Calibration and modeling support for instruments at ESO

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ABSTRACT

We describe the activities of the Physical Modeling Group in ESO's Instrumentation Division related to the calibration and physical description of an instrument with the objective to support the data reduction of science data and to facilitate operations. We will use CRIRES and X-shooter as examples to describe the general concept. The core contribution of the group consists of four parts: a) Optical model: describing the configurations of the optical elements of the spectrograph based on engineering information; b) Calibration Reference Data: examples are: Wavelength standards traceable to laboratory standards form the basis for the application of the 2-D wavelength calibration; spectro-photometric standard stars to support flux calibration; physical properties of optical components such as the refractive index (T, λ) of a disperser. c) support for Data Reduction Software (DRS) development: simulated data based on a model based description of the instrument; d) general Project Support such as participation in Testing, Commissioning and Science Verification**.** These tasks have been performed and documented in close collaboration with the project teams and the software development groups. In summary, we have found that the use of instrument physical modeling techniques can be beneficial during all phases of the life of an instrument: design, optimization, manufacture, testing and operations. Once fully integrated in the project plan and scheduling direct and tangible benefits to the overall project result. Hence planning for VLT 2nd generation and E-ELT instruments should make full use of these capabilities.

Keywords: calibration, model, physical, instrument, experiment, reference data

1. INTRODUCTION

The ultimate goal of all calibration efforts is to remove all relevant signatures imprinted on the light from the target throughout its way to the observer. While other astronomical objects such as intervening dust or gas will also leave their mark most of the complicating artifacts are added in the final few kilometers by e.g. Earth's atmosphere, the telescope and the measuring instrument and its detectors. In order to extract the intrinsic physical properties of the astronomical objects and in order to obtain quantitative results, it is essential to remove such artifacts to the maximum extent possible.

1.1 Aspects of experimental physics in astronomical observations

Traditionally, astronomy is not considered an experimental science simply for the fact that the objects of interest are located far beyond the sphere of influence of the scientist. Hence the astronomer has to take the role of an observer who tries to understand the various conditions of objects in nature.

In contrast, in experimental physics the object of scientific study will be subjected to varying environmental conditions that are controlled by the scientist. As a result a solid understanding of the measuring apparatus and all statistical and systematic errors associated with the measurement process is a prime requirement of all experimental work. The effort required to understand and minimize all sources of errors can be a very substantial fraction of the overall work.

It is a truism that – sometimes very complex – physics needs to be employed to understand the properties of astronomical objects. By the same token it is very appropriate to use physics to understand the performance of astronomical instruments and to properly describe the errors associated with the measuring process. Here some lessons may be learned from experimental physics.

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Given the fact that most of the modification of the information contained in the photons coming from the astronomical source takes places on Earth – most of it is actually done in the instruments built and operated by scientists – it seems worth having a closer look at some of the experimental aspects of astronomical observations. A schematic description of astronomical observations and associated calibration efforts is depicted in Figure 1. Some of the items shown, such as the net effect of the turbulent motion in the atmosphere, are highly complex and we are just beginning to be able to actively measure some of the relevant properties. Others, such as the description of the light dispersing action of a grating, have been well understood for more than 100 years.

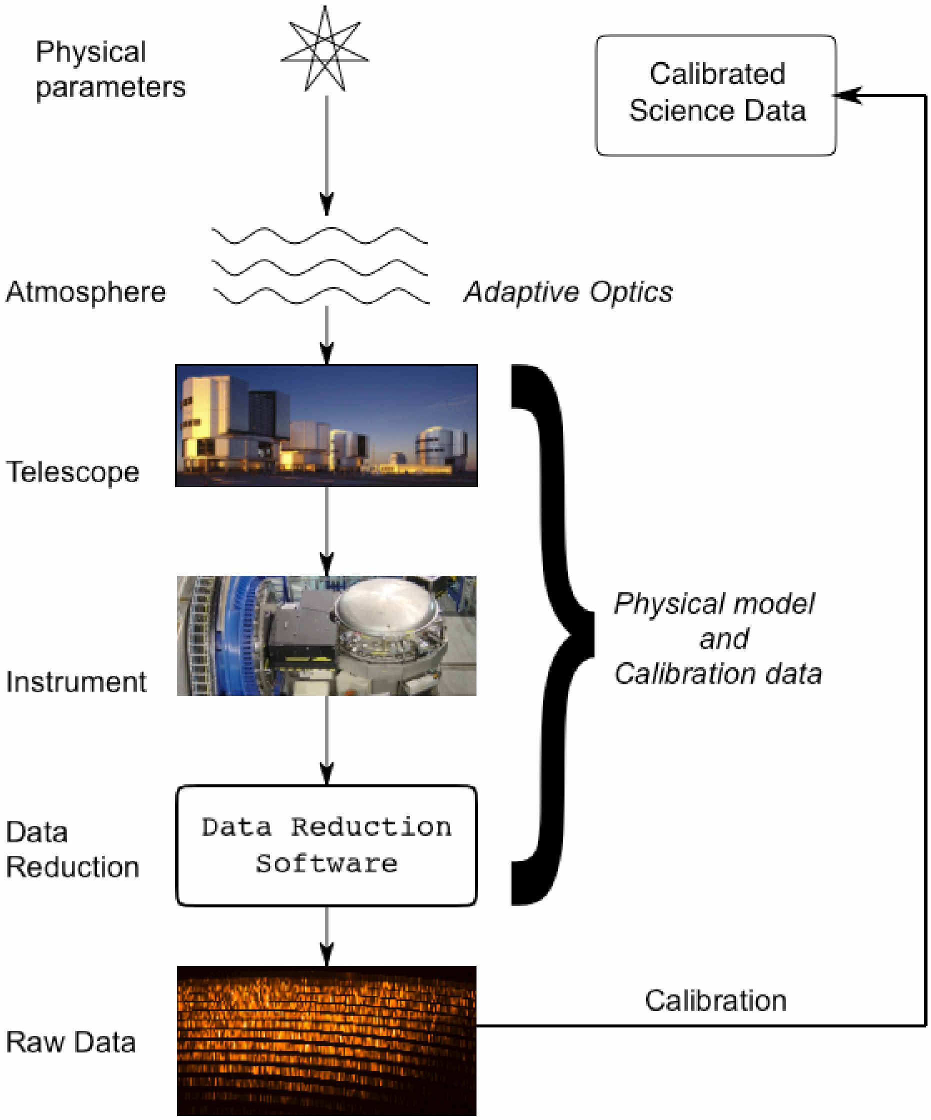

Figure 1: Schematic description of an astronomical observation and the calibration efforts needed to extract quantitative physical results by removing the signatures of Earth's atmosphere, telescope, instrument and detectors.

1.2 Physics for better calibration

The activities within ESO's Calibration and Model Support Group are aimed at employing the relevant physics related to the calibration of instruments with the objective of supporting the reduction of science data and facilitating operations. The two main components for this work are the adoption of physical instrument modeling techniques (section 2) and the use of calibration reference data (section 3). In addition, for very practical reasons the group provides support for the development of the Data Reduction Software (DRS), e.g. simulated data based on a model based description of the instrument; and participates in testing, commissioning and science verification of the instrument**.**

Two considerations are always to be made in this kind of work. First, *will the physical description improve the final science product?* A case in point is replacing a polynomial fit for deriving a dispersion solution by using the grating equation. Here the advantage is rather obvious since the relevant physics is easily described and the physical description provides predictive power which is limited for a polynomial and actually zero outside the range for which calibration features are available in a wavelength calibration exposures. Moreover the accuracy of the wavelength calibration can be significantly improved relative to the standard empirical methods as shown in section 2.2. The use of physics will usually be advantageous as long as the instrument remains stable during operations and as long as the physics can be well described. If these conditions are not met the effort associated with physical modeling can become very large and its benefit may become questionable. Therefore the second point to consider will be *is it worth the effort?* Here of course each instrument has to be assessed individually but the well-established 80/20 rule can serve as a general guideline. Experience has shown that a pragmatic approach is to be preferred over trying to do physics all the way. This may sound a bit confusing since one should certainly be able to describe a man-made instrument in terms of physics. The main reason for this is in the fact that many modern instruments are very complex both mechanically and electronically and the physics of the overall system quickly becomes very complex indeed. In addition the instrument will respond to environmental factors such as temperature or a variable gravity vector adding a time dependency.

It will be prudent to use the same pragmatic approach for physical modeling of future instruments such as the 2nd generation of VLT or E-ELT instruments. It is safe to say that at least some of these instruments will be complex at a level that can no longer be successfully (and economically) treated by empirical means but that requires physical modeling. Many of the science cases for ELTs require full quantitative analysis of the observations again stressing the need for excellent understanding of the instruments' physical state and performance.

2. INSTRUMENT MODELING

One crucial aspect for calibration is a proper understanding of the performance of the instrument and the errors associated with the measuring process. The life cycle of an instrument can be described as illustrated as follows:

1. Science Requirements
2. Optical Design, Optimisation
3. Engineering Expertise
4. Testing and Commissioning

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5. Operation and Data Flow
6. Calibration of Instrument
7. Scientific Data and Archive

Experience shows that it is difficult to ensure that the know-how and expertise that went into designing and building the instrument (steps 1-3) is brought to full use in the instrument calibration and scientific operations (steps 6 & 7).

A case in point is the wavelength calibration in which well-understood physics is employed to design a spectrograph with an optimal format while during operations the dispersion solution is then derived time and again in a purely empirical manner by, for example, fitting polynomials to a sparse calibration line spectrum.

One way to ensure that the engineering data propagates from instrument building to operations is to capture all the engineering information in a physical model-based description of the instrument. This model accompanies the instrument throughout its life cycle and is used to drive the science data reduction pipeline. In our concept the model is combined with validated physical data of the instrumental components and calibration reference data.

Our approach comprises an instrument specific model kernel and associated software to optimise the model parameters and to apply the model's predictive power to the calibration of science data.

2.1 Modeling approach

The concept of using the relevant physics to describe the performance of an astronomical spectrograph was developed more than 10 years ago by M. Rosa and P. Ballester[1] at ESO and has matured into the following strategy. We first construct a streamlined model of the dispersive optics based on the (e.g. Zemax/Code V) optical design. This model has a parameter file that describes the orientation, relative positioning and optical properties (e.g. grating constants, detector array dimensions) of the relevant components. The core of the model is a function that will return the detector co-ordinates for a given wavelength and entrance slit position. By making iterative calls to the core function for a range of wavelengths and slit positions we can create simulated 2D data (see Bristow et al. [2]) and other products such as detector array wavelength maps.

The model parameter set can be optimised to reflect the performance of the operational instrument with suitable calibration data in a similar way that a polynomial dispersion solution would be fit. The difference is that the parameters optimised here have physical meaning and represent the actual configuration of the instrument. They can always be adjusted to match the observed behaviour of the instrument or to predict the effects of tilting/modifying a component. For example, adjusting the camera focal length will change the scale on the detector.

In order to perform the optimisation we iteratively call the core model function for a list of standard wavelengths, comparing the results of each iteration to the measured centroids for these wavelengths as measured in the calibration data. We employ the simulated annealing technique[3,4] to continually adjust the model parameters until the best match between predicted and measured centroids is found. Figure 3 shows an example of a change in spectral format after an intervention that requires a re-optimization of the model. Full details of the method are given by Bristow et al.[5].

As it has evolved, variations of this strategy have so far been applied to FOS and STIS (where the application was recognised by a NASA group achievement award) on HST and UVES, CRIRES and X-shooter on the VLT.

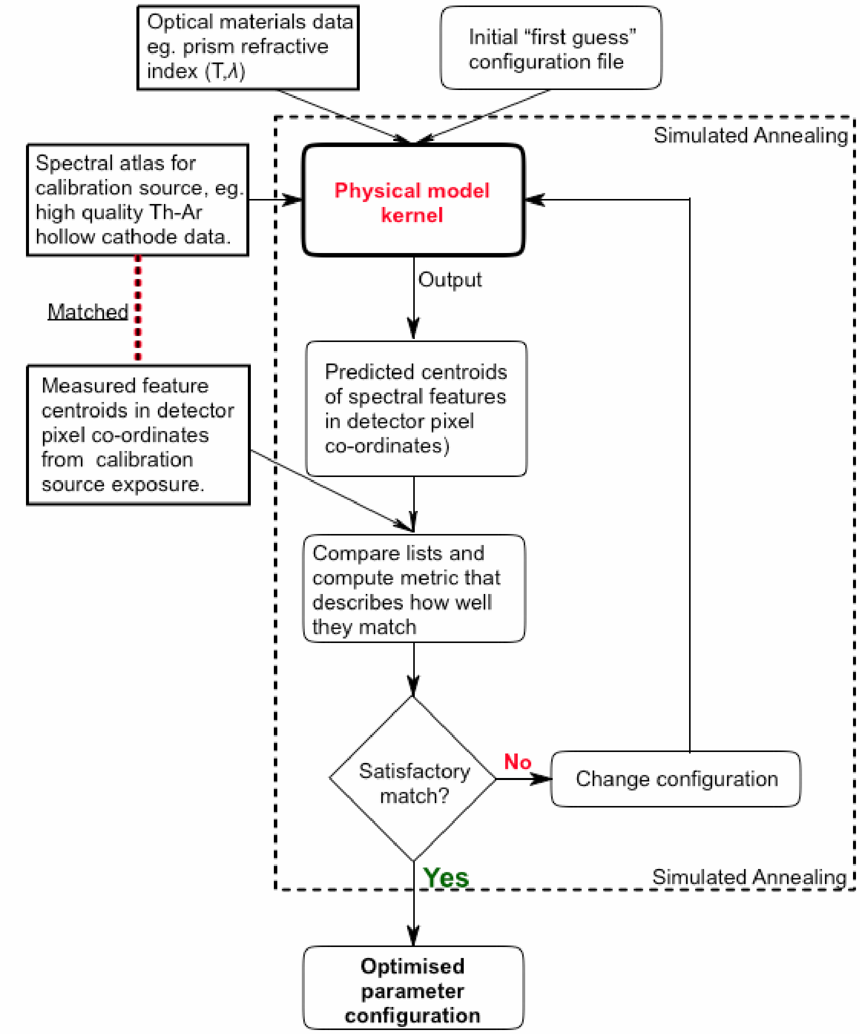

Figure 2: Schematic representation of the optimisation process for instrument physical models

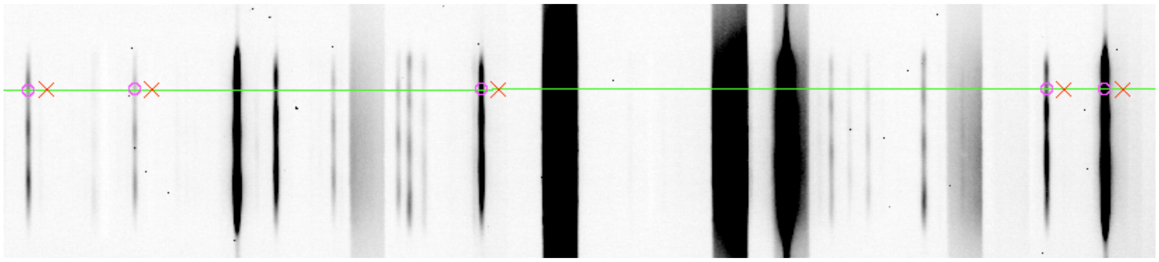

Figure 3: A CRIRES full slit Th-Ar calibration exposure used to discover the change in spectral format. The solid line is the locus of a chosen entrance slit position on the detector array. Crosses mark the predicted positions of isolated spectral features according to the baseline model parameter configuration. Open circles give the actual position of these features after a shift in spectral format.

2.2 Calibration

The principal purpose of the physical modeling approach is to provide accurate wavelength calibration for spectroscopic science data. Once the physical model parameter set is optimised to match the instrument reality and, where necessary, fine tuned to match the actual operating conditions, it is trivial to recover the wavelength corresponding to each pixel in the 2D detector array or each bin in extracted 1D spectra. For CRIRES and X-shooter this is incorporated in the standard data reduction software (DRS) pipeline.

The application to the Space Telescope Imaging Spectrograph (STIS) provided encouraging verification of the validity of wavelength calibration using this technique. Many spectral features occur in adjacent spectral orders in cross-dispersed Echelle spectrograms. An accurate dispersion solution should assign identical wavelengths to these features regardless of which spectral order they are measured from - see Kerber at al.[6] for details. Figure 4 is a histogram of the wavelength offset between wavelengths assigned to line positions on adjacent orders. The dashed histogram is found for the standard STIS data reduction software, *calstis*. Note that STIS is arguably one of the best empirically calibrated modern astronomical spectrographs. The solid histogram is what we obtain with the physical model approach. The goodness of the latter dispersion solution is even more impressive if one recalls that it is a global solution across the entire 2D dispersion map, while the 2D polynomials of the canonical *calstis* pipeline are matched locally (per order).

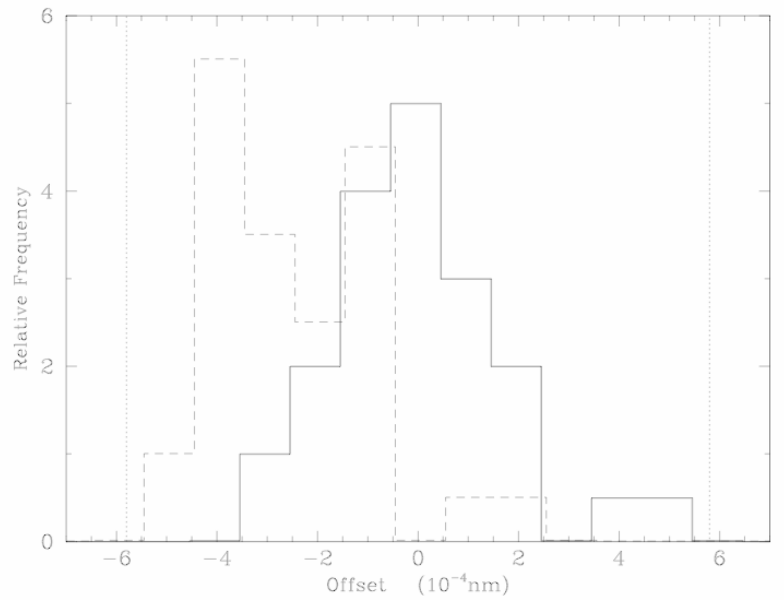

Figure 4: Histograms of the discrepancy in the wavelength assigned to features appearing in adjacent orders in STIS E140H exposures by the standard STIS DRS (dashed line) or the physical model derived dispersion solution (solid line). The dotted vertical bars indicate the size of one STIS pixel. (Figure taken from Kerber et al.[6])

The physical model can also be used to drive the extraction of 1D spectra from 2D data since it will predict the locus on the detector array of wavelengths entering at a given entrance slit position. A further possibility, which has not yet been fully exploited, is to use physical model to fully map flux in the 2D detector pixel array plane back to the slit position/wavelength plane.

2.3 Simulation Tools

An instrument model can also be used to simulate spectroscopic data. In addition to the geometric capabilities of the physical model, basic photometric simulation is also implemented. Blaze efficiency can be computed directly from the model parameter set, whilst other throughput issues such as quantum efficiency, dichroic transmission etc are incorporated through reference data (see section 3) for the materials used. Details of this method and its application to science observations are given in Bristow et al[2] (these proceedings). Figure 5a shows a section of a Th-Ar hollow cathode lamp X-shooter VIS exposure made using a nine pinhole mask, while 5b shows the equivalent section from a model based simulation. The predictive power of the model is excellent.

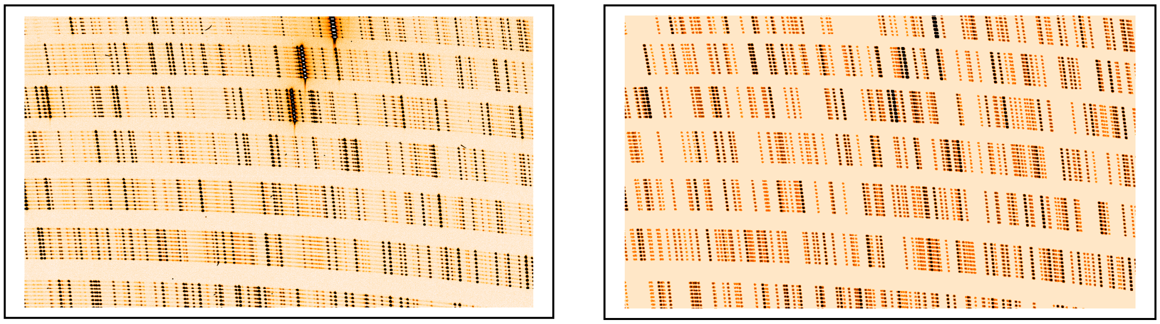

Figure 5: Left- Section of an X-shooter VIS 180s exposure of a Th-Ar HCL through a 9 pinhole mask obtained in the laboratory. Right - Physical model based simulation of the same exposure.

2.4 Physical model in the data reduction software

The wavelength calibration of X-shooter will be driven by a model-based description of its three arms each of which is a cross-dispersed echelle spectrograph[5]. The spectral format in X-shooter has been chosen such that each spectral order has some overlap with neighbouring orders where unique wavelengths are imaged in both. Traditionally, this overlap region is difficult to handle empirically. Usually, polynomial solutions are fitted independently to each order and often diverge at the extremes of the orders. Hence a comparison of wavelengths assigned in adjacent and overlapping order is a stringent test of the accuracy achieved by wavelength calibration (cf STIS, Fig. 4). Obviously, the wavelength assigned to a spectral feature should be the same regardless of which order and which part of the chip the flux was extracted from. Since the physical model is fitted simultaneously to data from all orders it is much better able to achieve a consistent fit in the order overlap regions. Figure 6 shows the excellent correspondence between the model wavelength solutions for neighbouring orders in X-shooter VIS data. One goal for the X-shooter DRS will be to make use of this capability to provide better merging of orders, a perennial weakness of many Echelle pipelines.

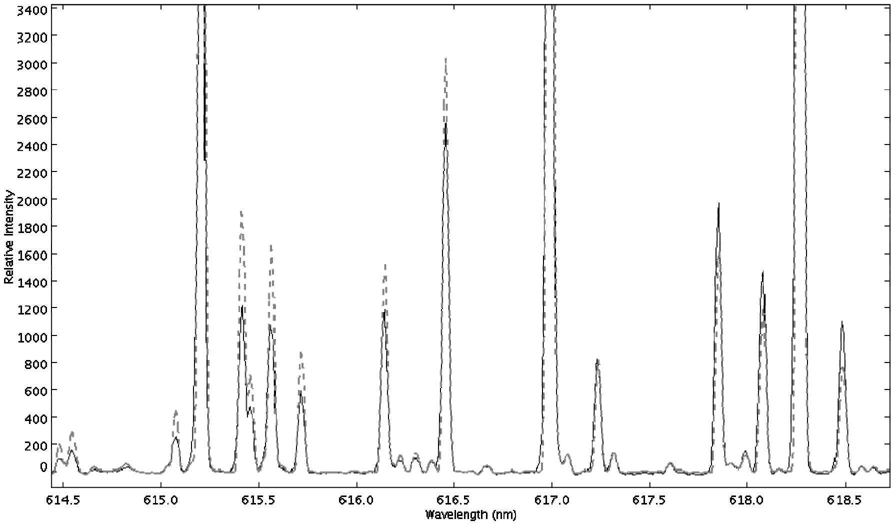

Figure 6: X-shooter VIS arm: orders 26 (dashed) and 27 (solid). The difference in relative intensity for a given feature seen in two orders is due to the changing blaze function along the order. Systematic differences in the centroids of features detected in different orders are well below the centroid uncertainty caused by shot noise.

3. CALIBRATION REFERENCE DATA

Calibration reference data serve as a “ground truth'” to operational instrument calibration efforts. The Calibration and Modeling Support Group performs several activities that are aimed at producing or obtaining data that will ensure optimum calibration of the science instruments at ESO. Our goal is to only use data that are traceable to laboratory standards as calibration reference data. All such data need to be fully described by meta-data explaining how they were obtained and what accuracy can be expected. In the following we give some recent examples.

3.1 Properties of Physical Materials

A realistic description of an instrument requires data describing the physical properties of critical components. For example, in CRIRES a ZnSe prism is used as a pre-disperser prism making it essential to quantitatively know the properties of ZnSe at CRIRES' cryogenic operating temperature. Since no such data were available in the literature new laboratory measurements taken at NASA's CHARMS facility (Kerber et al.[7]) were included in the model. The validity of the model in this respect was verified by comparing it with data taken during a temperature ramp during testing.

3.2 Spectro-photometric Standard Stars for the Near Infrared (IR)

In preparation of the operations of X-shooter a need for better IR flux calibration standards was identified. The aim of this ESO observatory program is to establish a set of spectro-photometric standard stars over a very wide wavelength range from 320 nm to 2500 nm. The strategy is to extend the useful range of the well established optical flux standards[8,9] into the near IR using a few well selected windows where atmospheric transmission is >99%. Interpolation between these measurements is done with state-of-the-art stellar atmosphere models for the white dwarfs (see T. Rauch's web site http://astro.uni-tuebingen.de/~rauch/). Three HST white dwarfs serve as primary reference[10]. For these agreement between flux measured above the atmosphere and stellar models is 1-2%. Early results detailed by Vernet et al.[11] indicate that an accuracy of between 2-6% can be achieved in J, H and K bands; significantly better than the original goal of 10%. Once fully validated this new set of standard stars will be useful to other near-IR spectrographs.

3.3 Wavelength Standards

Traditional approaches to wavelength calibration in the near-IR relied on atmospheric features, in particular the rich OH emission spectrum of the night sky[12]. This approach has significant limitation for high resolution spectroscopy and we decided that in order to realize the potential accuracy of ESO's Cryogenic High-Resolution IR Echelle Spectrometer (CRIRES)[13] an external calibration source would be desirable. To this end ESO, in collaboration with the Space Telescope European Co-ordinating Facility (ST-ECF) and the US National Institute of Standards and Technology (NIST), embarked on a project to establish Th-Ar wavelength standards in the 950-5000 nm operating range of CRIRES. Th-Ar hollow cathode lamps (HCLs) are a well establish wavelength standard in the ultraviolet (UV) and Visible providing a rich spectrum[14]. Since there is only one isotope in nature and the nuclear spin is zero the use of Th avoids the complexity of isotope- and hyperfine structure in the spectrum. Dedicated laboratory measurements at NIST have resulted in about 2400 lines between 750 and 4800 nm with highly accurate (accuracy: 0.001 cm^{-1} for strong lines) wavelengths. The calibration accuracy relative to laser measurements of Th[15] is $\approx 1.4\ 10^{-8}$. Details of this effort and the operations of HCLs are described in Kerber et al.[16] while the line list is published in Kerber et al.[17]. The Th-Ar HCLs provide a high density of sharp well-characterized emission lines combined with the ease and efficiency of operation of a commercial discharge lamp. They now are the backbone of wavelength calibration of CRIRES up to 2500 nm.

For longer wavelengths gas cells (N_2O and OCS) are being established as calibration sources by using NIST calibration reference data and laboratory measurements with ESO's FTS to characterise the gas cells as a function of fill gas pressure and temperature. Other gases with more specialized application have been measured at ESO in collaboration with a group in Hamburg (Gaedke & Kerber, in preparation).

With these developments wavelength calibration in the near-IR will become very similar to the UV-visible region, and it is possible to support high accuracy absolute wavelength calibration without having to rely on atmospheric features. In a related development ESO is undertaking - in collaboration with NIST - a dedicated effort to identify the best calibration sources for wavelength calibration of E-ELT spectrographs. The instruments currently under study cover a significant range in wavelength and spectral resolution but our knowledge of near-IR from various elements is rather limited. Aldenius et al.[18] (these proceedings) describe in detail the status of the project and present first results.

3.4 Optimising Calibration Systems

The combination of laboratory measurements with a physical instrument model is a very powerful tool for assessing the predicted performance of an instrument or its calibration subsystem. For the selection of the best-suited wavelength calibration sources for the near-IR arm of X-shooter we did an in-depth analysis[19,20]. As a result we have been able to identify a combination of the noble gases Ne, Ar and Kr as the best three-lamp combination. Our analysis provides a quantitative order-by-order prediction about the number of lines available from a given source, their relative intensities - including the effect of the blaze function - and an estimate of the line blending between sources. The prediction is currently being validated by laboratory measurements with X-shooter.

3.5 ESO Laboratory Facility

ESO operates a commercial Fourier Transform Spectrometer (FTS) (Thermo 5700) in its IR laboratory. The spectrometer is equipped with an external port that allows one to feed the light from external light sources to the FTS (Fig. 7) for analysis. ESO's Integration and Cryo-vacuum Department in Instrumentation Division has built a permanent set-up for the external feed which replicates part of the optical train of the FTS. Different combinations of detectors and beam splitters can be used to observe the wavelength range 700 nm - 10000 nm. The maximum spectral resolution is about 100000 at 1000 nm.

While proper calibration reference data can only be obtained by dedicated measurements at qualified physics laboratories such as NIST (see section 3.3) or PTB this in-house facility offers great benefit for studying several aspects of instrument operations. Recent routine examples are measurements of filters transmission curves (search for leaks) and transmission of optical fibers. Dedicated laboratory campaigns have resulted in analysis of the spectra of pen ray lamps for X-shooter calibration (Kerber et al.[19,20]), fundamental research into the near-IR spectra of hollow cathode lamps from various elements for E-ELT and their variation as a function of current (Aldenius et al.[18] their Figs. 6 & 7). In addition the spectra of various gases have been characterized as a function of pressure and temperature for use in CRIRES gas cells. The capability to perform such measurements in-house has proven to be a quick and very efficient way of obtaining relevant information for calibration purposes.

Figure 7: Commercial Fourier Transform Spectrometer in the ESO IR laboratory. On the right hand side part of the optical train of the FTS is replicated feeding the light from various sources to the external port of the FTS.

3.6 ESO Calibration Proposals

As of the beginning of 2008 ESO has introduced a new category of observing proposals aimed at enhancing calibration for ESO instruments. This was done in direct response to the feedback from the community and discussions at the 2007 ESO Instrument Calibration workshop[21]. ESO operates a large suite of complex instruments, many of which provide a significant number of possible configurations and observing modes. On the one hand the observatory already executes a rigorous calibration plan for each instrument and its most important modes. On the other hand ESO does not have the resources to calibrate fully all capabilities of all instruments. Astronomers are encouraged to submit proposals in the category of Calibration Proposals if their results and products can be used by the ESO observational community for existing or future programs. Calibration Proposals are evaluated and selected by the Observing Programmes Committee (OPC) consisting of scientists from the user community, who balance the potential added calibration value for future science on ESO telescopes with the more immediate return of the regular science proposals. The OPC is supported by a dedicated ESO calibration program committee that reviews the technical and operational feasibility. The raw calibration data, as well as the advanced calibration products that are based on Calibration Proposals will be non-proprietary and are made available to the entire community through dedicated web pages and the archive. ESO anticipates that Calibration Proposals will produce significant amounts of valuable calibration reference data in the future. The next call for proposals will be available from the ESO web page http://www.eso.org/sci/observing/proposals/index.html.

4. SUMMARY AND OUTLOOK

We have presented the activities of the Physical Modeling Group in ESO's Instrumentation Division related to the calibration and physical description of an instrument with the objective to support the data reduction of science data and to facilitate operations. It is advantageous to use the physics of astronomical instruments to gain insight in their performance and to properly describe the errors associated with the measuring process. The two main components for such work are the adoption of physical instrument modeling techniques and the use of high quality calibration reference data.

We have developed streamlined physical models for a variety of astronomical spectrographs that are characterised by a model kernel with an associated set of parameters; each parameter has a clear physical meaning. In addition we have implemented the tools necessary to optimise the parameter sets to match the actual configuration of the real instruments using dedicated calibration observations. Once optimised, the physical model drives the wavelength calibration inside the data reduction pipeline. This is already an option for CRIRES and is being realised for X-shooter. We have also produced a suite of software to simulate 1D and 2D spectroscopic data using such models. These simulations aid the initial alignment of the instrument in the laboratory, the development of the DRS and, potentially, the planning of observations.

Calibration reference data traceable to laboratory standards provide the ground truth needed for quantitative calibration. We have given several examples of such standards produced at ESO or in collaboration with other partners. A combination of the modelling techniques and calibration reference data can be used to optimise instrument performance throughout all phases of the life cycle of an instrument: design, manufacture, testing and operations.

Key to success and to achieving the best science product is an integrated approach that combines the development of physical instrument models, application of and feedback from these models during instrument integration, testing, commissioning and science verification and their integration in the data reduction software.

Second generation VLT instruments and E-ELT instruments clearly stand to benefit from this approach.

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