Spectroscopy Methods Summary
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Abstract

This paper is a summary of the methods I use for my spectroscopic work. This information is specifically to allow the user of the spectra to understand the general techniques I use. If more information is desired concerning the backup information and alternative methods I have investigated, please contact me. My intention is that all information on software, spreadsheets, microprocessor control, etc shall all be available to any interested party.

Introduction

For spectroscopy, I generally use my f3.5 18 in. Newtonian on an AP1200 mount in a Pro Dome observatory as described at www.menkescientific.com. The spectrometer is an SBIG DSS7 coupled to an SBIG ST402 camera. I can and do operate the entire system remotely from my home 400 ft. away. Once started on a target, I generally run the spectrometer observation unattended.

Because the DSS7 is designed for f/10 optics, using it on the f3.5 N18 would waste about 90% of the light as the large light cone is lost inside the DSS7. After theoretical and experimental investigation, I have settled on using an f3 Barlow lens (2 inch from Siebert Optics) to match the DSS7 to the telescope. The star image size is usually around 4-5 pixels (2.7a-s), which slightly overfills the 50u narrow slit on the DSS7. Where possible, I operate using the 100u slit (10pixels wide) to assure total light capture and to reduce guiding requirements.

I should note that the DSS7 is a low dispersion spectrograph of R=100. Using the ST402, it will display the entire visual spectrum over about 700 pixels at a best resolution of about 35A (somewhat better for guided star images). The DSS7 is a wonderful device, but as supplied does have features that limit its use or make it very awkward. These include
- At f10, it has limited ability to operate with faster optical systems
- Awkward to change among Slit/Direction/Spectrum operational modes
- Difficulty in placing target object on the slit
- No provision for tracking (keeping target on slit)
- Very limited software for data taking and analysis

The modifications to the DSS7 operation that I describe here take advantage of the wide variety of user software accessible functions in the imaging software MaximDL working with Visual Basic scripts (programs). I use MaximDL both during imaging, and to read (measure) the resulting images, and then an Excel spreadsheet to produce the final spectrum.

Mode Changing and Target Alignment

The DSS7 spectrometer is a slit spectrometer with a resolution of approximately 7A per pixel when used with an ST402 9u CCD image. The DSS7 can be operated in three modes:
- Slit. For giving an image of the slit, so that you know where the slit is on the image.
- Direction. This yields a fair quality sky image through the system and shows you the position in the field of where the various objects (stars, comet) are. The problem is to place the object on the slit location by moving the telescope.
- Spectrum. This mode takes a spectrum of whatever is on the slit.

SBIG uses the telescope guiding ports built into SBIG cameras to provide the control signals to switch among the four modes. The DSS7 software working in CCDOPS allows choosing the mode or one can use Maxim manually to change modes; however, either method is very awkward. To make it easy to control, I developed my own VB software to provide automatic mode control using a small menu program. For a

variety of reasons, I then developed a simple microcontroller under RS232 serial control (from a program in the PC) to control the mode directly without using the guide ports, thus freeing the ports for use in guiding the telescope as discussed below.

Using this system, I can select the "Slit" mode, and then expose to make an image of the slit. The control software makes an outline of the slit, and then can superimpose the outline onto an image taken in the "Field/Direction" mode. The user can manually or with a control button adjust the telescope pointing to place the target into the slit outline. Then, selecting the "Spectrum" mode, the user takes an image of the spectrum. Using my own control program with MaximDL, I can automate this entire operation. These operations are described in more detail on the website.

Tracking

Once a target object is on the slit, the question becomes how to keep the target on the slit over many minutes or hours of exposure. After review and experimentation, I implemented a method of taking and saving the spectral image (typically 120s), then switching to the direction mode to re-image the target field. The software then adjusts the telescope to realign the target to the known slit location, and the cycle repeats. In general, the tracking rms error of positioning is about 1 pixel over two hours. I orient the DSS7 so that the slit is E-W, i.e., mount periodic error shifts the spectrum "up and down" in the slit so that wavelength or capturing the photons is not affected. The figure shows an image of the control software "window". Note that rather than use after the fat guiding corrections, one could use a pickoff mirror to continuously sample the image coming to the DSS7 and to correct the telescope pointing on a real-time basis. There are both pros and cons of this method; however, a major drawback is that the steep light cone of a fast telescope makes it very difficult to insert an effective pickoff device.

Fig XX shows a screen shot from a typical observing session.
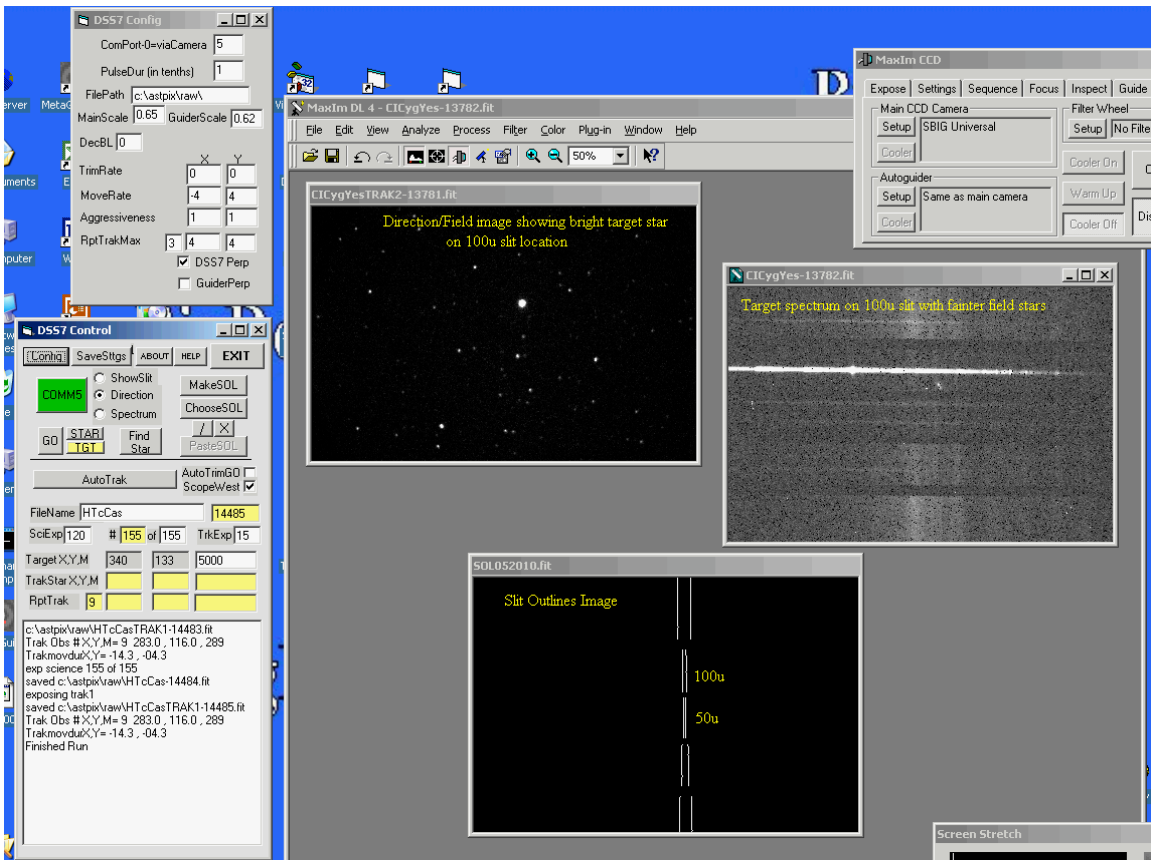
Data Reduction and Calibrations

I use TheSky5 for telescope control, and MaximDL (and ASCOM) for camera control to take the spectral and other images, and to make the measurements from the images. I then use Excel to tabulate and analyze the spectral data.

After taking the spectrum, one would need to perform a dark and bias (and perhaps flat) calibration on the image. In general, the image will likely be slightly rotated with respect to horizontal, so I use the MaximDL Edit/Rotate function to align the spectrum parallel to the edge of the image. Hot and cold pixel removal and other mild processing may also be appropriate (using the Maxim View/CommandSequence automates all these steps).

There are, as always, complications! For example, with a faint object, one might take 20-100 2-minute spectra, each of which shows a very faint spectrum. Using the automated tracking, these are usually very well aligned vertically. If not, using Maxim/Overlay one can quickly align them to the same position without affecting the wavelength calibration. One can then do a simple combine to yield the final spectrum to be measured.

To convert the spectral image to a (digital) line graph, I use MaximDL View/LineProfile function by drawing a narrow box around the desired part of the spectrum. The result is a graph that is saved as a simple comma separated variable (CSV) text file for later pasting into Excel or another program. I then move the same narrow box up and down the slit to obtain measures of the background for later subtraction (using the spreadsheet) from the spectrum. Although MaximDL supports various forms of pixel math that would allow one to perform calculations directly on the spectra, I find it better to use Maxim to prepare the best possible combined spectrum, then perform all calculations in Excel using data taken from the images. It is both easier, permits a clear record of the calculations performed on the data, and makes it easy to custom fit calculations to the data.

Calibration

Initial energy calibration may be done using a small fluorescent lamp (operated remotely shining on the interior of the observatory). Wavelength can also be checked by observing the inevitable atmospheric absorption (Telluric) lines in the red end of the spectrum of the target and reference star spectra, as well as known lines in the spectra.

Further calibration beyond wavelength calibration is needed to correct for the instrumental response of the instrument, as well as the effects of the earth's atmosphere. To accomplish this, we take a reference star spectrum (e.g., a B- or A-class star), and then divide the observed spectrum by the "true" spectrum taken from a spectrum library (I use the library in Vspec). This ratio then gives the calibration correction for use on the target (unknown) spectrum.

This calibration process is quick and easy using my own spreadsheet. The sheet has several areas
- Fluorescent calibration. This allows the user to identify the pixel number of two known lines, then calculate the wavelength of each pixel across the spectrum
- Target Spectral data. The text file data for the spectrum and upper and lower background that were generated in Maxim are copied from the csv files and pasted into the spreadsheet. This immediately gives the raw spectrum. The wavelength calibration can be adjusted if needed, as can the amplitude.
- RefStar Data. A similar portion of the spreadsheet allows the RefStar spectral data to be entered.

- Calibration. The intensity calibration has a space to paste the wavelength and intensity from the spectrum library (the "true" reference star spectrum). I usually use the convenient library spectra that are a part of VSPEC (see below). The spreadsheet then matches the library wavelengths to the RefStar wavelengths, and takes the ratio. The ratio usually has artifacts from inaccurate matches for emission or absorption lines, so an automated routine removes these (usually the H features, but not the red Telluric features) using linear interpolation. Note that the ratio curve is not otherwise smoothed. This final ratio is then applied to the target spectrum to generate the corrected final spectrum. Note that at the extremes of the spectrum, the corrections may exceed x2-4, so the results have less accuracy as one goes to the ends of the wavelength range. The figure shows a typical result of this analytic procedure.
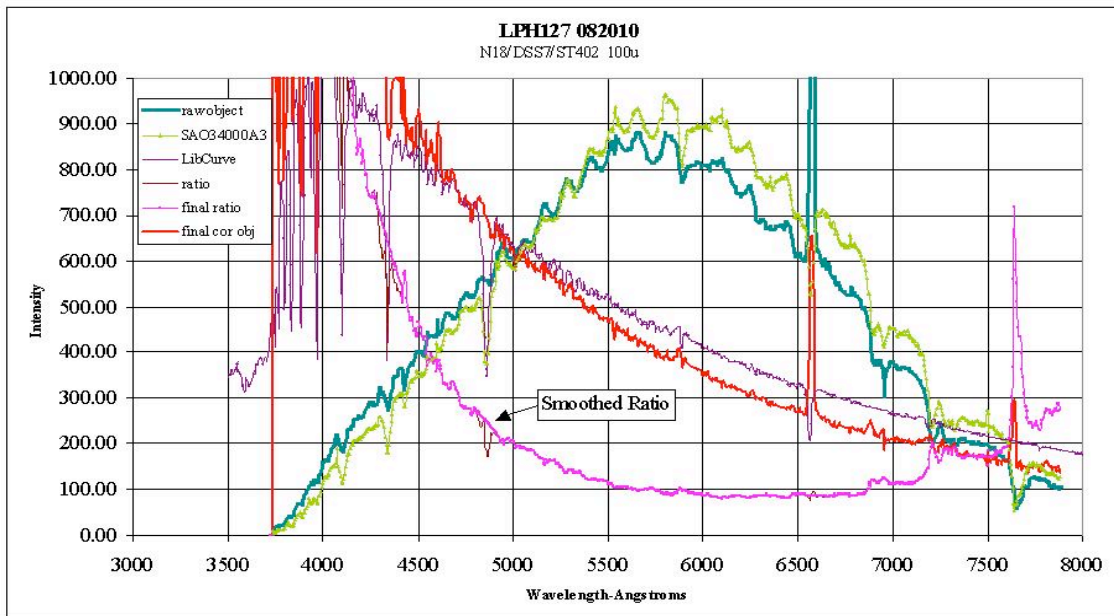
This method of analysis: using MaximDL to generate the spectral image and its text files, then using Excel for the quantitative analysis, has the great advantage of being fully under the user's control and observation, while making it easy to repeat or modify the method of analysis at any later time, and to allow easy preparation of graphs or other figures as desired. It is also easy to prepare a simple text file of wavelength and intensity for sending to users of the data.

VSPEC

I have mentioned using the library of reference star spectra that are a part of the VSPEC program. VSPEC is a free program written by Valerie Desnoux, and is available from the very active French spectroscopy group at http://www.astrosurf.com/buil/ and related web sites. VSPEC allows the user to open a fits spectroscopy image and perform the various manipulations hat are needed (rotation, scaling, calibration, division, etc). So, why do I not use that program and instead use Excel spreadsheets for my analysis and data display?

I have used Vspec, and have great respect for the writers and the many features that are in the program: Simply reading the HELP file is a good education! However, some users have found Vspec to be less than robust: if you do some things in the wrong order the program crashes. I would also note that Vspec does have a substantial learning curve, as does Excel for a new user. However, the learning put into Excel can also be used in many other applications. Some of us find that many of the steps and manipulations are not intuitive, and can be confusing.

Perhaps most important, when using Vspec for a complex series of calculations as discussed above, one has the result, but no real record of the steps taken to get there: one cannot go back and inspect, or check, or

modify, the process that was used to arrive at the final answer. Often, after a spectral analysis, the user will want to tweak some aspect of the analysis-this is difficult or impossible in Vspec, as compared to a spreadsheet that shows all the steps and allows them to be traced, copied, or modified. Indeed, the whole process of analysis in the spreadsheet is automated--more so than when using Vspec.

Also, after the job is done, one usually wants to present the results in a particular way--the graphs need particular scales or labels, or other steps need to be taken with the data. Often, one wants to customize a graph by putting several curves on the same graph--this is possible, but not easy, in Vspec. Excel, for all its faults, does have quite good facility with this.

Spectrometer Control Program

Fig XX shows an image of the spectrometer control program windows. Here is an outline of the controls and functions.

- The upper window is the configuration window. Scales are the image scales (a-s/pixel)
- TrimRate is the rate the user can impose on the telescope
- MoveRate is the rate (pixels/sec) of the telescope guide rate
- Aggressiveness is a multiplier for the MoveRate
- RptTrakMax is how many guiding images and corrections will be made in each cycle, and the pixel accuracy settings for the pointing
- DSS7Perp is whether the RA is on the X-axis or the Y-axis

The main window is as follows
- Comm5 starts the serial connection to the spectrometer controller
- ShowSlit/etc select the modes
- MakeSOL makes a slit outline from a SLIT exposure
- ChooseSOL chooses which image contains the slit outline
- PasteSOL pastes the slit outline onto a fresh Direction/Field image
- AutoTrak turns on/off the auto guiding
- AutoTrimGO turns on the user imposed telescope move rate (e.g., to follow a comet)
- ScopeWest tells whether the scope is on the west or east of the mount
- FileName and number is for the image names, plus a running image counter
- SciExp is spectrum exposure duration, TrkExp is the tracking exposure duration
- Target X,Y,M is the S,Y for the guiding star (may be different from the target) and the ADU as measured by a R=20pixel aperture
- TargetStar and RptTrak show the X,Y,ADU for the successive tracking exposures
- Large window shows the latest entries in the running log of actions

DSS7 Config

ComPort-0=viaCamera 5
PulseDur (in tenths) 1
FilePath c:\astpix\raw\
MainScale 0.65 GuiderScale 0.62
DecBL 0
                    X   Y
TrimRate   0   0
MoveRate   -4   4
Aggressiveness   1   1
RptTrakMax   3   4   4
☑ DSS7 Perp
☐ GuiderPerp

DSS7 Control

Config SaveSttgs ABOUT HELP EXIT

COMM5 ○ ShowSlit   MakeSOL
       ● Direction   ChooseSOL
       ○ Spectrum
                      / X
GO STAR/TGT Find Star   PasteSOL

AutoTrak   AutoTrimGO ☐
                  ScopeWest ☑

FileName HTcCas   14485
SciExp 120   # 155 of 155   TrkExp 15
Target X,Y,M 340   133   5000
TrakStar X,Y,M
RptTrak   9

c:\astpix\raw\HTcCasTRAK1-14483.fit
Trak Obs # X,Y,M= 9 283.0 , 116.0 , 289
TrakmovdurX,Y= -14.3 , -04.3
exp science 155 of 155
saved c:\astpix\raw\HTcCas-14484.fit
exposing trak1
saved c:\astpix\raw\HTcCasTRAK1-14485.fit
Trak Obs # X,Y,M= 9 283.0 , 116.0 , 289
TrakmovdurX,Y= -14.3 , -04.3
Finished Run