Advanced 2D Spectroscopic Predicted Data

Paul Bristow^a, Florian Kerber^a, Michael R. Rosa^b

^aESO - ESO, Karl-Schwarzschild-Str. 2, 85748 Garching, Germany; ^bESA - ST-ECF, Karl-Schwarzschild-Str. 2, 85748 Garching, Germany

ABSTRACT

We have developed physical models of the dispersive optics of several astronomical spectrographs (STIS, CRIRES, X-shooter). The primary goal is to use these models to provide a physically motivated wavelength calibration of these instruments. However, a further advantage of this approach is the possibility to produce detailed simulations of spectroscopic observations as they would appear on the instrumental detectors in 2D. In the case of operational spectrographs, such data can be further processed by the instrument pipeline creating all of the products that would be produced for real data. This enables observers to project existing spectra or theoretical model spectra of their proposed target onto the resolution, sensitivity and format of a given instrument. For instruments in the planning phase, this approach provides a highly accurate method for visualising the capabilities of the proposed instrument under a wide range of possible operating conditions - such as alignment errors, setting angles of gratings, miss-rotation of detector grids to name a few. Mitigation strategies and operational concepts can thus be integrated into the design at a very early stage.

Keywords: Spectroscopy, Wavelength Calibration, Instrument Modelling

1. INTRODUCTION

We have developed a physical model of the principle dispersive optics in astronomical spectrographs that allows rapid and accurate simulation of the performance of these instruments. The model parameters can be optimised to match the observed behaviour of the instrument via the use of wavelength calibration exposures. The principal use of the physical model is to provide an accurate wavelength calibration based upon physical knowledge of the instrument as opposed to the classical empirical approach. Our approach is discussed in detail by Bristow et al,¹ while specific instances of physical models developed for the VLT instruments CRIRES and X-shooter are described in Bristow et al² and Bristow et al³ respectively.

We discuss here a further possibility opened up by the availability of such physical models. Since the models are relatively streamlined compared to full fledged optical codes such as Code V or Zemax, performing only the calculations necessary to evaluate the location on the detector that photons of a given wavelength arrive at the resolution of the instrument, they are extremely fast. This makes the simulation of two dimensional spectrograph exposures via the iterative use of the physical mode code possible in realistic execution times. Hence, given a suitable source input spectrum, we are able to simulate the raw data that the instrument would produce. This raw data can then be processed by the instrument's standard data reduction pipeline, providing observers with unprecedentedly accurate predictions of the data set that they can expect that is only limited by the input spectrum that they are able to provide.

The basic function of the physical model is accurate mapping of the wavelength and entrance slit position onto the detector. All of the X-shooter examples below also include modelling of the throughput (dichroics, blaze function and quantum efficiency) and in some cases (where stated) readout noise. A rigorous treatment of the dark, flat field and biases properties of each arm, so that the simulated data could be processed by the full data reduction pipeline would not be technically difficult but would require considerable further development.

A fully automated way of offering this kind of synthetic preview data has yet to be implemented and the examples given were generated with considerable interaction and tweaking of the physical model code. However, all of the required algorithms already exist and, as the examples below show, can be used in the ways described.

Further author information: (Send correspondence to Paul Bristow)

Paul Bristow: E-mail: bristowp@bristowp@eso.org, Telephone: +49 89 32006454

2. REQUIRED INPUT

Naturally the observation must be specified by providing detailed information regarding the intended astronomical target and the observing conditions. The more accurate the input data, the more realistic the simulation will be.

- Representative target spectrum/spectra for the X-shooter wavelength range
- Sky background spectrum for the X-shooter wavelength range
- Atmospheric attenuation for the X-shooter wavelength range
- Intensity profile of the target(s) along the entrance slit
- Observation parameters:
 - Exposure times Entrance slit parameters Use of Integral Field Unit or Similar Readout mode(s)

Some of these, for example sky background and atmospheric attenuation, could be made available in a library of standard inputs for the instrument in question, whilst others are already standard options in existing exposure time calculators (readout modes, entrance slit options) such as those provided by ESO

(http://www.eso.org/observing/etc/). The possibility of the observer choosing a target spectrum from a list of templates or even supplying this from his own sources is also becoming common in exposure time calculators for modern spectrographs. Specification of the illumination along the slit is a new requirement, necessary to produce 2D simulated data. However this does not need to be an additional complexity for observers who have no special observational requirements in this respect, default options of uniform illumination or a point source will be sufficient for most users. On the other hand, others may wish to specify the intensity variations due to the structure of an extended source along the slit (this could even be directly computed from finding charts). Moreover observations of complex targets that have components with different spectra falling at different positions along the slit could easily be accommodated, the chief difficulty would be constructing an interface that allows observers to efficiently characterise this kind of observation.

3. EXAMPLES

We present here a number of examples intended to illustrate what is possible with this approach. These examples are simply mock ups made using easily available data. In some cases we have enhanced aspects of the data so as to make certain features apparent with the limited dynamic range offered by printed figures. The reader should not be tempted to infer the signal to noise or resolution characteristics of the X-shooter or CRIRES instruments based upon these figures.

The sky background spectrum⁴ and atmospheric attenuation spectrum⁵ used in all of the examples below were obtained from the Gemini Observatory web pages.

3.1 Orion Nebula with X-shooter UVB and VIS arms

X-shooter is a single target spectrograph for the Cassegrain focus of one of the VLT UTs covering in a single exposure the spectral range from the UV to the K band (320 -2500 nm). It is designed to maximize the sensitivity in this spectral range by splitting the incoming light into three arms (UVB, VIS and NIR) with optimized optics, coatings, dispersive elements and detectors, operating at intermediate resolutions (R=4000-14000). Each of the three arms constitutes a cross dispersed Echelle spectrograph. See⁶ for a full description of X-shooter.

Figure 1 shows simulated full slit exposures of the Orion nebula captured with the UVB and VIS arms. Well known spectral features are identified in the figure. The input for this simulation was simply emission lines and continuum appropriate to the target. There is no sky background, atmospheric attenuation or readout noise. The slit is uniformly illuminated and the only noise is shot noise.



Figure 1. Simulated UVB and VIS exposures of the Orion nebula with some well known spectral features identified.

3.2 Standard star with X-shooter

Figure 2 shows a simulated exposure of a standard star at the centre of the slit captured on all three X-shooter arms. The input here was the spectrum of the star and the sky background spectrum. Note the sky background features all along the slit (especially visible at longer wavelengths).

3.3 Sa type Galaxy with X-shooter

Figure 3 shows a simulated full slit exposure of a Sa type galaxy spectrum⁷ with a variable intensity along the slit. Also on the slit is an emission line region. The input was a standard galaxy spectral template, a profile for how the intensity varies along the slit, a hypothetical list of emission line features, the sky background spectrum and an atmospheric attenuation spectrum.

The atmospheric attenuation of the galaxy spectrum is mostly visible at longer wavelength, as is the sky background. The emission lines appear always at the same location along the slit as if they come from a compact region. The features from the global galaxy spectrum extend across the slit but variable in intensity. Readout noise is also included, barely visible between the orders.

With this kind of complex simulation observers can see how the varying signal to noise regimes at different wavelengths and on different detectors compare for a given exposure time on an instrument like X-shooter. This may help to choose strategies for multiple readouts on one detector while the others continue to integrate.



Figure 2. A complete (top to bottom: NIR, VIS, UVB; inset: detail from UVB) synthetic X-shooter exposure of a point source and sky background, sky background and atmospheric attenuation.



Figure 3. A complete (top to bottom: NIR, VIS, UVB) synthetic X-shooter exposure of an extended source showing variable luminosity along the slit, emission lines from a compact region, sky background and atmospheric attenuation.



Figure 4. Top: A section of a solar spectrum exposure obtained via a fibre with the VIS arm on X-shooter during testing at ESO HQ. Bottom: A simulated VIS arm X-shooter exposure of a point source solar spectrum.

3.4 Solar spectrum with X-shooter VIS arm

Figure 4 shows a section of a real X-shooter VIS arm exposure of the solar spectrum obtained through a fibre while the instrument was being tested at ESO headquarters (a) compared to the same section of a simulated VIS arm exposure of the solar spectrum as a point source (b): agreement is excellent. The inputs here were a solar spectrum and a sky background spectrum.

3.5 Stellar spectrum with CRIRES

CRIRES is a cryogenic Echelle spectrograph covering the wavelength range from 950-5300nm at high spectral resolution (Rmax~100,000) now operating at the VLT on UT1. It is not cross-dispersed, instead the pre-dispersed spectrum falls on a linear array of four 512x1024 pixel detectors separated by ~300 pixel gaps. Owing to the high resolution, a single exposure only covers a small fraction of the total spectral range available, different wavelength ranges are accessed by setting the two adjustable optical components (the pre-disperser prism and the diffraction grating) appropriately. See⁸ for a full description of CRIRES.

Figure 5 shows a simulated exposure at $\sim 1.25 \mu$ m of a stellar source illuminating part of the slit. The inputs were a simplistic stellar model (a 6000K black body with some arbitrary emission features), the sky background spectrum and an atmospheric attenuation spectrum. For an instrument such as CRIRES with adjustable components that determine the wavelength range of the exposure, such simulations allow the observer to see where features in their target spectrum will fall relative to the detector array. In the case of CRIRES



Figure 5. A simulated CRIRES 1.25μ m exposure of a simplistic stellar model (a 6000K black body with some arbitrary emission features) with atmospheric attenuation as it would appear across the four detectors.



Figure 6. Comparison between the input spectrum (open diamond symbols) for the simulated exposure of the Sa type galaxy shown in figure 3 and the 1D spectrum after data reduction that can be extracted from such a simulation (grey line). The solid black line is the spectrum extracted directly from the 2D data. The grey line is the extracted spectrum once it has been corrected for the instrument signature (i.e. flat fielded to correct for the blaze function, dichroic function and quantum efficiency, corrected spectral bin size stretching and corrected for atmospheric attenuation). The spectra have been scaled and shifted in order to show them in the same graph.

the positioning of the spectrum on the array is especially important because of the gaps between the detectors. Usually interlaced exposures are obtained. An observer could request 2D simulations of both interlaced exposures and process them with the instrument DRS pipeline in order understand what the implications are for signal to noise around the detector gap overlap areas in the combined data.

3.6 1D input vs 1D extracted spectra

Usually the spectrum used as input for these kind of simulation will not have been obtained with the spectrograph being simulated but with one or more different instruments. Since it is possible to reduce the simulated 2D data and extract a 1D spectrum, it may be instructive to compare the input with the output. Clearly this will not enable the observer to benefit from higher resolution or signal to noise that might be offered by a new spectrograph, but it will give an indication of what can be expected.

Figure 6 shows such a comparison for the galaxy spectrum of figure 3 for order 21 of the VIS arm. One can easily see that the X-shooter exposure will offer better resolution but that with the short exposure time simulated the spectrum is relatively noisy.

4. SUMMARY

We have shown that the implementation of a physical model of astronomical spectrographs, whose principal purpose is to drive wavelength calibration, opens up new possibilities for advanced 2D data previews. The simulated data products could be developed to the stage where they could be reduced by the instruments data reduction pipeline, producing the full suite of secondary data products.

The full implementation and automation of the concepts discussed here, from user interface to simulated products that flow through the data reduction pipelines, would require a significant investment of effort. However, as astronomical instruments become ever more sophisticated and ambitious, devoting resources to these kind of tools would seem increasingly worthwhile.

Such simulations can also potentially aid the instrument design phase, enabling a better understanding of how critical parameters influence 2D data products. Second generation VLT instruments and the E-ELT project stand to benefit from this additional simulation tool.

Moreover, the development of the data reduction software benefits from the availability of semi-realistic simulated 2D data before the instrument is built. This latter possibility has already been realised for the X-shooter DRS development.

Perhaps the ultimate projection of the concepts presented here would be the following intriguing idea: The best available existing spectra (for example from the VO) are used to make the most realistic synthetic data for every observation. This data is run through the DRS pipeline in parallel with the real observational data and the observer deduces the useful new information contained in his new observational data via a comparison between the synthetic and real data products.

Acknowledgements

It is a pleasure to thank both the CRIRES and X-shooter instrument teams for useful collaboration.

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