Recent developments in the optimal extraction of UVES spectra

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UVES

Instrument

- The VLT-UT2 UV-Visual Echelle Spectrograph
- Operated by ESO Paranal Observatory in service and visitor mode since 2000-04-01

Pipeline

- Automatic reduction of UVES data at the telescope
- Generation of trending Quality Control parameters
- Master calibration and science data products
- User support for personalised data reduction

New algorithms

Methods

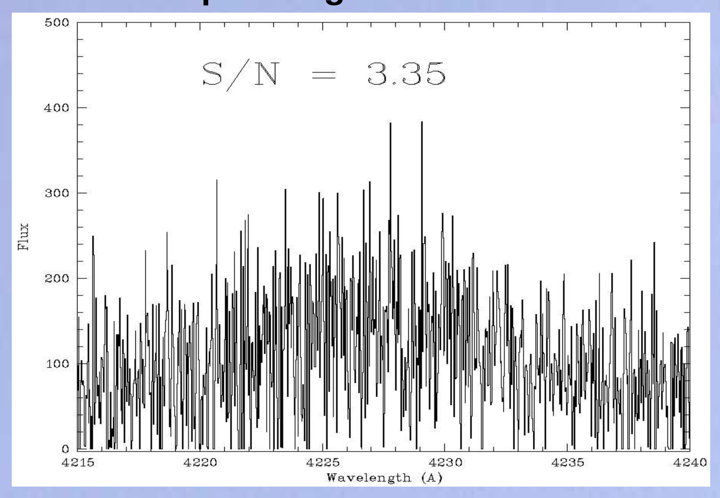
- Virtual resampling method described by Marsh and Mukai, generalized to multiple echelle orders
- Analytical methods for measuring the cross-order profile using Moffat or Gauss profiles, robust at low S/N
- New sky subtraction method
- Detection and handling of CCD cold pixels
- Implemented using ESO's Common Pipeline Library

Main results

- Elimination of ripple patterns at high S/N
- More robust against cosmic rays and generally at very low S/N

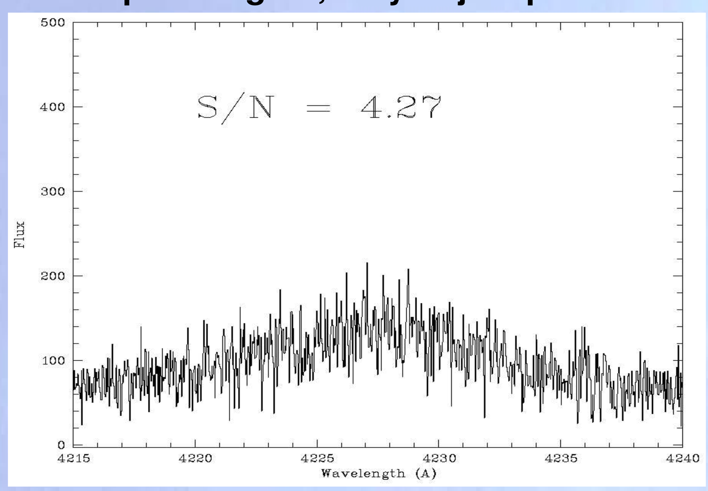
Why optimal extraction?

Equal weights extraction



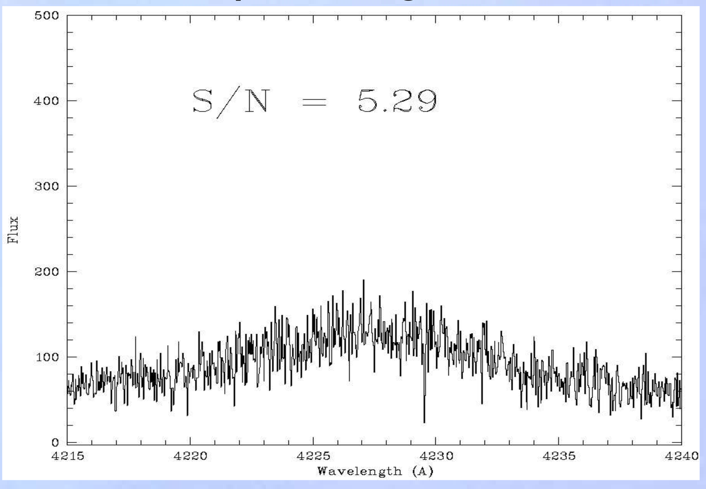
The straightforward way to extract the data is to sum all pixels along the slit, for each wavelength. Problem: Pixels near the slit edges contain little or no signal, but contribute with noise, leading to a noisy spectrum (simulated data).

Equal weights, only object pixels

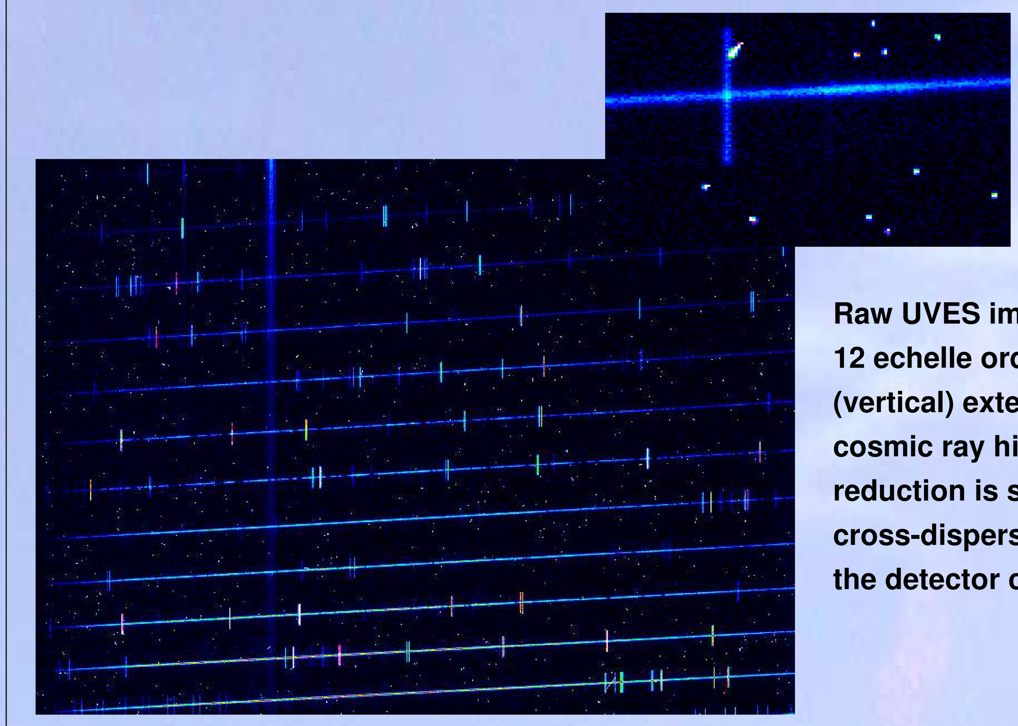


The spectrum signal-to-noise (S/N) may be improved by summing only the few (in this example 4) pixels at the slit center, which contain most of the object signal. Problem: The object flux outside the extraction window is lost.

Optimal weights



Horne showed that the optimal S/N is achieved using a weighted sum of all pixels, with weights proportional to p/V, where p is the relative illumination fraction (spatial profile), and V is the pixel flux variance.



Raw UVES image (and a zoom) showing 12 echelle orders, sky emission lines (vertical) extending over the entire slit and cosmic ray hits (white dots). The data reduction is simplified by the fact that the cross-dispersion direction is aligned with the detector columns (QSO-1101-264).

Optimal extraction

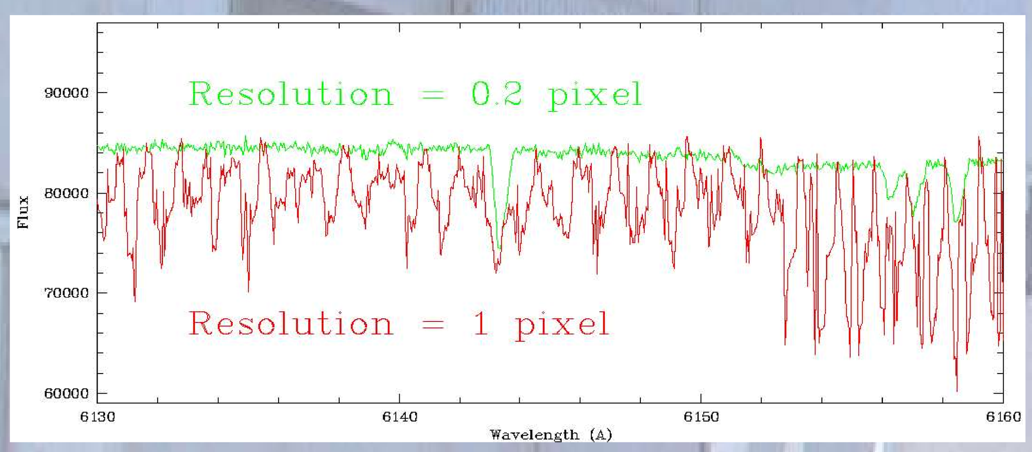
- is a minimum variance estimator of the flux at each wavelength,
- improves the extracted spectrum S/N in comparison with simpler methods (especially for faint sources), corresponding to an increase in effective exposure time,
- allows identifying cosmic ray hits as pixels which deviate significantly from the average spatial profile.
- But: requires measuring the object spatial profile, difficult for faint objects.

References

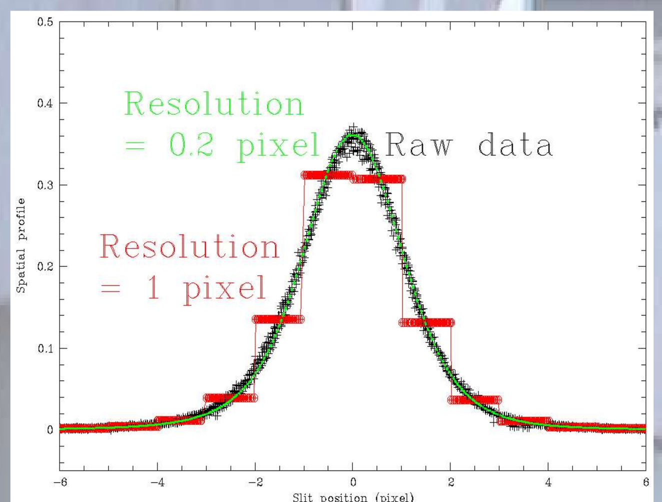
- Horne, K., 1986, An optimal extraction algorithm for CCD spectroscopy, PASP, 98:609-617
- Marsh, T.R., 1989, The extraction of highly distorted spectra, PASP, 101:1032-1037
- Mukai, K., 1990, Optimal extraction of cross-dispersed spectra, PASP, 102:183-189

Profile measurement at high S/N

At high S/N, the usage of a too crude low resolution model to measure the spatial profile introduces an error that depends on the position of the object with respect to the center of a pixel. This leads to characteristic quasiperiodic ripples in the extracted spectrum. The problem was solved by using a higher resolution model (see below).

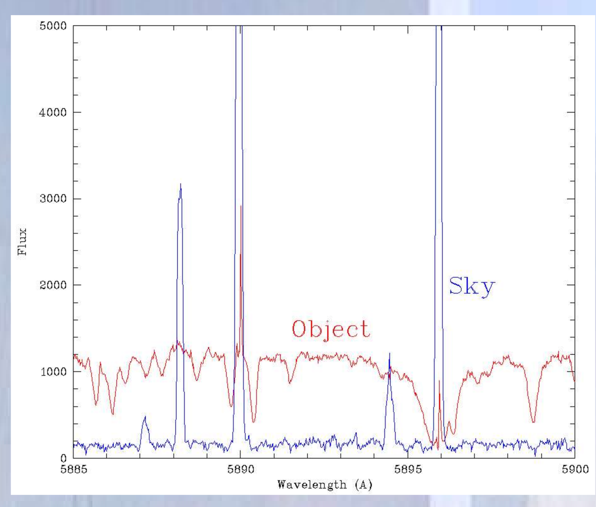


The empirical (raw) spatial profile, a high resolution (0.2 pixel) and a low resolution (1 pixel) model. Additionally, the high resolution model uses bilinear interpolation to evaluate the spatial profile.



Sky subtraction

The packages provides two sky subtraction methods.



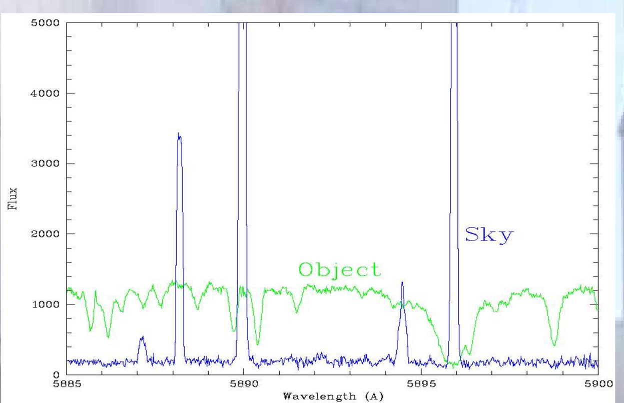
Strong sky emission lines are not fully subtracted, thereby leaving residuals in the object spectrum.

1. The sky level is determined by a two-parameter minimization of

$$\chi^2 = \sum_i \frac{\left(f_i - \left(S + F p_i\right)\right)^2}{V_i}$$

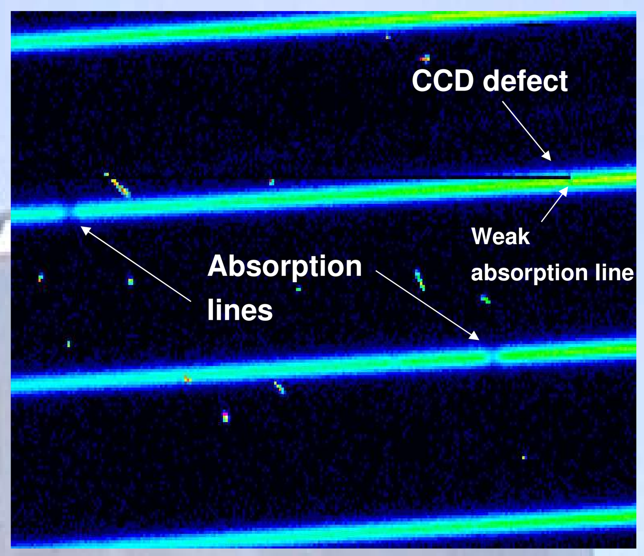
where (f_i, V_i, p_i) are the flux, variance and spatial profile at the i'th pixel, and (S, F) are the sky and flux levels of the current extraction bin. While theoretically this gives the combined optimal sky and object spectra, in pratice the object spectrum contains residuals from strong sky emmission lines (left).

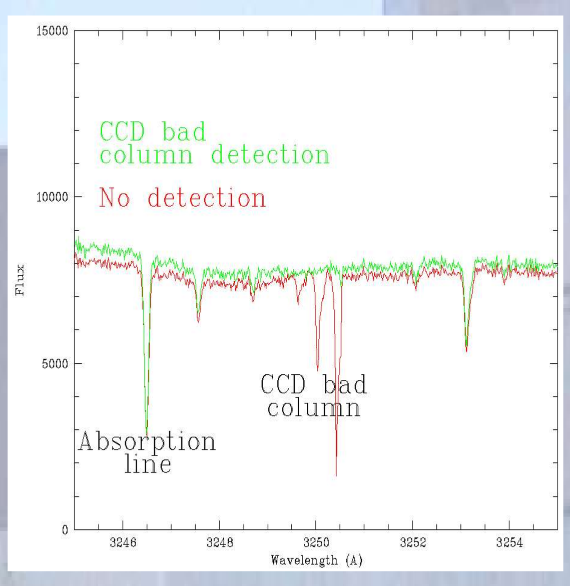
2. Alternatively, the sky can be determined as the median of all pixels along the slit after masking out the object. This gives a better sky estimation, thereby eliminating the residuals from the previous method (right).



CCD defects

Raw data showing a CCD trap column (black horizontal line, upper right) and absorption lines.



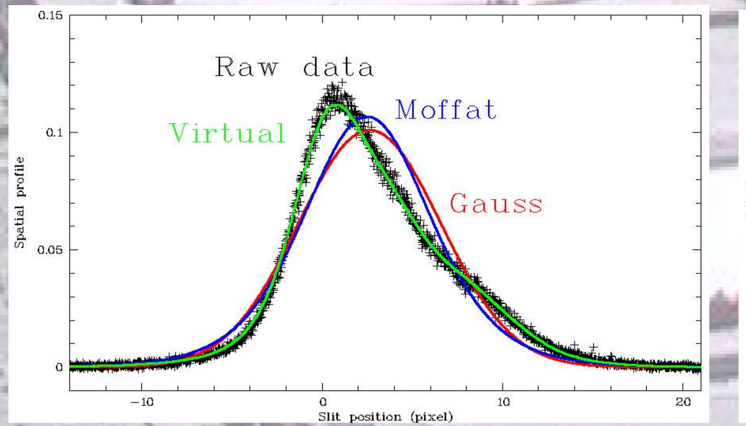


Extracted spectrum showing the effect of detecting and handling CCD defects. Kappa-sigma clipping is used to detect outlier pixels, which are then excluded from the optimal extraction. The three absorption features around 325 nm are due to the CCD defect and might be mistaken for real absorption lines, if not handled. Also note that the very weak absorption feature at the beginning of the CCD defect is recovered.

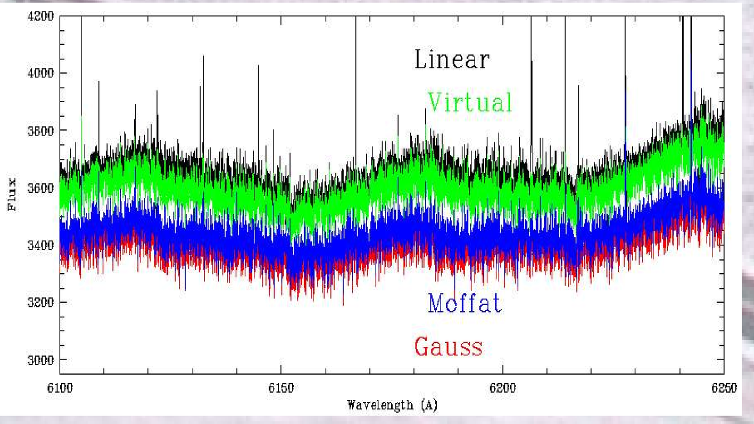
Cross-order profiles

For measuring the spatial profile, the package provides two analytical methods (using either a Moffat or Gauss profile), and the (non-analytical) virtual resampling method described by Marsh and Mukai.

At high S/N, the UVES asymmetric instrumental PSF makes the simpler analytical methods inappropriate (see below). At low S/N, however, the analytical methods are more robust due to the lower number of free parameters, and the raw cross-order profile does not show a clear asymmetry. The algorithm selects at runtime the appropriate profile measuring method based on an initial estimate of the object S/N.



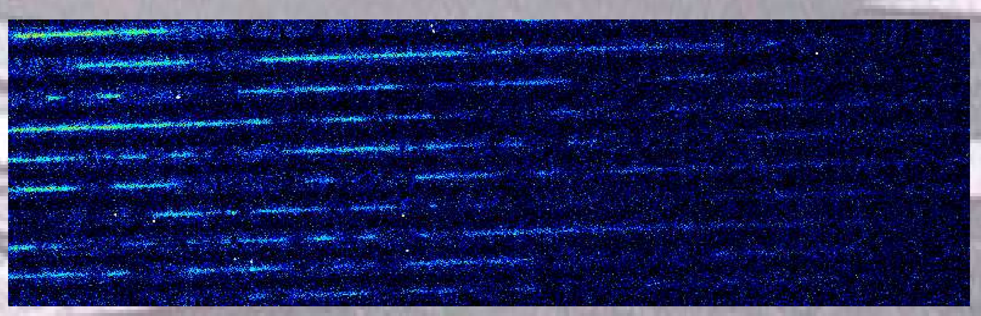
The object spatial profile (black), two analytical (Moffat/Gauss) models and the non-analytical Virtual model. Clearly, the asymmetrical object spatial profile is well fitted only by the non-analytical model. (The high asymmetry in this data is due to an asymmetric source and is not representative of the UVES spatial profile for a point source.)



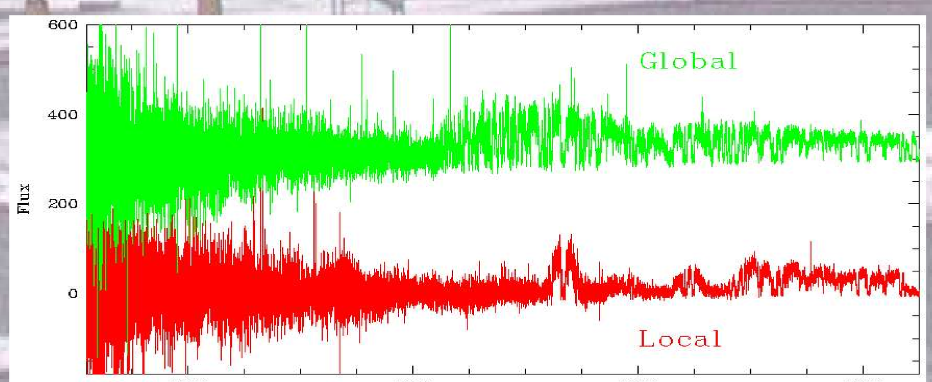
The optimally extracted spectrum is underestimated if the model profile does not match the empirical object profile well. For reference, we show also the results of a linear extraction (notice the cosmic ray spikes). The slight shift between the normalisation of the virtual and linear methods might result from a slightly imperfect fit of the cross-order profile using the virtual method. Still, the improvement is very significant compared to the two analytical methods.

Profile measurements at low S/N

The S/N improvement of optimal extraction with respect to linear extraction is largest at low S/N. But this is also when measuring the spatial profile is more difficult due to low statistics.

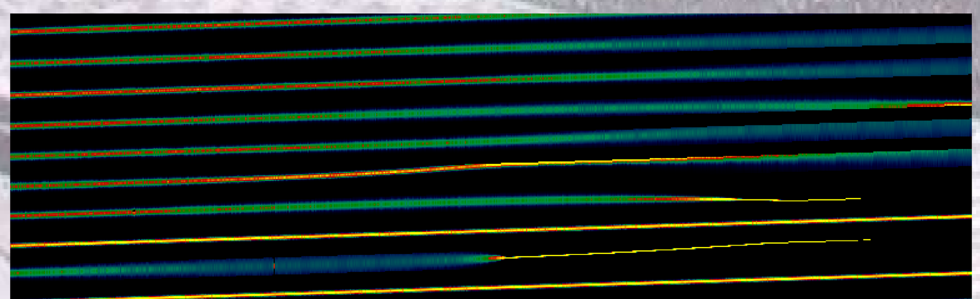


Quasar raw data (zoom) with broad absorptions lines (S/N ~ 0-10) .



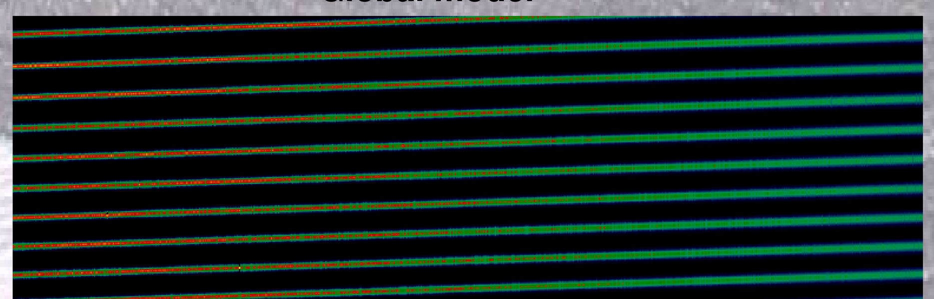
Extracted spectra from the global/local models described below (the global spectrum is shifted +300 units for easier comparison). The local model fails to properly trace some of the orders, which causes spuriously low flux in parts of the Lyman-alpha forest (> 343 nm).

Local model



Reconstructed order traces using an order-by-order model where each of the 33 orders (only 10 orders shown) is modelled by a Gaussian whose centroid and width vary as 3rd degree polynomials. The irregular shape of the traces indicates that the large number ((4 + 4)*33 = 264) of free parameters cannot be reliably determined from the low S/N quasar data.

Global model



Same plot as to the left, except that the Gaussian centroid and width are fitted using two-dimensional (3, 3)-degree polynomials as function of wavelength and order number (only 4*4 + 4*4 = 32 free parameters). This exploits the fact that the spatial profile is expected to vary slowly as function of wavelength *and* from one order to the next, and allows interpolating the regions with no signal, leading to a regular (better) object tracing.