Goodman HTS Pipeline User Manual

version 0.1

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Contents

Introduction

This is the User Manual for the *Goodman Spectroscopic Data Reduction Pipeline*. It provides an overview of the pipeline's main features, instructions on its use and how to run it on our dedicated *SOAR Data Reduction Server*, and installation instructions for those who wish to run it on their own computers.

Overview

The Goodman Spectroscopic Data Reduction Pipeline - GOODSPEC - is a Python-based package for producing science-ready, wavelength-calibrated, 1-D spectra. The goal of **goodspec** is to provide SOAR users with an easy to use, very well documented software for reducing spectra obtained with the Goodman spectrograph. Though the current implementation assumes offline data reduction, our aim is to provide the capability to run it in real time, so 1-D wavelength calibrated spectra can be produced shortly after the shutter closes.

The pipeline is primarily intended to be run on a data reduction dedicated computer. Instructions for running the software are provided in the Using Pipeline section of this guide. The Goodman Spectroscopic Data Reduction Pipeline project is hosted at GitHub at it's GitHub Repository.

Currently the pipeline is separated into two main components. The initial processing is done by `redccd`, which trims the images, and carries out bias and flat corrections. The spectroscopic processing is done by `redspec` and carries out the following steps:

- Identifies multiple targets (spectra of more than one object in the slit)
- Trace the spectra
- Extract the spectra
- Estimate and subtract background
- Find the wavelength solution. Defaults to automatic wavelength solution, but can be done interactively
- Linearize data (resample)
- Write wavelength solution to FITS header
- Create a new file for the wavelength calibrated 1D spectrum

Features

- Self-contained, full data reduction package for the most commonly used spectroscopic setups with Goodman. Given the almost limitless number of possible configurations avaliable with the Goodman instrument, only the most popular configurations will be supported, though we will try to add as many modes as possible.
- Python based, using existing Astropy libraries as much as feasible.
- Extensively documented, using general coding standards: PEP8 – Style Guide, PEP257 – Docstrings Convention (in-code documentation) – Google Style
- Multiplataform compatibility (tested on Linux Ubuntu, CentOS and MacOSX).
- Modular design. Could be used as a library within other Python applications.

Ways to run the pipeline

There are two ways to use the pipeline.

1. **Run it directly on a SOAR data reduction server** that you can access using VNC.
2. **Download and install the pipeline** (go to the Install section of this manual). Though we will try our best to provide answers to quick and simple installation issues, we cannot provide general installation support.

What the pipeline does not do

- In its current version the pipeline does not perform combination of individual spectra. If you obtained several individual exposures of the same object, they will be output as separate 1-D, wavelength-calibrated spectra
- There is yet no flux calibration. We are working on a module that will do this.
- This pipeline does not evaluate nor select data by quality. It will simply try to run using all existing files. **Make sure you only have good data in the folder that will be reduced**.

General Considerations on using the pipeline

The Goodman Spectroscopic Pipeline is meant to work as a single package. However, the full process is split in two separate modules: `redccd` and `redspec`. The first does the basic 2D image reduction, applying bias and flat field corrections, and cosmic ray removal. The second module, `redspec`, takes the corrected 2D images output by `redccd` and produces wavelength-calibrated 1D spectra.

The pipeline is run from the command line in a terminal window. Each module is run separately, first `redccd` followed by `redspec`, however, you could run both sequentially from e.g. a shell script.

In order to make things easier you should organize your data:

1. Make sure all the data in your folder corresponds to the same binning, readout mode, region of interest (ROI), and grating/wavelength mode combination.
2. You should have bias, flats (quartz or dome flats), and the appropriate comparison lamps. Other files like acquisition images, slit images and focus images should be deleted.
3. Do not mix dome flats with quartz lamp flats. As an example, suppose you took both quartz lamps and dome flats for your targets. You could create two folders, one with the science data and the dome flats, and another with the same science data and the quartz lamps. Then, if you run the pipeline in each folder you can compare the results and decide which type of flat works best for my particular case.

Command line arguments

For a list of the options and command line arguments type `--help` argument:

For `redccd`

```
usage: redccd [-h] [--auto-clean] [--cosmic <method>]
              [--dcr-par-dir <dcr.par_directory>] [--debug]
              [--flat-normalize <normalization_method>]
              [--flat-norm-order <order>] [--ignore-bias] [--ignore-flats]
              [--keep-cosmic-files] [--log-file <log_file>]
              [--raw-path <raw_path>] [--red-path <red_path>]
              [--saturation <value>]

Goodman CCD Reduction - CCD reductions for Goodman spectroscopic data.

optional arguments:
  -h, --help            show this help message and exit
  --auto-clean          Automatically clean reduced data directory
  --cosmic <method>     Clean cosmic rays from all data. Options are: 'dcr',
                        'lacosmic' or 'none'. Default is 'dcr'. See manual for
                        full description of dcr.
  --dcr-par-dir <dcr.par_directory>
                        Directory of default dcr.par file
  --debug               Show detailed information of the process.
  --flat-normalize <normalization_method>
                        Choose a method to normalize the master flat
                        forspectroscoy. Choices are: mean, simple (model) and
                        full (fits model to each line).
  --flat-norm-order <order>
                        Defines the order of the model to be fitted. Default
                        to 15
  --ignore-bias         Ignore bias correction
  --ignore-flats        Ignore flat field correction
  --keep-cosmic-files   After cleaning cosmic rays with dcr, do not remove the
                        input file and the cosmic rays file.
  --log-file <log_file>
                        Name for log file. Default name is goodman_ccd.log.
                        The file is written in <red_path> and will be deleted
                        each time you run this program
```

```
  --raw-path <raw_path>
                        Path to raw data.
  --red-path <red_path>
                        Path to reduced data.
  --saturation <value>  Saturation limit. Default to 65.000 ADU (counts)
```

And for `redspec`

```
usage: redspec [-h] [--data-path <Source Path>]
               [--proc-path <Destination Path>]
               [--search-pattern <Search Pattern>]
               [--output-prefix <Out Prefix>] [--extraction <Extraction Type>]
               [--reference-files <Reference Dir>] [--interactive] [--debug]
               [--log-to-file] [--max-targets <max targets>] [--save-plots]
               [--plot-results]

Extracts goodman spectra and does wavelength calibration.

optional arguments:
  -h, --help            show this help message and exit
  --data-path <Source Path>
                        Path for location of raw data. Default <./>
  --proc-path <Destination Path>
                        Path for destination of processed data. Default <./>
  --search-pattern <Search Pattern>
                        Pattern for matching the goodman's reduced data.
  --output-prefix <Out Prefix>
                        Prefix to add to calibrated spectrum.
  --extraction <Extraction Type>
                        Choose a which extraction to perform. Simple is a sum
                        across the spatial direction after the background has
                        been removed. Optimal is a more advanced method that
                        considers weights and profilefitting.
  --reference-files <Reference Dir>
                        Directory of Reference files location
  --interactive         Interactive wavelength solution.Disbled by default.
  --debug               Debugging Mode
  --log-to-file         Write log to a file
  --max-targets <max targets>
                        Maximum number of targets to be found in a single
                        image. Default 3
  --save-plots          Save all plots in a directory
  --plot-results        Show wavelength calibrated spectrum at the end.
```

Lists of Reference Lamps Available

The automatic wavelength calibration relies on having previously calibrated reference lamps obtained in the same configuration or mode. It is also important that the lamp names are correct, for instance `HgAr` is quite different than `HgArNe`. For interactive wavelength calibration, reference lamps are used as a visual aid only. It lets you find the matching laboratory lines values that will be used to fit a pixel to wavelength relation that we call *Wavelength Solution* The list of lamps is the following.

Grating	Mode	Filter	Lamp
400	M1	None	HgAr
400	M1	None	HgArNe
400	M2	GG455	HgAr
400	M2	GG455	HgArNe
600-old	Blue	None	HgAr
600-old	Blue	None	CuHeAr
1200	M2	None	CuHeAr
1200	M3	None	CuHeAr
1200	M5	GG455	CuHeAr

Adding new reference lamps

It is possible to add new lamps very easily you just need a raw lamp that meets the following specifications with respect to your science project:

- Same instrument configuration or mode
- Same Grating
- Same order blocking filter if present
- Same binning
- Same lamp/combination that you use in your observations
- Smallest slit possible. Equal is OK too.

Then you can use the interactive mode or other software (such as IRAF) to produce a wavelength-calibrated 1D spectrum. Now you have to options, identify the system folder where the lamps that come with the package are saved and simply put it there or put it in another directory and use the argument `--reference-files`

```
redspec --reference-files /path/to/ref-lamp-location
```

Or contact `storres [at] ctio [dot] noao [dot] edu` and we will make it available as a package file.

Running the pipeline in the SOAR data reduction computer

The Goodman Spectroscopic Data Reduction Pipeline has been installed on a dedicated computer at SOAR. The procedure is to open a VNC session, for which you need to be connected to the SOAR VPN. The credentials for the VPN are the same you used for your observing run, provided by your *Support Scientist*, who will also give you the information for the data reduction computer VNC connection.

Note

IRAF is available in all three data servers. Running `iraf` will open an *xgterm* and *ds9* windows. `iraf-only` will not open *ds9*

Establish a VNC connection

Separately, you should receive a server hostname, IP, port and VNC-password. If you don't you can ask for it. We have decided to use a similar organization of vnc desktops:

For the rest of this tutorial we will assume your host name is `vnc-server` the port is `1` and your password is `password`. Though we recommend using RealVNC, most other VNC clients will work fine (e.g., Remmina in Linux). For GNU/Linux and Mac OSX machines we suggest the RealVNC Viewer client. For Windows machines, we suggest either the RealVNC Viewer client or the UltraVNC viewer client. We also know that Vinagre and vncviewer on GNU/Linux work fine.

VNC from the Terminal

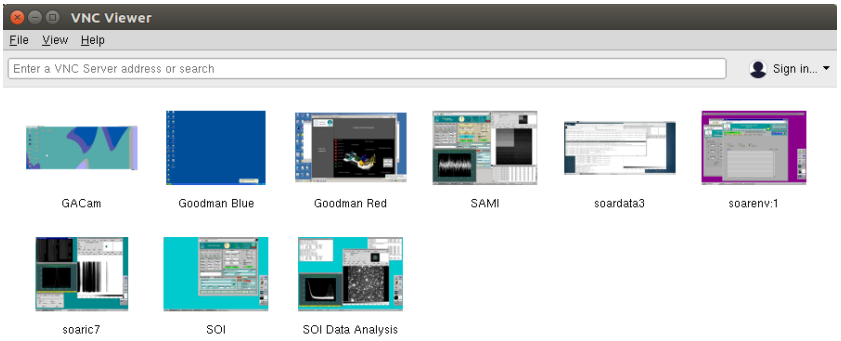
Open a terminal, and assuming you have installed `vncviewer`.

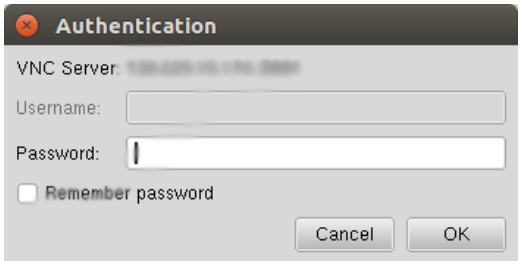
```
vncviewer vnc-server:1
```

You will be asked to type in the *password* provided.

VNC using a Graphical Client

Using a graphical VNC client is quite similar and intuitive





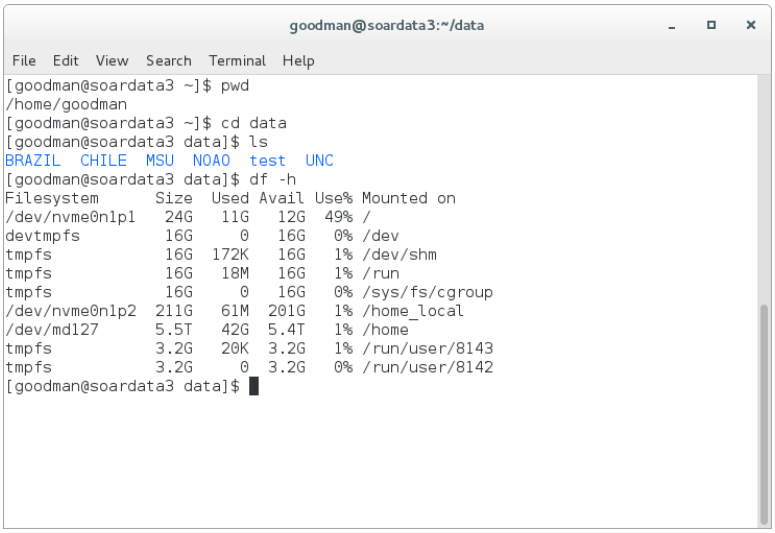
In this case the *IP address* was used, which is equivalent and sometimes better.

Running the Pipeline

1. Open a Terminal
2. Go to `/home/goodman/data`

   ```
   cd /home/goodman/data
   ```

3. Here you have a workspace to put your data according to your institution.



4. Create a data folder inside your workspace.

   ```
   cd NOAO
   ```

   ```
   mkdir 2017-07-05
   ```

   ```
   cd 2017-07-05
   ```

5. Copy your data from Goodman Computer

   ```
   scp observer@soaric7:/home3/observer/GOODMAN_DATA/NOAO/2017-07-05/ ./
   ```

6. Make sure you have a full data set. At this point your observing logs will become very useful, eliminate focus sequence, aquisition exposure and any other file present that will not be needed for the processing. The following list summarizes the kind of data that you need to fully process your data.

   - BIAS: Bias
   - FLAT: Flats
   - COMP: Comparison Lamps
   - OBJECT: Science Frames

   Also make sure your data has the same *readout speed*, *binning*, and *ROI*. If you used different configurations during the same night, we recommend you to set up a separate folder for each.

7. Run `redccd`:

   If you are running `redccd` for the first time you can use `redccd` alone but if it's a second or third time you will need to use `--auto-clean` which is a built-in protection for your data, in case you don't want to delete what has been done. Also you might want to consider `--saturation <new value>` to change the saturation level if you get all your flats rejected due to saturation. Sometimes there is a hot column at the end that produced very high values.

   ```
   redccd --auto-clean
   ```

   In case you want to use `--saturation` here is an example:

   ```
   redccd --auto-clean --saturation 70000
   ```

This changes the saturation level to *70000 ADU*` in this context the saturation value works as a threshold for rejecting images and it varies from one instrument configuration to another.

By default, `redccd` puts reduced data in a subdirectory `RED`, you can provide a different one by using `--red-path`.

An image `image_file.fits` that has been fully (and propperly) processed should have the new name (including the reduced data folder):

```
cfzsto_image_file.fits
```

The meaning of every letter in `cfzsto` is summarized in the following table:

Letter	Meaning
c	Cosmic ray cleaned or mask created depending on the method
f	Flat corrected
z	Zero or Bias corrected
s	Slit trimmed, trims off the non-illuminated sections of the detector
t	Initial Image trimming
o	Overscan corrected

8. Run `redspec`:

   By default `redspec` will search for images with the prefix `cfzsto`, in case you have produced a different prefix you can change it by using `--search-pattern`

   You can just run `redspec` in case everything is the default but if this is the first time you run the pipeline we suggest:

   ```
   redspec --plot-results
   ```

   In that way two important plots will be shown full screen, the comparison lamp fitted to a reference comparison lamp and some values for the wavelength solution fit and the extracted spectrum plotted with the wavelength solution.

   The final image has a `g` added to the start of the name, following the above example your final 1D and wavelength calibrated image will be named:

   ```
   gcfzsto_image_file.fits
   ```

Using the Interactive Mode

If you need to make sure that your solution is the best possible you can use the *Interactive Mode*. Some of the key features are:

- Manually match spectroscopic lines
- Zoom in to get a better reference
- Evaluate the quality of your solution
- Uses a visual reference for matching the lines
- Uses laboratory values for reference lines

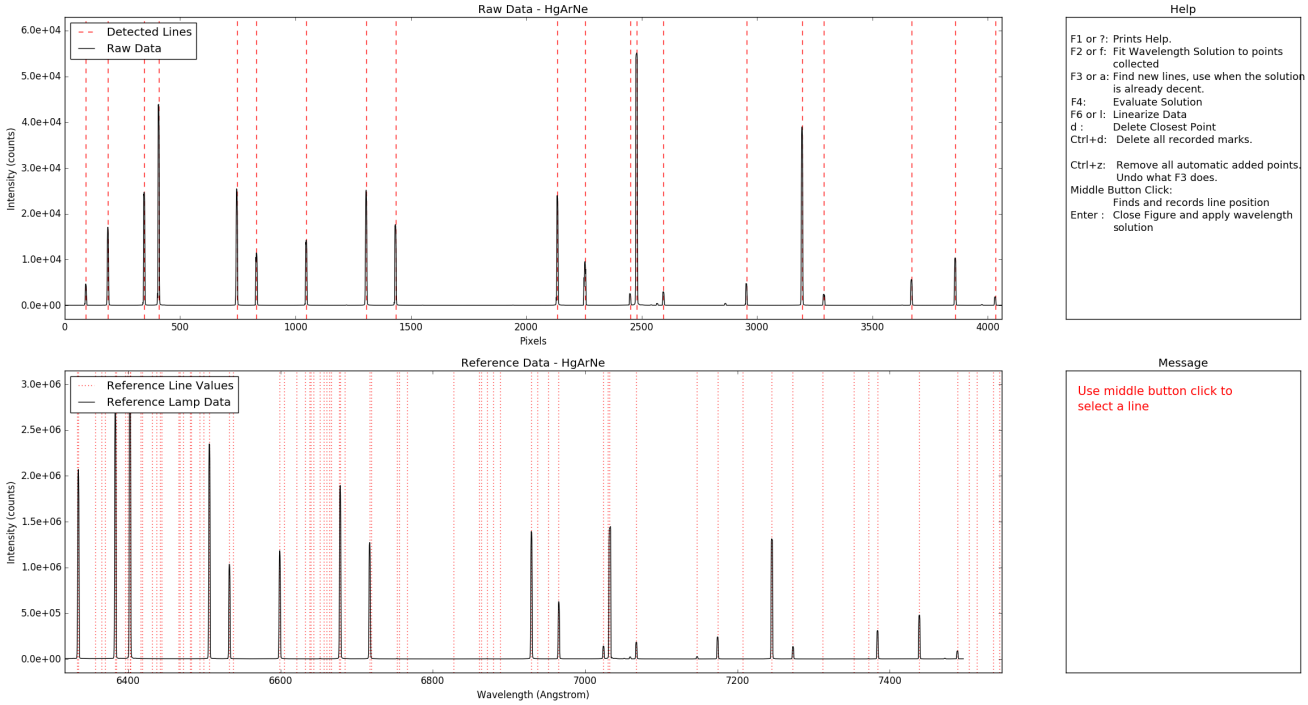
Right now it uses matplotlib as the underlying tool to enable interaction.

Below you will see a sequence as well as a description of the procedure to use the interactive mode.

1. The interactive screen has four subplots. In the *Upper main panel* you have the raw comparison lamp, i.e. your comparison lamp 1-D-extracted but without wavelength solution, the dashed red lines represent the lines found by the pipeline. In the *Lower main panel* you have the reference lamp. This is a previously calibrated lamp that is distributed with the package (also you can use your own). In this case the red lines are the laboratory values obtained from the NIST Atomic Spectra Database site (https://physics.nist.gov/PhysRefData/ASD/lines_form.html). The *Upper right panel* is a static help, intended to give you a quick and easy-to-reach help. Finally, the *Lower right panel* is an information window, in fact it

serves three main purposes:

- Display messages and warnings.
- Shows you a zoomed line.
- Displays the wavelength solution quality information.

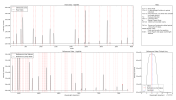


2. The way you interact is by using your mouse and keyboard. The following table describes all the available keyboard commands with their respective keys and/or buttons, and a summary of their functionality.

Main Key	Alternative Key	Mouse Equivalent	Description
?	F1	None	Print Help message on the terminal
f	F2	None	Fit a function to collected points
a	F3	None	Find lines automatically
None	F4	None	Evaluate wavelength solution
d	F5	None	Remove point closest to the mouse pointer
l	F6	None	Linearize and smooth spectrum
m	None	Middle Button	Register the line closest to the mouse pointer
ctrl+z	None	None	Deletes ALL automatically added points
ctrl+d	None	None	Deletes all recorded points
ctrl+q	None	None	Ends the program
Enter	None	None	Accepts wavelength solution and closes the figure

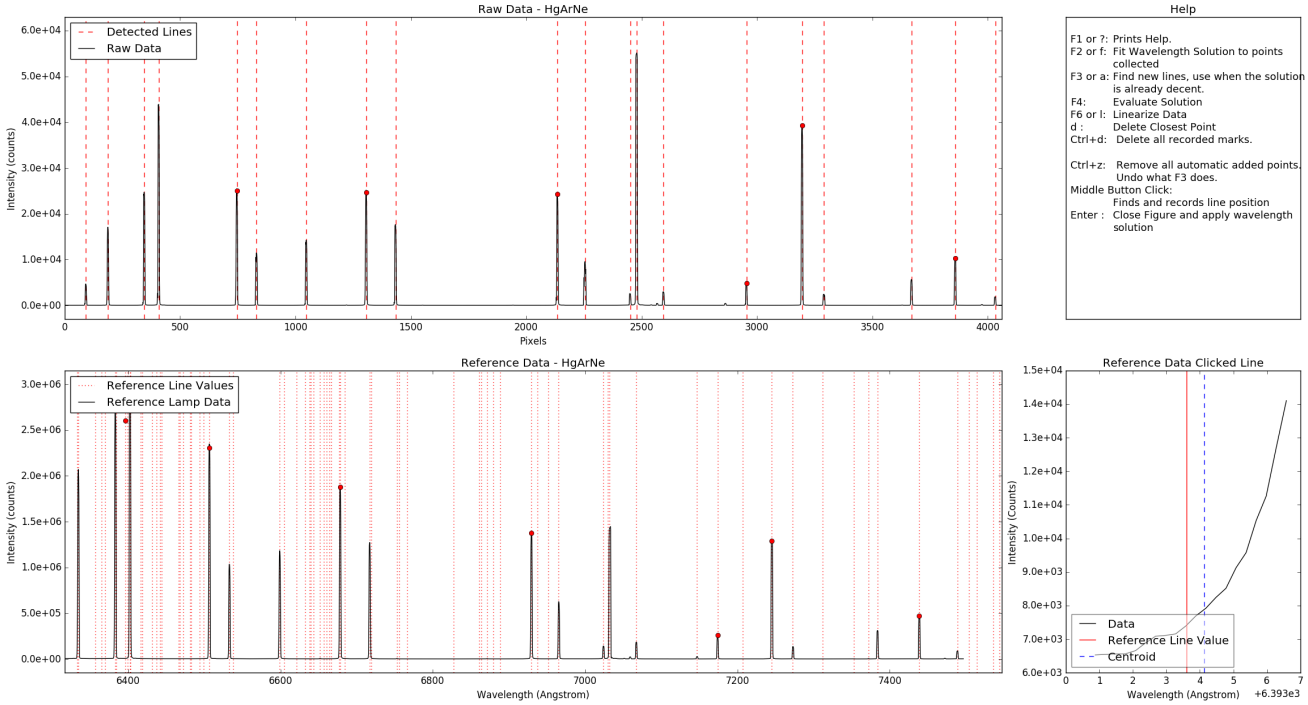
It is advisable to practice a little bit to get familiar with this combination of keys and functions. Since we are still in the development stage, if you feel that the use of a key creates problems for you let us know.

In the following image the mouse pointer was placed very close to the center of the line and then with a middle button click the line is marked with a red circle. The software will calculate a centroid (vertical dashed blue line) and then will try to find the closest reference value (vertical red line). Keep in mind that the reference data (red dotted lines) are not the *reference lamp* lines themselves but values obtained from the NIST site indicated above.

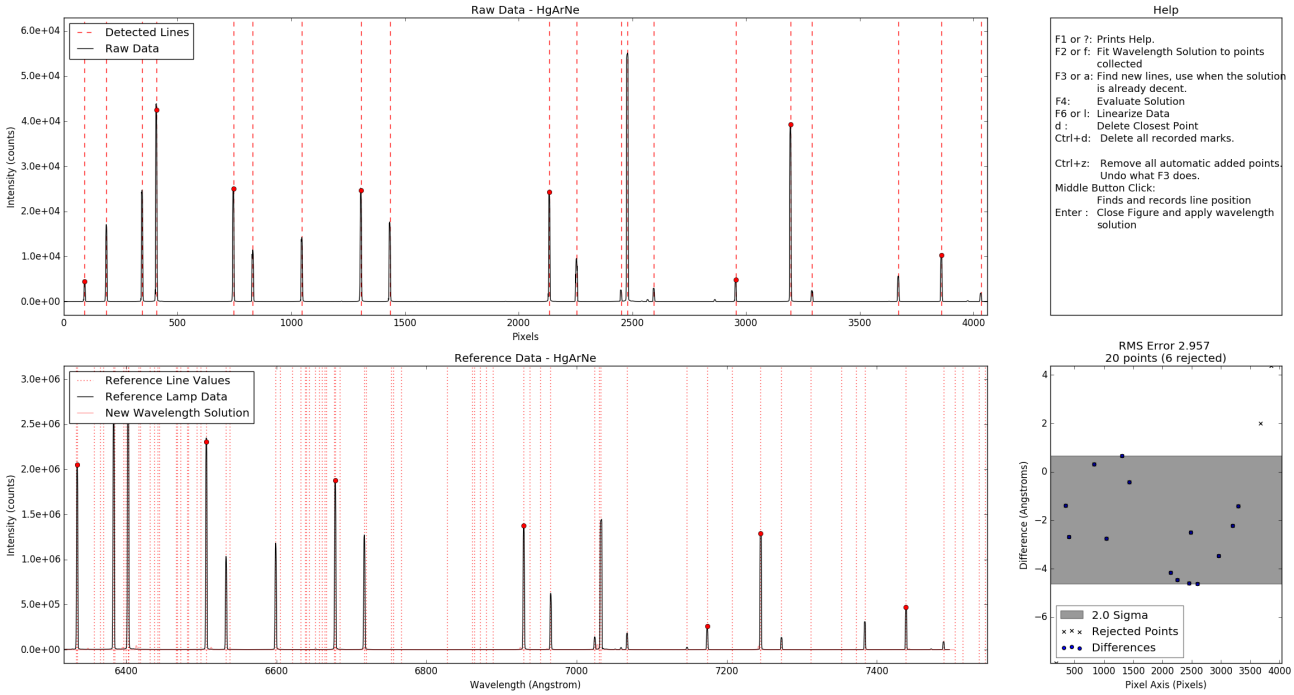


Then you have to find the corresponding line in the opposite plot. There is no preferred plot to start as long as you are consistent with the order in which you mark the lines.

3. In case you miss-identified a line, like in the image below, you can place the mouse pointer above the corresponding red circle and press **d** to delete it. It will search for the closest mark along the horizontal axis and remove it. If there is a counterpart in the opposite plot it will delete it too.



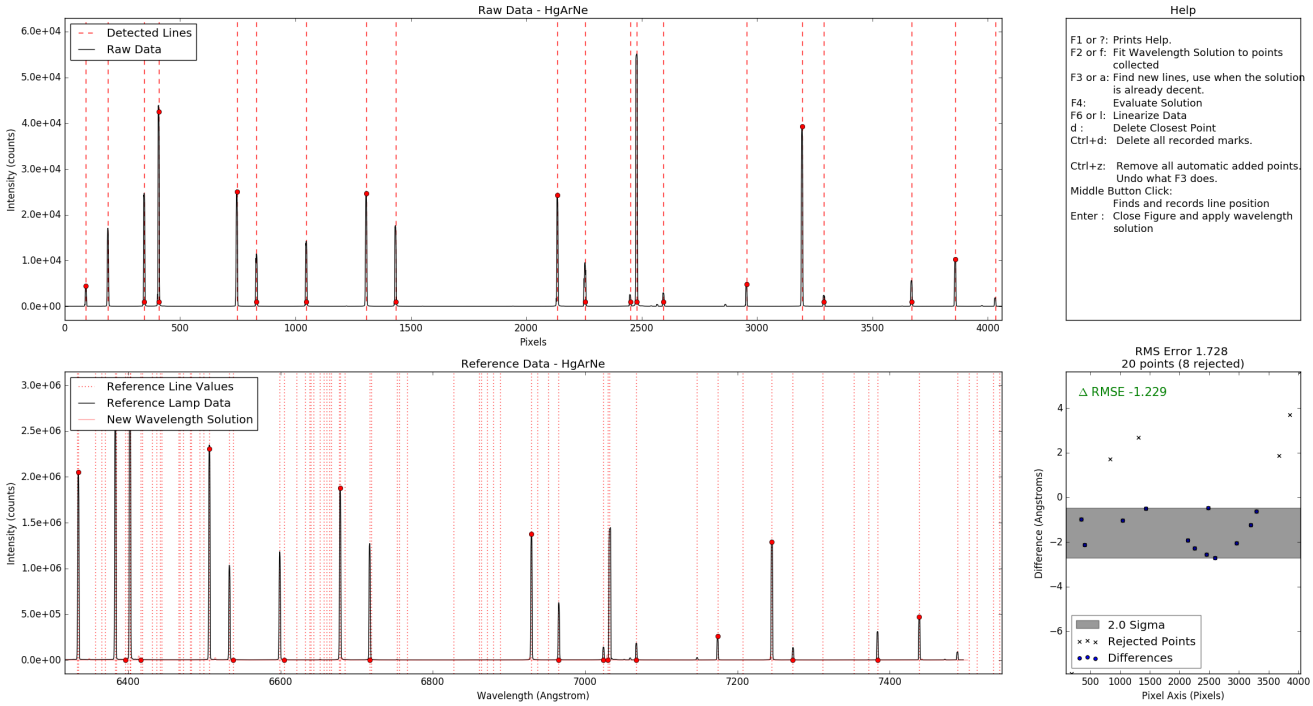
4. Once you matched a good number of lines, the minimum required by the fitting routines are four, you can either press F2 or **f** to make a fit of the pixels and angstrom values collected. Now the *Lower Right panel* will show the scatter plot of the fit. It is important to note here that the points in this plot do not represent the points you marked but rather each of the lines detected in your extracted 1-D comparison lamp spectrum (red dashed lines in the *Upper main plot*) It does one iteration of a 2-sigma clippinp to reject outliers, and then it uses those values to calculate the Root Mean Square Error. In the example we show here the RMS is a bit high, but we will fix that below.



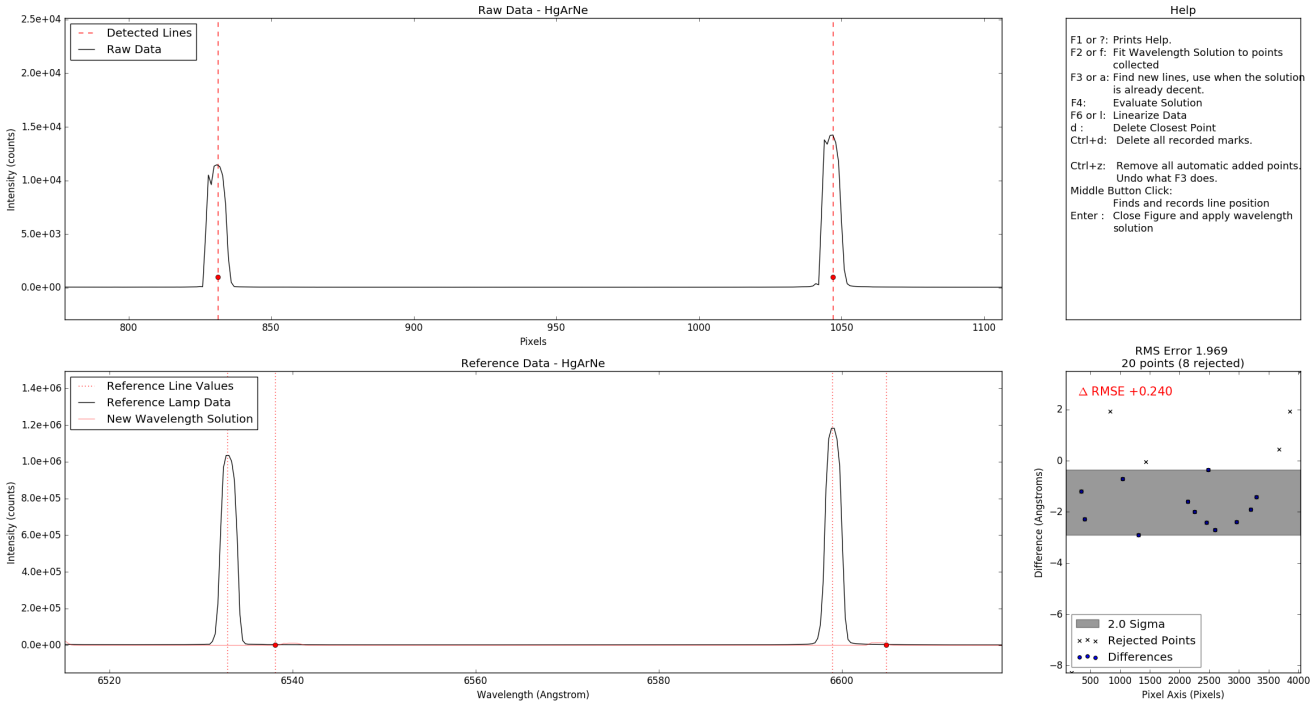
5. If you see that your current solution is decent you can press F3 or **a** and the pipeline will try to find more points automatically. The new matches found

by the software are shown as red dots at the base of each line in the two main *Upper* and *Lower* panels.

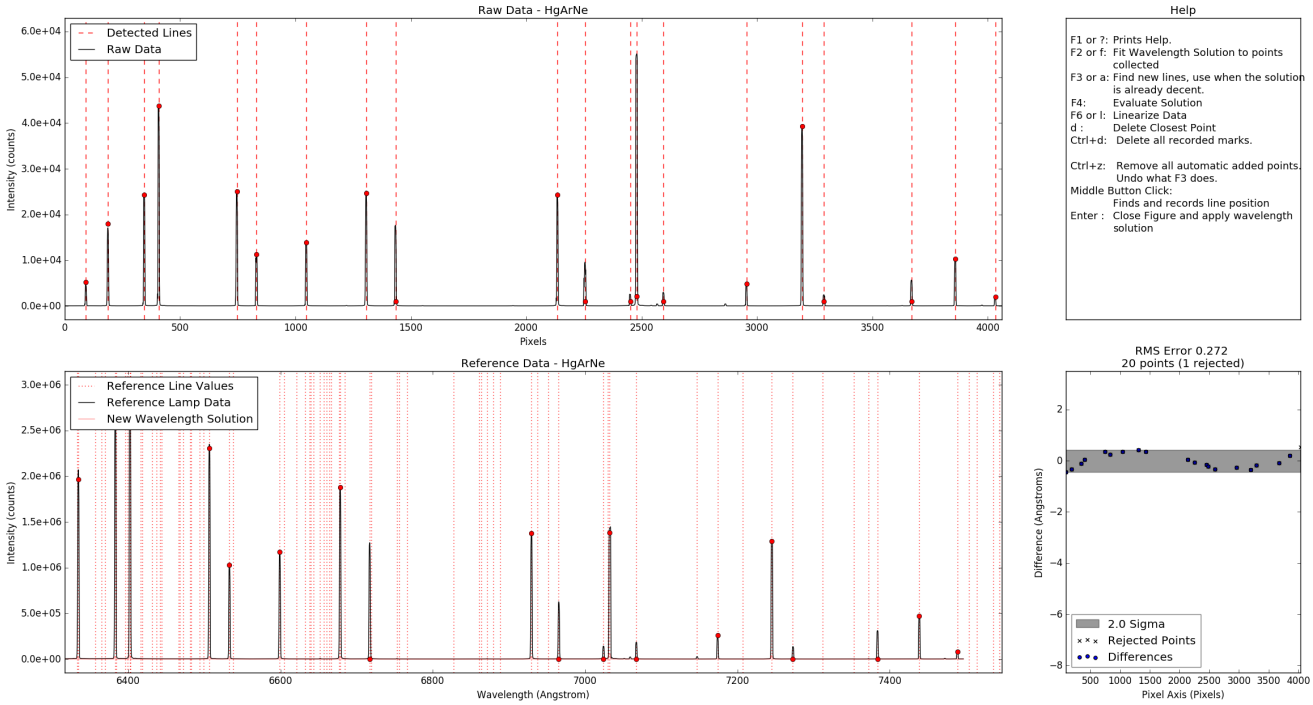
The automatic finding routine is not perfect, and indeed it depends on the preliminary wavelength solution. It uses the detected lines in the uncalibrated 1-D lamp, applies the preliminary solution and tries to find a match in the reference line values. In most cases it improves the solution, but not always so keep that in mind. In this case the RMS error is reduced by almost half, which is good, but if you look closely you can see the mismatches; also the *Bottom right* panel will show you this.



6. Now you we show an example of when the match is apparently good but in fact it's not. Here you need to zoom-in to see that there is an offset between the line centers and the matched laboratory line values, as shown in the figure below. You may have to apply different zoom values to your lamp and the reference lamp to get the plot to look like show it here. The solution in this case is locate the offending line(s), and delete it(them) pressing **d**. Then do a new match by clicking with the middle mouse button on the lines in the laboratory/reference plot, and the respective line in your 1-D uncalibrated lamp.

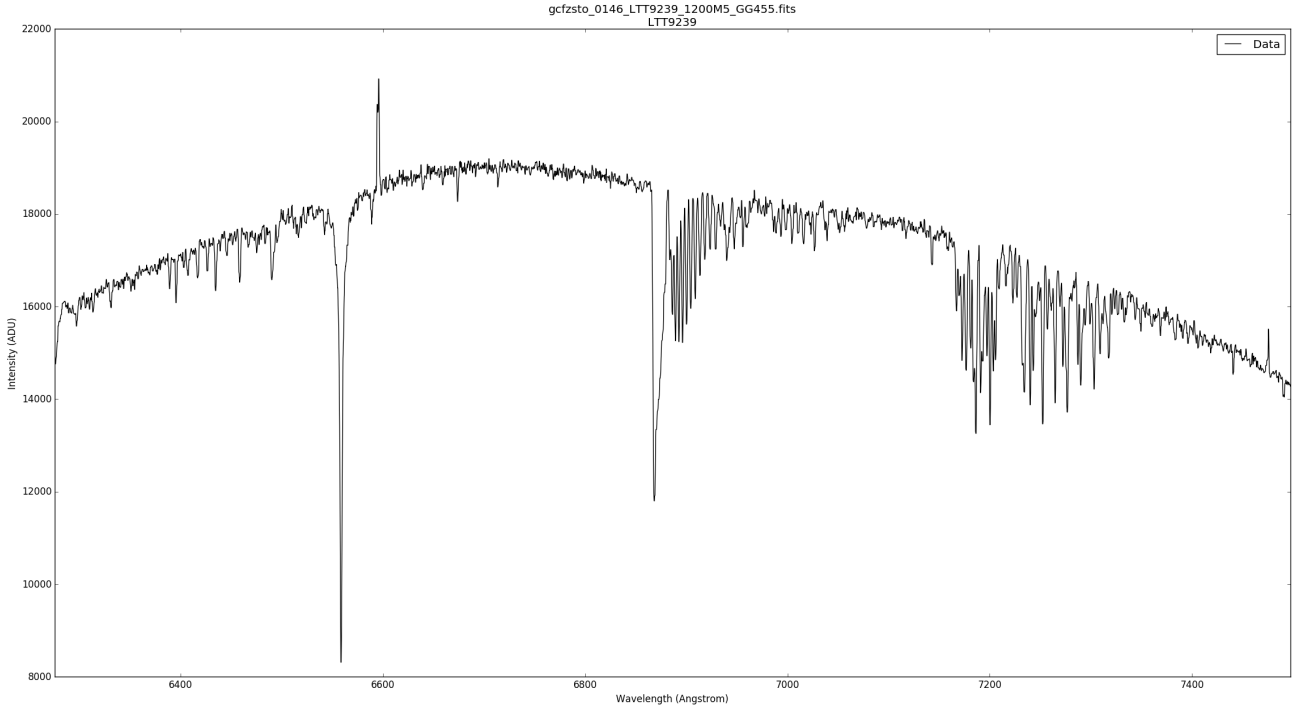


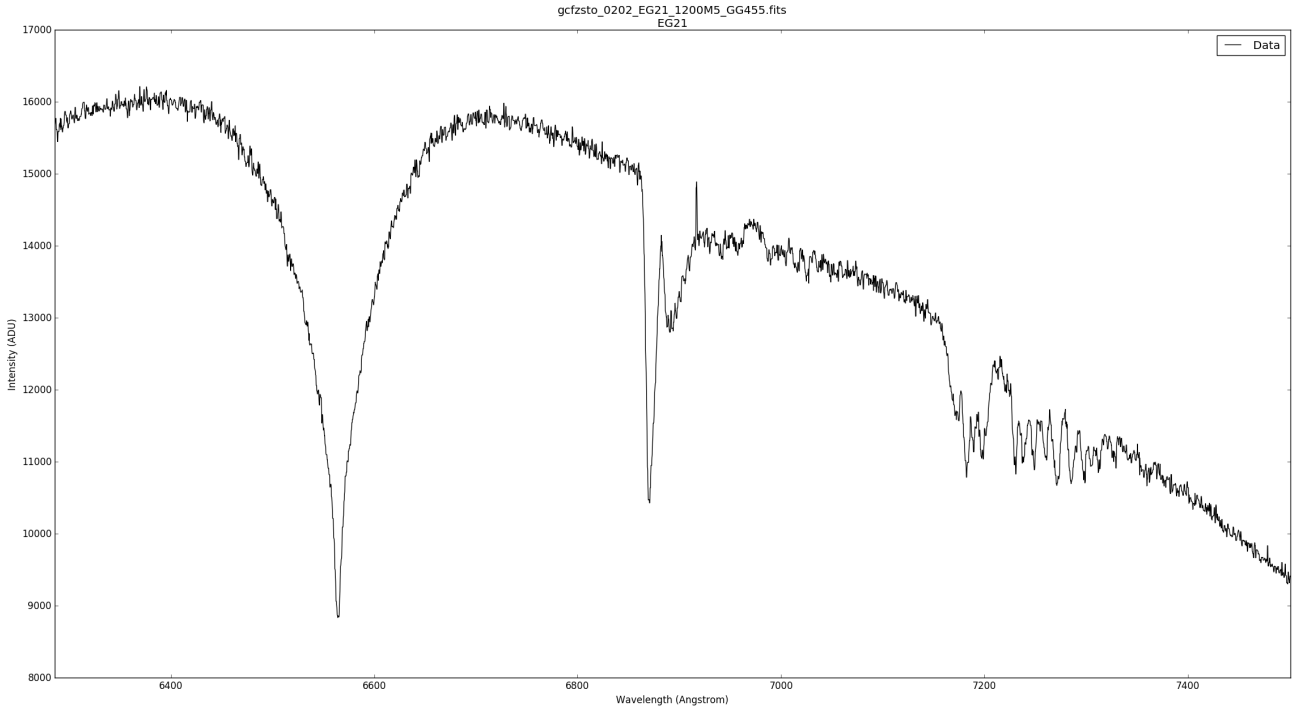
7. After you checked all the identifications and are happy with it, fit the solution again and you will obtain something like this:

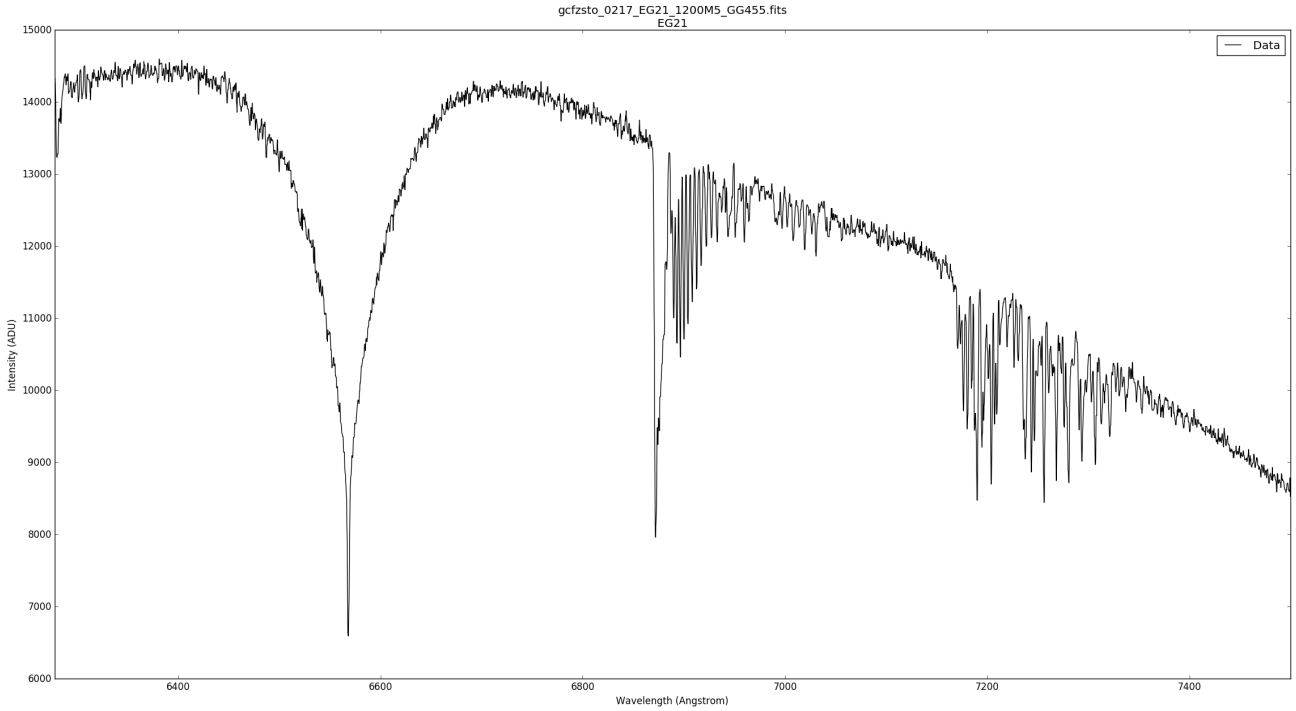


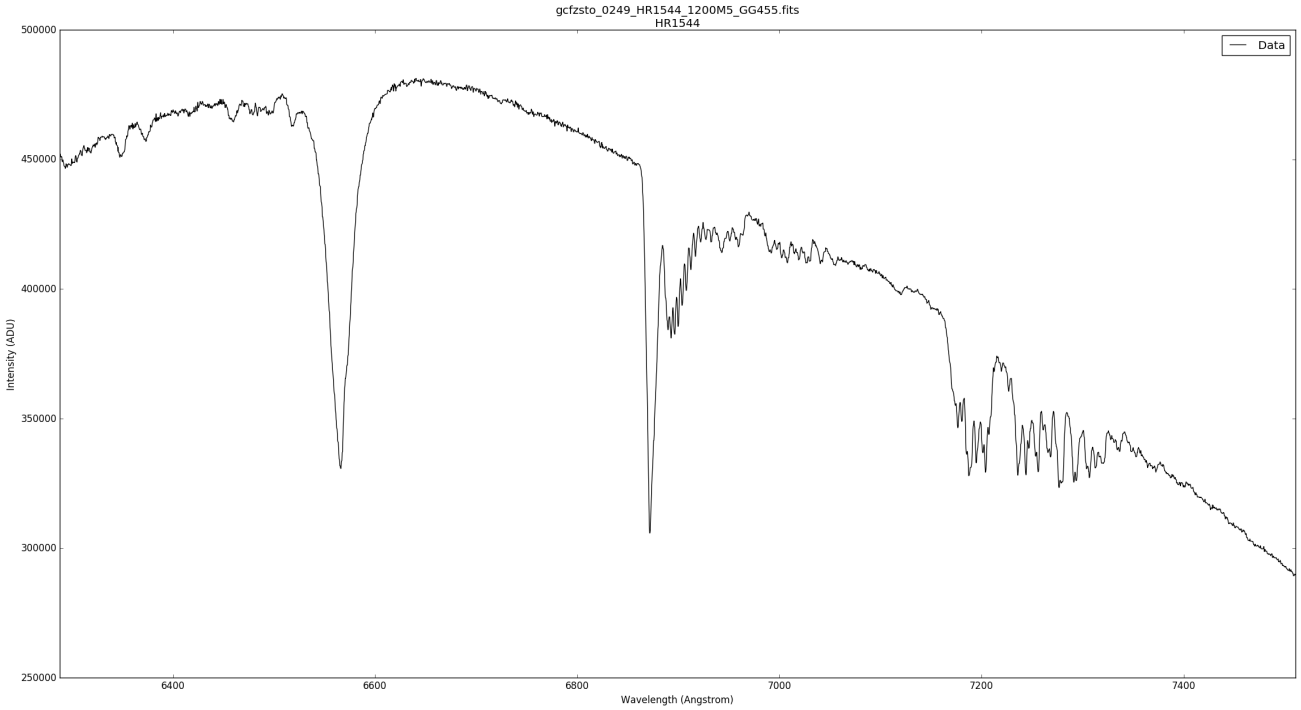
Here you can see that the *Bottom Right* panel shows the differences have a sinusoidal shape, which is also a sign that the solution can be improved. There are ways this can be implemented to refine the fit even further, but this is at present deferred to a later version.

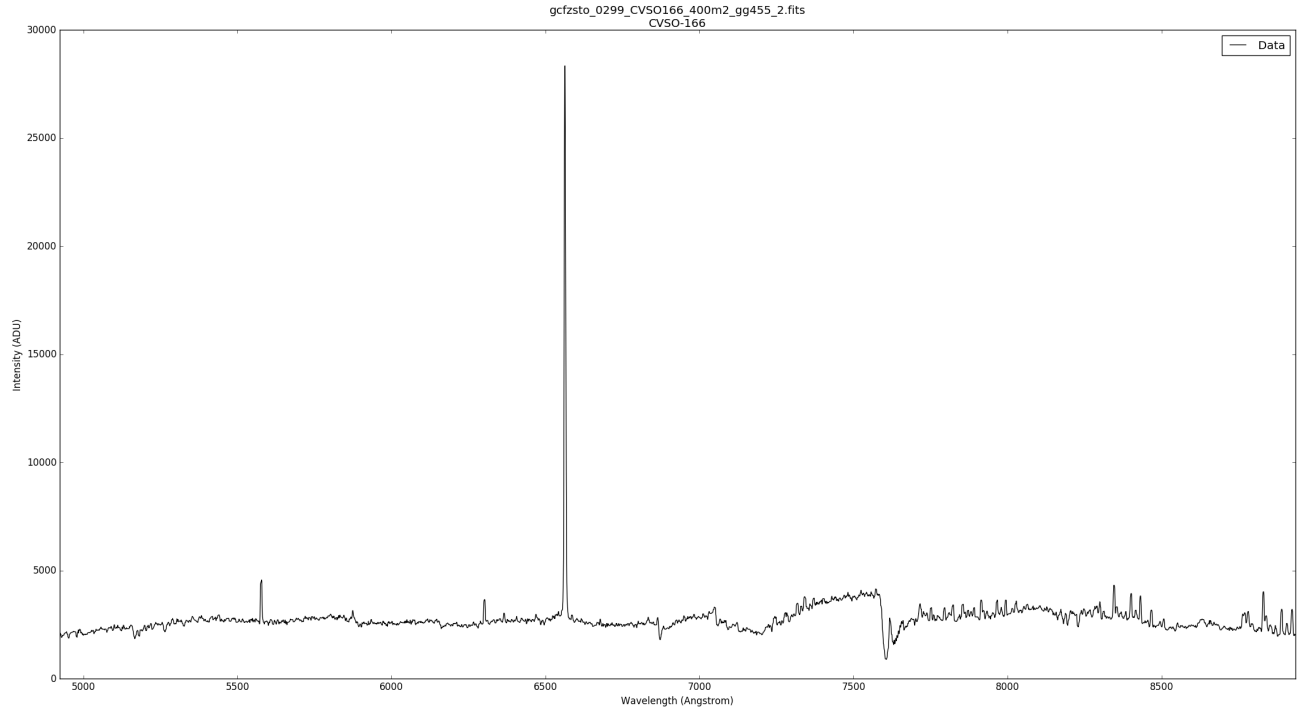
8. Finally, a few samples of the spectra extracted by the pipeline.

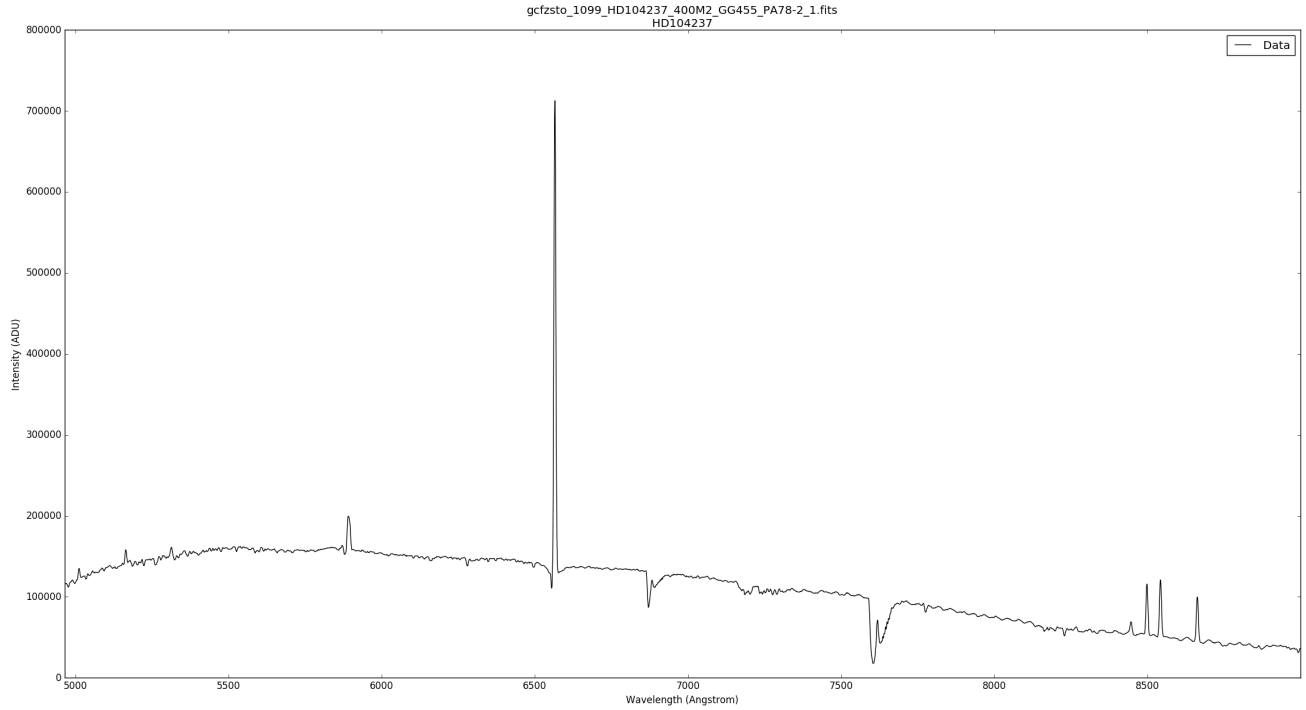



gcfzsto_0202_EG21_1200M5_GG455.fits
EG21
Data
Intensity (ADU)
Wavelength (Angstrom)
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
6400
6600
6800
7000
7200
7400


gcfzsto_0217_EG21_1200M5_GG455.fits
EG21
Data
Intensity (ADU)
Wavelength (Angstrom)
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
6400
6600
6800
7000
7200
7400


gcfzsto_0249_HR1544_1200M5_GG455.fits
HR1544
Data
Intensity (ADU)
Wavelength (Angstrom)
500000
450000
400000
350000
300000
250000
6400
6600
6800
7000
7200
7400


gcfzsto_0299_CVSO166_400m2_gg455_2.fits
CVSO-166
Data
Intensity (ADU)
Wavelength (Angstrom)
30000
25000
20000
15000
10000
5000
0
5000
5500
6000
6500
7000
7500
8000
8500



Troubleshooting

- The wavelength Solutions is way off: Check that the lamp was correctly registered in the header. Also check that the corresponding reference lamp exist. for instance is not the same to have `HgArNe` to `HgAr`
- Can't detect any objects: Check that the keyword `OBSTYPE` is correct.
- The reference data plot, in interactive mode, doesn't show anything or only vertical dotted lines: The reference lamp doesn't exist for that configuration, since this is used only for visual reference sometimes it will display the same lamp but in other instrument configuration, this will not affect the quality of the solution.

Installation Instructions

We strongly recommend installing the pipeline using *virtual environments*. Below you will find a summary of installation steps.

> ***Warning***
>
> Remember that we are not providing any kind of support for installation. This documentation will be the only existing.

- Install `anaconda`
- Add `astroconda` channel
- Create virtual environment
- Activate environment
- Install requirements
- Install pipeline

Anaconda

For anaconda installation we recommend you to check the astroconda channel's documentation page. The instructions will be reproduced here but they might change for newer versions.

> ***Warning***
>
> Anaconda installer requieres BASH. Don't try with other shell.

1. Installing `anaconda` - Go to https://www.anaconda.com/downloads and download the appropriate

   anaconda installer for your platform, most likely it has been automatically selected.

   - Run the installer.

     ```
     cd <download_directory>
     ```

     ```
     bash <install_script>
     ```

   - Once completed, check the bottom of `~/.bash_profile` or `~/.bashrc` there should be a new `PATH` definition with anaconda included.
2. Check `anaconda` installation

   ```
   which conda
   ```

   You should get a response similar to this:

   ```
   ~/bin/anaconda3/bin/conda
   ```

   If you don't get this response check the detailed instructions on the astroconda site. Otherwise continue to the next step.
3. Configure Conda to use the *Astroconda Channel*

   ```
   conda config --add channels http://ssb.stsci.edu/astroconda
   ```
4. Create a virtual environment. Here you have two options, one with `iraf` and one without it.

   - Standard: Without Iraf (Python 2 or 3).

     ```
     conda create -n astroconda python=2.7 stsci
     ```

     or

```
conda create -n astroconda python=3 stsci
```

astroconda is the name of your environment, you can use any name you want.

- Legacy software stack: Iraf included (Requires Python 2.7).

```
conda create -n astroconda python=2.7 iraf-all pyraf-all stsci
```

5. Activate your environment.

   ```
   source activate astroconda
   ```

6. Get latest release of the *Goodman Spectroscopic Pipeline*

   visit https://github.com/soar-telescope/goodman/releases/latest and download the `*.zip` or `*.tar.gz`

   ```
   cd <download_location>
   tar -xvf <pipeline_file>.tar.gz
   ```

   or

   ```
   unzip <pipeline_file>.zip
   ```

7. Install requirements from `requirements.txt`

   ```
   cd <goodman_pipeline_unpacked_location>
   pip install -r requirements.txt
   ```

8. Install the pipeline

   ```
   pip install .
   ```

Install DCR

In terms of cosmic ray rejection we shifted to a non-python package because the results were way better compared to LACosmic's implementation in astropy. LACosmic was not designed to work with spectroscopy though.

Visit this Link to download the code and find the instructions for compiling. I have added a few pre-compiled binaries and if you are lucky they will work right away. The available binaries are located in `goodman/dcr` and the options are:

- dcr.Ubuntu16.04
- dcr.Centos7
- dcr.MacOSSierra
- dcr.Solaris11

Choose whatever version fits your needs and rename it `dcr` and put it in a folder that at the same time is in your `$PATH` variable. If you don't know what that is follow the next section.

Install binary DCR

1. Open a terminal
2. In your home directory create a hidden directory `.bin` (Home directory should be the default when you open a new terminal window)

   ```
   mkdir .bin
   ```

3. Move the binary of your choice and rename it `dcr`. If you compiled it most likey it's already called `dcr` so you can ignore this step.

   ```
   mv dcr.Ubuntu16.04 ~/.bin/dcr
   ```

4. Add your `$HOME/.bin` directory to your `$PATH` variable. Open the file `.bashrc` and add the following line.

   ```
   export PATH=$PATH:/home/myusername/.bin
   ```

   Where `/home/myusername` is of course your home directory.

5. Close and reopen the terminal or load the `.bashrc` file.

```
source ~/.bashrc
```