).

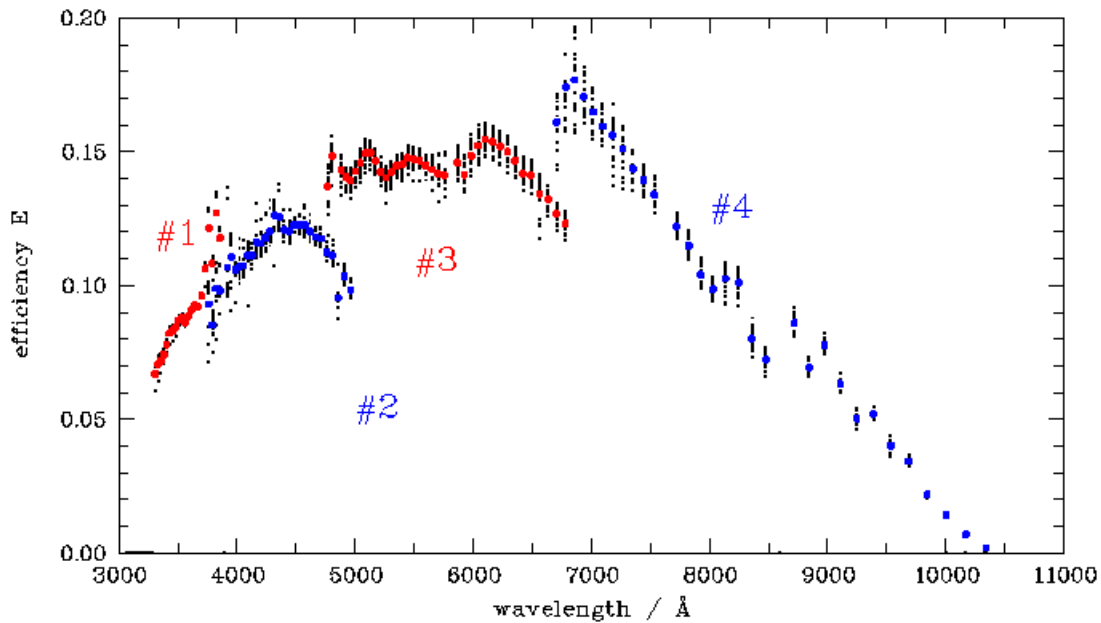


Figure 10. Chromatic system efficiency curve of UVES. The efficiency values at the blaze wavelengths of each echelle order have been collected to construct this curve. Dots mark single data points, filled circles mark averaged numbers. Data were obtained for each of the four crossdisperser gratings (#1...#4).

5 SOME SPECIAL SERVICES

5.1 Solar atlas

In any UVES exposure of sufficiently long integration time, the atmospheric air glow imprints a spectrum in addition to the scientific target. This spectrum is the combination of airglow emission lines, telluric absorption lines and the solar spectrum due to scattered moonlight.

In order to monitor the solar contribution, a high-resolution atlas of the solar spectrum has been created⁵, from observations of the Moon illuminating the slit. Its main purpose is to provide a high-resolution, high S/N template for solar absorption lines, useful e.g. for data reduction. Its resolution is about 85,000 in the blue, and 100-115,000 in the red. It ranges from 3100 to 10,200 Å.

5.2 Atlas of sky emission lines

Another project combines more than 10 hours of exposure time per wavelength region to derive a high-resolution atlas of sky emission (and absorption) lines⁶. These data have been obtained under dark conditions around new moon. The primary purpose is to provide line identifications and positions for checks of the stability of the wavelength scale. Furthermore, the sky spectra may be useful as templates for reducing spectra from extended objects. The faint airglow emission lines in the blue range have not yet been extensively monitored at all, in contrast to the much stronger sky emission lines in the red. The airglow lines may be useful for non-astronomical purposes as well, for instance in aeronomy.

⁵ http://www.eso.org/qc/UVES/pipeline/solar_spectrum.html

⁶ to be published soon

6 SUMMARY AND PROSPECTS

It has been demonstrated that the UVES QC process has been tremendously useful for controlling the status of the instrument, to improve its performance and to assess and guarantee its data quality. Being a built-in part of the pipeline from the beginning of operations, the QC process has continuously evolved over the past 2 years and has become an integral part of science operations on Paranal and of data flow operations in Garching. The processed QC information is used by the VLT staff to quickly react to instrumental problems. It is also made available to the end user through the Service Mode packages, and to the community through the web pages. These feedback loops are essential to grow confidence within the community in the UVES data quality. The QC process, as a central memory of the instrument status, will deliver invaluable information for reprocessing scientific and calibration data from the Science Archive in the framework of the Astrophysical Virtual Observatory.

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