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Physical Modeling of Scientific Instruments

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Abstract. This contribution revolves about computer models of astronomical instruments and their application in advanced calibration strategies and observation model based data analysis. The historical connection between calibration and data analysis is reviewed. The success of physical models in the analysis of observational data with strong instrumental signatures is shown, and a concept for model based calibration developed. A discussion of advantages for observatory operations, observing, pipeline processing, and data interpretation is accompanied by a briefing about the current status of the Observation Simulation and Instrument Modeling project at the ST-ECF and ESO.

1. Introduction

The increasing importance assigned to tasks circumscribed by the terms "calibration" and "data reduction" reflects the evolution of equipment and the fact that purely morphological investigations have largely been superseded by the demand to turn the last bit of useful information in raw data into significant astrophysical quantities.

Calibration strategies currently adopted are empirical methods aimed at "cleaning" raw data of instrumental and atmospheric effects. Since it is only through the empirical determination of calibration reference data (e.g., dispersion relations, flat fields, sensitivity curves) that both evils—changes of the instrument and changes of atmospheric conditions, respectively—are detected and their effects removed, these calibration strategies often take on the form of a defensive battle repeatedly fought every night.

Space based instrumentation, in particular IUE and HST, has taught that once the effect of the human desire to tweak the instrumental parameters every so often is nullified, pipeline calibration of the raw data can efficiently be implemented. Monitoring and trend analysis of the calibration parameters also shows that predictions made about the instrumental characteristics are usually very reliable. Operational scenarios with pipeline calibration are now also being planned for ground based observatories (e.g., ESO's VLT), and it is easy to show that once instrument stability through configuration control is achieved, all that remains of nightly calibration data taking is to address environmental aspects, e.g., the atmospheric transmission.

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Nevertheless, the calibration process remains of the "instrument signature removal" type, even if based on predicted, less noisy calibration data. A long learning process is required to determine the optimum deployment of resources—manpower and observing time—for the calibration task as a whole, and for its subprocesses. This approach also hides the direct link between the engineering parameters of instruments and the differing characteristics in closely related configurations (e.g., the 2-D pattern of echellograms obtained with different grating tilts).

Repeatedly, situations arise where the scrutinizing analysis of science data, in particular when combined with very specific theoretical expectations (e.g., stellar atmospheric models, evolutionary color diagrams), reveals shortcomings or omissions in the "signature removal" calibration. Usually the effects found are neither new to the type of instrument (e.g., non-linearity of a detector) nor unexpected on physical grounds (e.g., scattered light in grating spectrographs). To be fair, almost always the embarrassing situation is not a result of an oversight but rather a consequence of the calibration strategy employed—dealing piecemeal with a highly complex interrelation of physical effects.

Can we do any better? In the following I will lay out the arguments for a radically new approach, highlighting a few examples, and briefly report on the activities in an collaborative ESO/ST-ECF effort to implement observational data calibration and analysis on the basis of physical models.

2. From Observations to Astrophysical Interpretation

Usually the calibration and data analysis process is conceived as a well defined activity, detached from, but linking the observational process with the astrophysical interpretation. The direction is from raw data to better (i.e., "cleaned") data, from counts per pixel to H_0. What really happened during the observation was, however, the application of an operator $\mathbf{O}$ onto a vector $\mathbf{u}$ representing a subvolume of the many-D universe. $\mathbf{O}$ describes the equipment used as well as any other environmental circumstances (e.g., the atmosphere).

Were it not for the ultimate limitation imposed by noise, we could try to just find and apply the inverse operator $\mathbf{C}$ to calibrate, i.e., recover $\mathbf{u}$ from the raw data $\mathbf{d}$, and then go on to interpret $\mathbf{u}$. Eventually the more rewarding "data analysis" strategy is to subject a range of probable $\mathbf{u}'$ to a model of the data taking process $\mathbf{O}'$ and to compare the resultant simulated data $\mathbf{d}'$ with the actual $\mathbf{d}$.

Practically, finding $\mathbf{C}$ empirically is hampered not only by noise, but also by the fact that $\mathbf{O}$ is huge, while we can spend only so much time exploring the parameter space—science exposures are certainly more rewarding. It would help if we had a good idea of what $\mathbf{O}$ looks like. All that is necessary, on paper, is a complete description of the important physical aspects of the instruments. We will see below how far one can go in reality.

In essence, one can implement a two stage process to achieve substantial improvements over the canonical "signature removal" data analysis. Step 1 consists of casting physical principles into code which is capable of simulating observational data. This can be used to generate calibration references that are noise free and contain controllable engineering parameters. At this stage it is straightforward to generate calibration data for a large array of modes that would otherwise have to be covered painstakingly by individual calibration exposures.

After having gained confidence in stage 1, application of optimization techniques, e.g., simulated annealing to simulated data using the physical instrument model, will be step 2 (cf. Rosa 1995).

3. Related Schemes

It is important to note that the process described above differs substantially from many seemingly similar schemes, in that the kernel is an instrument model based on first principles. In observation planning, it is now common practice to simulate the outcome of proposed observations by convolving target models with empirical spectral response curves, adding noise and whatever else the calibration data base can provide. Good examples are the WWW planning tools for the HST instruments. It has also become standard technique now, thanks again to HST, to apply deconvolution techniques and derivatives such as multiple frame analysis (see Hook 1997) to data sets—techniques that usually work best if fed by sophisticated models of the PSF (e.g., TinyTim of HST). Calibration data for HST instrument modes that can not be obtained for reasons of limited time are usually supplied by interpolation between neighboring modes and for all modes forecasted by trend analysis.

The complete physical model of an instrument, in principle, incorporates many of those capabilities. In fact its construction and tuning to actual performance requires a deep understanding based on the experiences gained with many of the tools described above. The big difference is its predictive power.

4. How Far to Go

Exercises such as the FOS scattered light correction (Rosa 1994; Bushouse, Rosa, & Müller 1995) or the FOS dispersion model (Dahlem & Rosa 1997,in preparation) demonstrate that a software model, covering just one particular aspect (here the diffraction and interference properties of gratings and apertures, and the reimaging electron optics of digicons), but going beyond a simple throughput calculation, i.e., correctly describing all relevant physical effects, can be very beneficial in solving problems encountered during the scientific analysis of data. Used in this way, the model appears simply as an additional data analysis tool in support of the calibration process. However, the purpose of this paper is to go one step further, i.e., to advance beyond the "signature removal" calibration strategy currently in use. Had the FOS model been available early on, it would certainly have influenced the specifications for the pipeline, and even earlier the introduction of solar blind detectors.

Obviously, it is necessary to correctly describe all aspects of an instrument to such a degree that the typical percent level accuracy of the canonical calibration can be surpassed. The FOS models mentioned above do not need to incorporate geometric and intensity aspects at once. On the other hand, a model designed to completely cope with the analysis of long slit echelle spectra must be able to predict the geometrical pattern (curvature of orders, of slit images and field distortions), and the blazed sensitivity variations in dispersion direction as well as the spatial intensity profiles (LSF and interorder background).

5. Current Activities

A generic echelle spectrograph model, such as described above, is currently under construction in a collaborative effort between ESO and the ST-ECF. Its immediate application will be to the UVES spectrograph under construction for the VLT observatory and the STIS instrument to be working on HST after the servicing mission in February 1997.

The basis of this effort is a library of C++ classes that provide equipment modules, e.g., grating, mirror, filter, detector, and optical rays (the targets passing through the equipment), as well as modules for other ingredients such as targets, interstellar extinction, and atmospheric properties to compose instrument models and simulate observations (see also Ballester, Banse, & Grosbøl 1997).

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