MEGARA

MtJohn Echelle General Algorithms for Reduction and Analysis

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Manual Version 1.6

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MEGARA?

Megara is a suite of codes that perform basic reduction and further of HERCULES spectra. Both reduction and processing can be done in a standard way or be adapted to the user requirements. Please note Megara is work in progress so contact me (emily.brunsden@york.ac.uk) with any problems. Please only use the most up-to-date release.

Contents

1 Things Everyone Should Know

Megara is a suite of Matlab routines that have been developed to reduce HERCULES spectra for analysis. The code was developed in the framework of understanding line-profile variations from pulsations and has been generalised for other tasks.

- **In order to reduce spectra**, you will be running the script `Run_megara`. This is found in the `User_codes` directory. All other Megara code is in the subdirectory `Reduction_code`. It is not recommended you change scripts in the `Reduction_code` directory and its subdirectories.
- **Information on HERCULES** can be found in Hearnshaw et al. [2003].
- Information on **getting started with Matlab** can be found at https://uk.mathworks.com/help/matlab/getting-started-with-matlab.html
- Megara has a built in **tutorial**, see section 3.
- A description of **other code provided** with MEGARA users may find useful is in section 4.4.
- **For common errors** see section 5.
- **For support** contact emily.brunsden@york.ac.uk.

2 Setting up Megara on your machine

2.1 Requirements

Megara can run on Mac or Linux systems. You will need to have a licensed version of Matlab and access to a terminal. All directories from home to Megara files or data files should not have spaces in their names. This version of Megara has been tested on the versions and toolboxes in table 1.

Software	Version	core or option
MATLAB	24.2 (R2024b) Update 5	core
Optimization Toolbox	24.2	core
Signal Processing Toolbox	24.2	core
Image Processing Toolbox	24.2	core
Statistics and Machine Learning Toolbox	24.2	core
Curve Fitting Toolbox	24.2	core
Parallel Computing Toolbox	24.2	core

Table 1: Requirements for Megara. Software indicated by 'core' are required for operation.

2.2 Setup

- Unzip the Megara folder to your desired location.
- You will need to have `Raw_Data` and `Reduced_Data` directories. They can have any name and be any location on your machine but need to be distinct. `Raw_Data` should be structured with subdirectories for each observing period (this can be a month, a run or a single night- so long as thars and whites exist). These will be reduced independently. I recommend no longer than 1 month in each subdirectory as the flats may shift slightly.
- Move the pointer files to the correct locations so Megara can find your data. `pointer_file_megara` should be in the `Megara` directory. `pointer_raw_data_directory` should be in the `Raw_Data` directory. `pointer_reduced_data_directory` should be in the `Reduced_Data` directory.
- Open a terminal. Navigate to the `Megara/Reduction_code/barycentric_correction/new_hrsp_barycorr` folder. Type

  ```
  chmod 777 *
  ```

  This will give you permission to execute all files in the directory.
- In a terminal, navigate to the `Megara/Reduction_code/post_reduction/synspec/synspec` folder. Type

  ```
  chmod 777 *
  ```

  This will give you permission to execute all files in the directory.
- In Matlab, use `Set Path` (under the HOME tab) to add the Megara directory and subdirectories.
- If you have a multi-core machine then you can run parts of the code in parallel for speed. If you wish to run parallel code then under the HOME tab in the Parallel drop-down menu there are options in Parallel Preferences you can set to the specifics of your machine.
- In Matlab, open `Run_megara.m`

3 Tutorial

A tutorial with 15 observations of the star HD_48501 taken in December 2006 is included. It is in the directory `tutorial_data.m`. To run the tutorial go through the setup procedures as outlined in section 2.2. In Matlab, open `Run_megara.m`. The tutorial should have the following settings.

USER INPUTS

- `objectname='hd_48501';`
- `reduction_folders=;`
- `teff=[]; logg=[]; vsini=[];`

Note that if you have more than one folder with data for HD_48501 in the `Raw_Data` directory these files will also be reduced unless you specify `reduction_folders=['tutorial_data'];`.

USER OPTIONS

- `star_census=1;`
- `skip_reduction=0;`
- `skip_post_reduction=0;`
- `skip_reduction=0;`
- `blue_data_chop_value=500;`
- `apply_barycentric_correction=1;`
- `apply_continuum_fit=1;`
- `manual_continuum_fit=0;`
- `auto_continuum_fit=1;`
- `order_merge=1;`
- `overwrite_fulldata=1;`
- `overwrite_post_reduction=1;`
- `cross_correlation=1;`
- `rv_measurement=1;`
- `extend_velocities=0;`
- `suppress_figures=0;`
- `ascii_output=0;`
- `fits_output=0;`
- `FAMIAS_output=0;`

The code can then be run either by the `Run` button or by typing `Run Run_megara` in the command window.

3.1 Census

Megara will search all directories in the specified path (or those specifically specified in the `reduction_folders` parameter) for instances of stellar frames of the specified target. This is cross-matched with data in the `Reduced_data` directory and any frames already reduced are skipped. If there are new observations then this should be forced by setting `star_census=1;`. A summary is given on completion:

```
Running census on Month/Run 1 of 1
Reducing object hd_48501
A total of 15 observations have been found
A total of 0 observations have been previously reduced
```

3.2 File check routine

The reduction proceeds on unreduced data in the `Raw_data` directory. The command window outputs are:

```
Reducing Month/Run 1 of 1, This is tutorial_data
Testing calibration files
```

At this point a window appears for the user to manually check a frame (Figure 2. This happens when the file check routine is unsure of the classification of a frame. The window on the left is a trace in the vertical axis of the image in question. On the right are three sample traces for examples of a white lamp (flat field), Thorium (arc lamp) and stellar image. The user identifies of the classification of the image in the top left of the frame is correct by comparing it to the sample traces. If the user selects `Yes`, then the image is retained for reduction. If the user selects `No` then the image is removed from the reduction (but kept in a `removed_files` directory for later use if needed).

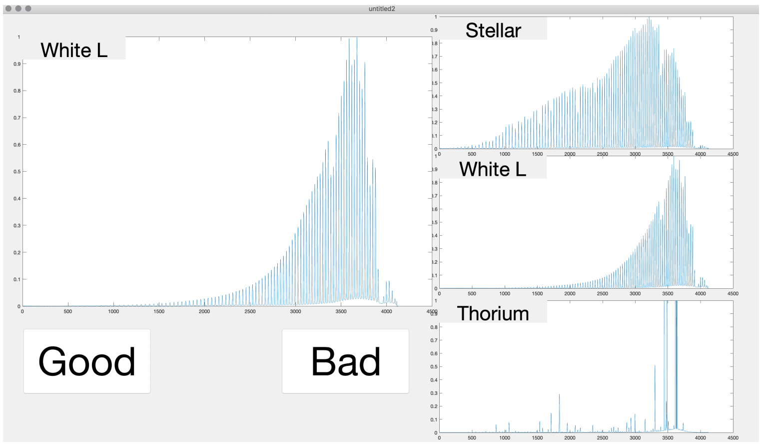

Figure 1: Classification of a file. The large image is the frame in question and the three smaller frames are to guide the user.

In this case the white frame is good so select `Yes`. The file check routine finishes and a summary window shows the results.

```
ans =
'J7731001 aWhite L is good'

Press enter to move bad files to a subdirectory or CTRL-C to change break out.
```

This window appears for the user to visually inspect the results of the file check. The three columns are three categories of file. The top image in the column displays the vertical trace of the queried files being kept for reduction. The bottom row shows the vertical trace of the queried files being removed from reduction. These can be useful to inspect if a problem is suspected with the directory being reduced, for example if shifts are detected. If this is the case, `CTRL-C` will break out of reduction leaving the

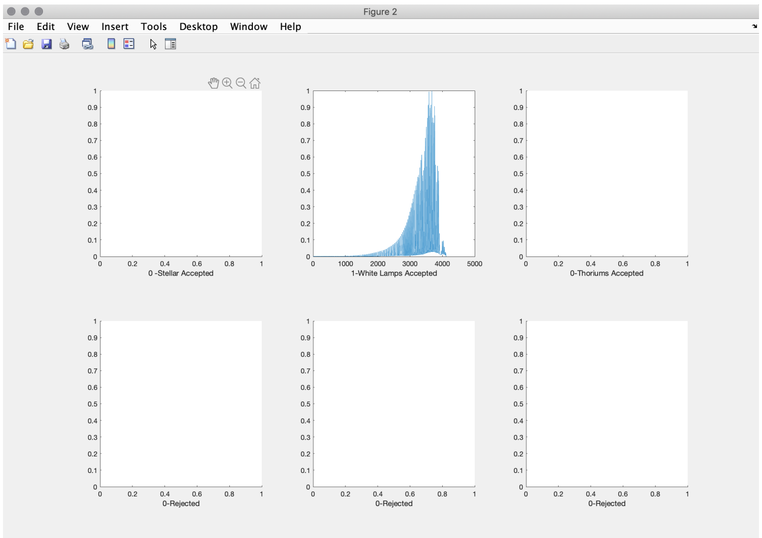

Figure 2: Classification results from thr file identification. The top row shows the stellar, flat and thorium files accepted and the bottom row shows the stellar, flat and thorium files rejected.

trace files in Matlab format in the directory to be examined. There are also two incomplete files in the directory which are only 9 MB instead of the standard 32 MB. These are automatically moved to the `removed_files` directory.

In the tutorial example the file is good. Only a trace of the white in the top middle plot is shown. Press `enter`.

```
The file check program is now complete.  The bad files have been moved to a
separate folder called removed_files and should not be reduced.  Everything else
remaining in the current directory is suitable for further use.  Reduction will
commence shortly.

A total of 15 stellar frames are suitable for reduction
```

3.3 Flat field calibration

The flat fields are identified and reduced into a summed master flat frame for each sub directory in the `Raw_data` directory.

```
reading file J7731001.fit
reading file J7731002.fit
reading file J7731003.fit
reading file J7731004.fit
reading file J7731005.fit
reading file J7731007.fit
flat summing complete
getting starting centre orders ...
tracing each order ...
fitting the background ...
extracting the data ...
extracting the background data ...
2532 cosmic ray affected pixels found and adjusted
finalising flat-field data
Flat-field images processing complete
```

On completion of this section the flat field data are saved as `flat_info_blue_500.mat` where 500 is the blue data chop value used in producing the flat. This file is used in any subsequent reduction in this directory.

3.4 Thorium calibration

The thorium frames are identified and reduced individually. They are saved collectively in a single file in each sub directory in the `Raw_data` directory. The below example shows the parallel processing of thorium frames and outputs will differ if this is not available on your machine (see section 2.2).

```
Starting parallel pool (parpool) using the 'local' profile ...
connected to 6 workers.
processing ThAr spectrum file:  J7733016.fit
processing ThAr spectrum file:  J7733028.fit
processing ThAr spectrum file:  J7731016.fit
processing ThAr spectrum file:  J7734024.fit
processing ThAr spectrum file:  J7731028.fit
processing ThAr spectrum file:  J7731042.fit
1025 lines found
1031 lines found
1003 lines found
931 lines chosen, 94 lines rejected
1007 lines found
1008 lines found
1017 lines found
908 lines chosen, 95 lines rejected
processing ThAr spectrum file:  J7733026.fit
1017 lines found
processing ThAr spectrum file:  J7734028.fit
1019 lines found
936 lines chosen, 95 lines rejected
processing ThAr spectrum file:  J7731026.fit
1028 lines found
914 lines chosen, 93 lines rejected
processing ThAr spectrum file:  J7731050.fit
1021 lines found
918 lines chosen, 90 lines rejected
processing ThAr spectrum file:  J7734018.fit
1012 lines found
928 lines chosen, 89 lines rejected
processing ThAr spectrum file:  J7731036.fit
1017 lines found
923 lines chosen, 96 lines rejected
processing ThAr spectrum file:  J7734026.fit
1015 lines found
920 lines chosen, 95 lines rejected
932 lines chosen, 96 lines rejected
processing ThAr spectrum file:  J7731018.fit
1025 lines found
925 lines chosen, 100 lines rejected
934 lines chosen, 87 lines rejected
processing ThAr spectrum file:  J7731048.fit
1018 lines found
923 lines chosen, 94 lines rejected
processing ThAr spectrum file:  J7733018.fit
1015 lines found
918 lines chosen, 97 lines rejected
926 lines chosen, 91 lines rejected
processing ThAr spectrum file:  J7731034.fit
1021 lines found
928 lines chosen, 93 lines rejected
916 lines chosen, 96 lines rejected
processing ThAr spectrum file:  J7734016.fit
1015 lines found
```

```
915 lines chosen, 100 lines rejected
processing ThAr spectrum file:  J7735052.fit
1017 lines found
923 lines chosen, 94 lines rejected
processing ThAr spectrum file:  J7735026.fit
1021 lines found
928 lines chosen, 90 lines rejected
processing ThAr spectrum file:  J7731044.fit
1015 lines found
processing ThAr spectrum file:  J7735044.fit
1025 lines found
920 lines chosen, 105 lines rejected
processing ThAr spectrum file:  J7735034.fit
1021 lines found 923 lines chosen, 92 lines rejected
processing ThAr spectrum file:  J7735050.fit
1018 lines found
922 lines chosen, 96 lines rejected
processing ThAr spectrum file:  J7735056.fit
1019 lines found
920 lines chosen, 99 lines rejected
processing ThAr spectrum file:  J7735058.fit
1012 lines found
916 lines chosen, 96 lines rejected
924 lines chosen, 97 lines rejected
processing ThAr spectrum file:  J7734032.fit
1016 lines found
918 lines chosen, 98 lines rejected
processing ThAr spectrum file:  J7735042.fit
1021 lines found
925 lines chosen, 96 lines rejected
processing ThAr spectrum file:  J7735028.fit
1016 lines found
921 lines chosen, 95 lines rejected
926 lines chosen, 95 lines rejected
processing ThAr spectrum file:  J7735036.fit
1018 lines found
925 lines chosen, 93 lines rejected
```

The filename, lines found and lines chosen data are displayed out of order during parallel processing. It is important that all thorium frames have a minimum of 900 lines found and 800 chosen. Fewer than this indicates a problem with the wavelength solution (see section 5). A warning will appear at the end of the reduction if this is the case. On completion of this section the thorium data are saved together as `ThAr_info_blue_500.mat` where 500 is the blue data chop value used in producing the thoriums. This file is used in any subsequent reduction in this directory.

3.5 Stellar (science) frames

```
reducing stellar spectrum file:  J7731049.fit
reducing stellar spectrum file:  J7733027.fit
reducing stellar spectrum file:  J7734017.fit
reducing stellar spectrum file:  J7731027.fit
reducing stellar spectrum file:  J7734031.fit
reducing stellar spectrum file:  J7731043.fit
saving J7731049.mat and J7731049_prc.mat
saving J7733027.mat and J7733027_prc.mat
saving J7734017.mat and J7734017_prc.mat
saving J7734031.mat and J7734031_prc.mat
saving J7731027.mat and J7731027_prc.mat
```

```
saving J7731043.mat and J7731043_prc.mat
reducing stellar spectrum file:  J7735057.fit
reducing stellar spectrum file:  J7735043.fit
saving J7735043.mat and J7735043_prc.mat
reducing stellar spectrum file:  J7733017.fit
saving J7733017.mat and J7733017_prc.mat
saving J7735057.mat and J7735057_prc.mat
reducing stellar spectrum file:  J7734025.fit
saving J7734025.mat and J7734025_prc.mat
reducing stellar spectrum file:  J7731017.fit
saving J7731017.mat and J7731017_prc.mat
reducing stellar spectrum file:  J7731035.fit
saving J7731035.mat and J7731035_prc.mat
reducing stellar spectrum file:  J7735027.fit
reducing stellar spectrum file:  J7735051.fit
saving J7735051.mat and J7735051_prc.mat
saving J7735027.mat and J7735027_prc.mat
reducing stellar spectrum file:  J7735035.fit
saving J7735035.mat and J7735035_prc.mat
Run reduced
```

As before the above outputs are out of order due to the parallel processing. The `J*.fit` stellar file will be reduced into a `J*.mat` file and a `J*_prc.mat` file. These are moved to the `Reduced_data` directory on completion. The above procedure will now repeat for all directories of interest in the `Raw_data` directory.

3.6 Post reduction

The second part of Megara processes the reduced data according to the user's needs. The tutorial is shows how to get a coarse corss-correlation profile from the spectra.

```
CONTINUUM FITTING
Loaded template continuum fit
COSMIC RAY REMOVAL
MERGING ORDERS
A total of 0 observations have been removed
FAMIAS-ready files written in reduced data directory
DATA PROCESSED
finaldata =
struct with fields:
fullwave:  [182673×1 double]
fullint:  [15×182673 double]
jd:  [1×15 double]
systemic_velocity:  50.8351
systemic_velocity_gauss:  50.8351
radial_velocity:  [1×15 double]
radial_velocity_error:  0.1542
vsini:  [1×15 double]
vsini_error:  1.0888
single_vsini:  32.6721
single_vsini_error:  0.2811
single_vsini_std:  13.7557
```

Four plots are produced to show the results for this star. A plot of the full order-merged spectra for HD_48501 is produced, figure 3. A second figure, figure 4, shows the cross-correlation profile for the star. The cross-correlation data are saved as `ccf_hd_48501.mat` in the `hd_48501` directory.

The third plot, Figure 5 shows the measurements of $v\sin i$ in kms^{-1} as against time. Note that for pulsating stars scatter is expected in these measurements. Two values of the $v\sin i$ are very low and should be removed. The final plot, Figure 6, shows the radial velocity measurements in kms^{-1} (centred around zero) for the observations with errors.

The final reduction result, `final_data`, is saved under `Reduced_data` in the directory `hd_48501`.

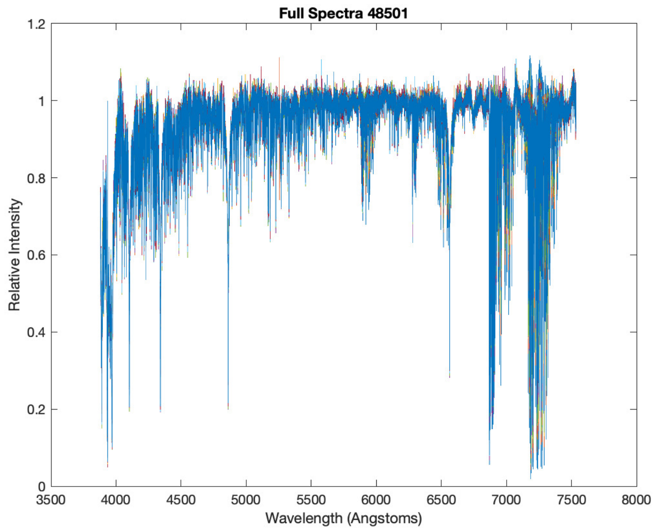

Figure 3: The full order-merged spectra of HD 48501. Each colour is a different observation.

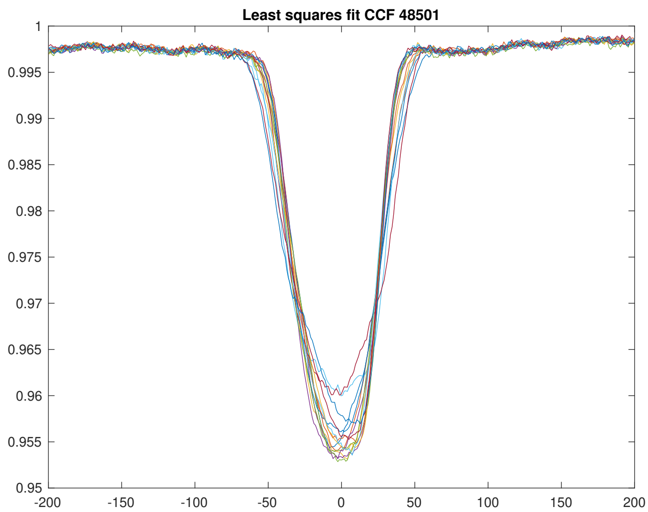

Figure 4: The cross-correlation line profiles of HD 48501. Each colour is a different observation.

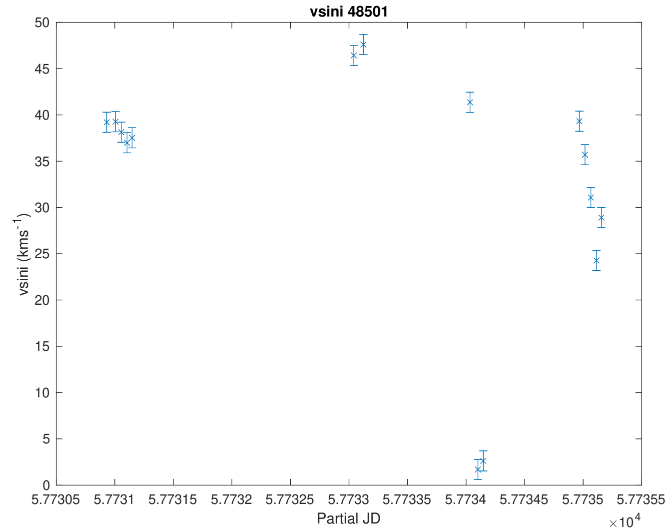

Figure 5: Measurements of $v\sin i$ from against time of observation. Two values of the $v\sin i$ are very low and should be removed for future analysis.

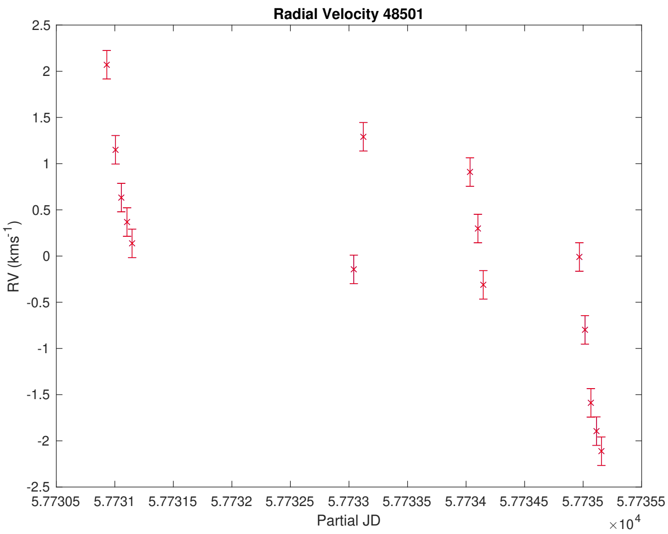

Figure 6: The radial velocity measurements for HD 48501.

4 Run_megara

4.1 A standard run

For most basic reductions the key steps are:

- In Matlab, open `Run_megara.m`
- Select your star. Under the `%USER INPUTS%` section, change the `objectname=[]` to your star name. The name is not case sensitive but user input variations such as HD49434 and HD_49434 have to be reduced separately. No input, `[];`, reduces all stellar images in the directory. To run all MUSICIAN stars use `'musician'`.
- Select directories to reduce. Under the `%USER INPUTS%` section, change the `reduction_folders=[]` to a comma-separated list of the directory names to be reduced, e.g. `reduction_folders=['Jan 2018', 'Feb 2018']`. The strings must match the subdirectory titles exactly. No input, `[]`, reduces all stellar images in the subdirectories where `pointer_raw_data_directory.m` is located.
- Input stellar values. Under the `%USER INPUTS%` section, change `teff=[]; logg=[]; vsini=[];`. These can be left blank for MUSICIAN targets.
- Select user options. Under the `%USER OPTIONS%` section, choose which parts of the reduction to run. For all the below `1` turns the option on and `0` turns it off. Section 4.2 shows all current options. Be careful selecting options with dependencies. Save your changes.
- Run the code. This can be done using the `Run` button in the Editor tab of Matlab or by using the Command Window and typing `Run_megara`.

4.2 User options

The below is a list of the current user options in Megara set in the `Run_megara` file. Defaults are given for a standard MUSICIAN run.

- `star_census` Do you want to redo census of observations? (default 1)
- `skip_reduction` Do you want to skip reduction? (default 0). Note that if the number of observations found matches the number of reduced files of a target then the reduction is also skipped. This is not valid if a subset of folders is specified to reduce.
- `skip_post_reduction` Do you want to skip processing and post-reduction? (default 0). This can be used if you wish to only reduce files to the *.mat stage.
- `blue_data_chop_value` Number of pixels to cut off the blue end of the spectrum due to incomplete flats (default=500). Using 500 captures more blue orders.)
- `apply_barycentric_correction` Do you want to apply the barycentric correction? (default 1). The barycentric correction is calculated using HRSP core code `barycorr_hrsp`. The default is to convert the target name to a HIP number for this calculation. In the case where no HIP number exists for an object (e.g. a Nova or Saturn) then the J2000 coordinates from the .fits header are used. Note that these coordinates are a user-defined header so must be correct when writing the fits header, or will need to be updated manually.
- `apply_continuum_fit` Apply a continuum fit to normalise the data (default=1). Continuum fitting uses a previous manual fit in the reduced data directory for the star by default. If this does not exist then either `manual_continuum_fit` or `auto_continuum_fit` must be set.
- `manual_continuum_fit` Do you want to manually continuum fit? Use this for precision work or non A or F type stars. This overwrites previous manual fits. See 4.2.1 for further guidance.
- `auto_continuum_fit` Do you want to apply an automatic continuum fit? Recommended only for A or F type stars.
- `order_merge` Do you want to merge orders? (default 1). Requires `apply_continuum_fit=1`.

- `overwrite_fulldata` Do you want to redo processing to order-merged spectra? (default 1)
- `overwrite_post_reduction` Do you want to re-do cross-correlation and related measurements? (default 1)
- `cross_correlation` Do you want to cross-correlate? Requires `order_merge=1`. Note that any previous cross-correlations will be overwritten. Two different cross-correlation calculations are performed.
  - The *Cross Correlation* (CCF) uses a list of wavelengths and widths of a synthetic spectrum to construct a delta-function template that is then cross-correlated with each spectrum.
  - The *Least-Squares-Fit Cross Correlation* (LSF CCF) takes the largest lines lines from the synthetic spectrum and fits them using a least-squares fit to the spectrum. This technique has the advantage that is weights the lines actually found in a spectrum highly. It is, however, more susceptible to small irregularities. See Wright [2008] for more information.
- `rv_measurement` Do you want to measure radial velocities? This calculates radial velocities, systemic velocity and $v\sin i$ with errors. Note that this is done with both the CCF and the LSF CCF. Results for the CCF are recorded in the `final_results` file. Results for the LSF CCF are recorded in the `supplementary_results` file.

  - Radial velocities are measured using the moment method [Aerts et al., 1992] with a standard error. The parameters are saved in `final_data.radial_velocity` and `final_data.radial_velocity_error` for all the observations corresponding to `final_data.jd`. These have units of have units of kms^{-1}.
  - The systemic velocity from average of all the CCF is given in `final_data.systemic_velocity`. The median systemic velocity from the Gaussian fits to the CCF is given in `final_data.systemic_velocity_gauss`. If these two are significantly different then it is likely the profile is noisy or contaminated enough that the radial velocity measurements may not be trustworthy. It recommended to do these measurements manually in this case.
  - The $v\sin i$ measurement is done using code based on that in Wright [2008]. The `final_data.vsini` is a direct fit of the line with standard error in `final_data.vsini_error`. All the above have units of kms^{-1}. Note that the above $v\sin i$ can be variable for pulsating stars and line profiles with large distortions may fail and give small (approx 1 kms^{-1}) values. An average is given in the parameter `final_data.single_vsini` with a standard error (`final_data.single_vsini_error`) and standard deviation (`final_data.single_vsini_std`). These should be inspected and bad fits removed from averages. The standard deviation is a reasonable error for pulsating variables.

    Note that the automatic $v\sin i$ measurements are very sensitive to binarity. If a single-lined binary is observed the radial velocity shifts mean the $v\sin i$ values may be very small (approx 1 kms^{-1}) and should not be used. Similarly if the star is a double-lined star then the fit fails and produces low values or NaN. Advice on how to measure the $v\sin i$ for these stars will be included in a later update.
- `extend_velocities` This extends the velocity axes for the cross-correlation from $\pm 200\mathrm{kms}^{-1}$ to $\pm 400\mathrm{kms}^{-1}$ (default 0)
- `supress_figures` Do you want to suppress figures during running of MEGARA?(default 0)
- `ascii_output` Do you want your output files in ascii format rather than matlab format? (default 0). See below for output file descriptions.
- `fits_output` Do you want your output files in fits format rather than matlab format? (default 0). See below for output file descriptions.
- `FAMIAS_output` Do you want to generate FAMIAS-ready cross-correlation files? (default 0). Requires `cross_correlation=1`. See below for output file descriptions.

4.2.1 Manual Continuum Fitting Guidance

If manual_continuum_fit is selected then the user can create a bespoke continuum fit for their object. This is done order-by-order and this fit is then carried forward to the order merging process if this option is chosen. The following is an example of how to manually continuum fit using the tutorial data. When manual_continuum_fit is selected the following will print in the command window.

```
CONTINUUM FITTING
Create new manual continuum fit.  Opening program for manual fit
Try to keep the function smooth and fit the top sides of the line profiles.
S Y N S P E C
Model atmosphere watch 86 mod
Line list gf3000
Job input files output
cp:  fort.6:  No such file or directory
cp:  fort.69:  No such file or directory
cp:  fort.18:  No such file or directory
cp:  fort.10:  No such file or directory
cp:  fort.86:  No such file or directory
cp:  fort.99:  No such file or directory
mv:  rename f99 to fort.99:  No such file or directory
vrot = 44.000
chard = 0.050
step(rot.conv) = 0.100
fwhm = 0.500
step(inst.conv) = 0.100
lambda initial = 3800.000
lambda final = 8000.000
irel = 1
1 - add point
2 - delete point
3 - move point
4 - exit
```

The final four numbers are the inputs for figure 100 (7) which is produced. In the figure blue line is the observed spectrum and the green line is the difference between the observed spectrum and the synthetic spectrum produced by synspec. Note the synthetic spectrum uses the input temperature, logg and *v*sin*i* and only produces a spectrum between Å and 7500 Å.

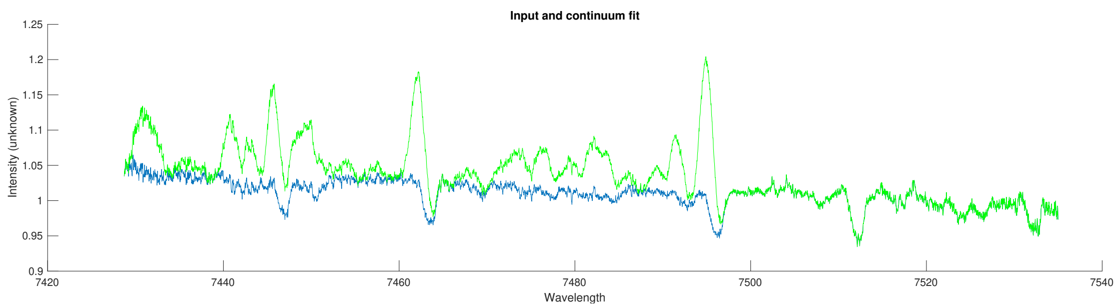

Figure 7: Figure 100 produced for continuum fitting. The blue line is the observed spectrum and the green line is the difference between the observed spectrum and the synthetic spectrum.

To fit a spectral order a minimum of seven points of continuum need to be selected on the spectrum. To choose a point enter '1' into the command window. This creates a crosshair on figure 100 and clicking a point on the curriculum will introduce a red cross. Repeating this process will continue to add crosses to the figure. Option '2' can be used to delete any points that and unsatisfactory and option '3' will move a point that is clicked.

Tips to get a good continuum fit:

- Shoulders of spectral lines can indicate good areas of continuum.
- Where the green line and the blue line intersect in the figure can also be good regions.
- It is good practice to 'anchor' the fit by placing points at each end of the order.
- Try to keep the fit smooth without sharp changes.
- Avoid placing points too close together as this creates spikes in the function.
- Be wary of the hydrogen absorption lines which can appear in multiple orders. Ensure the fit is a straight line over them.
- A minimum of seven points is required for the fit but you can add as many as needed. It is not recommended to have more than about 12 as this can indicate the spectral order is over-fitted and the fit may be interfering with the lines.
- Review the fit that is produced in relation to the synthetic spectrum. Disregard if the lines are offset in wavelength or are not the correct depth but review if the continuum levels seem right. Adjust the points to improve this as needed.

When the fit is acceptable enter '4' into the command window to move to the next order. A further example of the fit for a later order is given in figure 9.

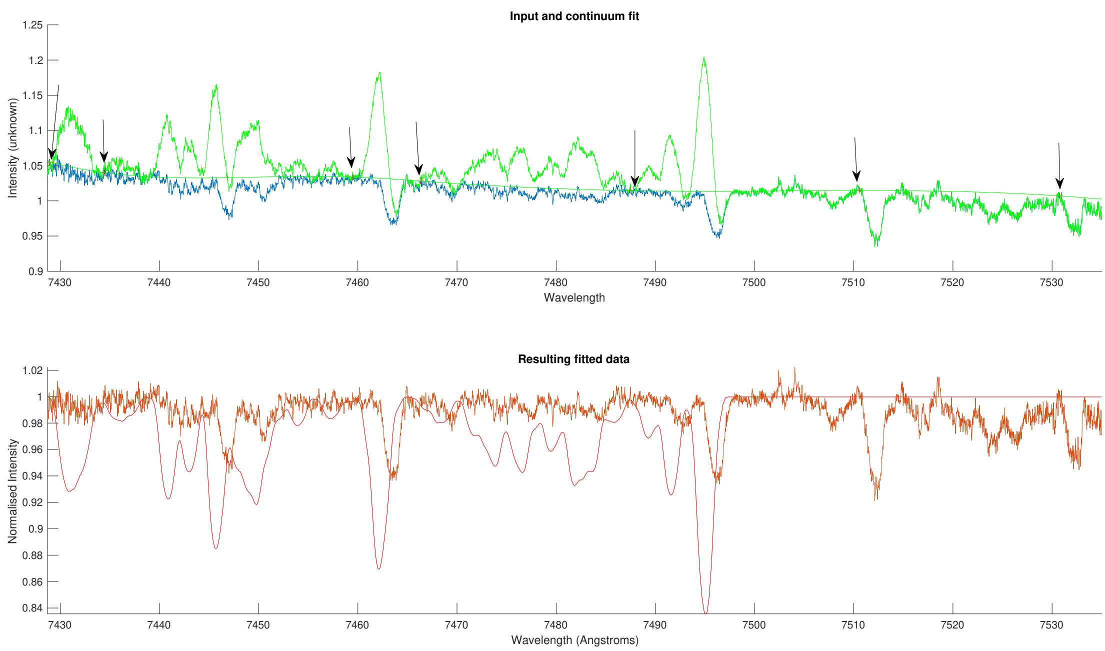

Figure 8: Figure 100 with selections for continuum fitting and resulting fit. In the top figure the blue line is the observed spectrum, the original green line is the difference between the observed spectrum and the synthetic spectrum and the new smooth green line is the fit function. In the bottom figure the orange line is the data after the fit is applied and the red line is the sythetic spectrum. Arrows have been added to highlight where the continuum fit points were added.

When the continuum fitting is completed, MEGARA contiunes with the processing of the object. The manual fit is saved as `data_cf_(objectname).mat` in the reduced data directory for the object. Note this fit will be used in subsequent reductions for this star. If the continuum fitting is interrupted the results may not save and will have to be produced again.

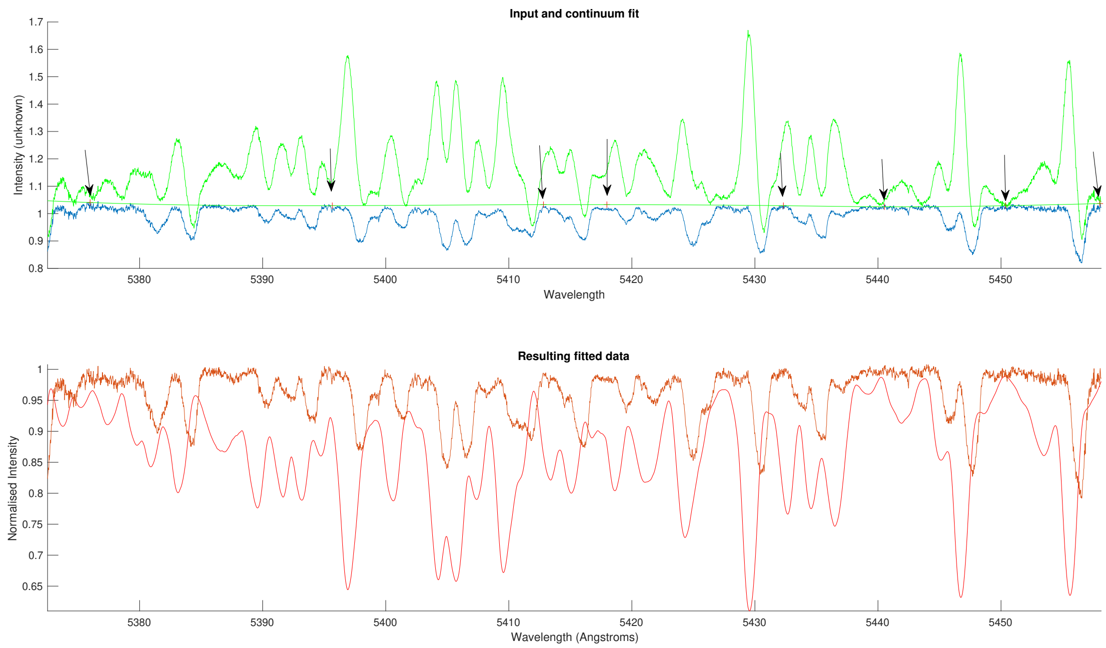

Figure 9: Figure 100 with selections for continuum fitting for a second region and resulting fit. In the top figure the blue line is the observed spectrum, the original green line is the difference between the observed spectrum and the synthetic spectrum and the new smooth green line is the fit function. In the bottom figure the orange line is the data after the fit is applied and the red line is the sythetic spectrum. Arrows have been added to highlight where the continuum fit points were added.

4.3 Outputs

As Megara runs the command window will display progress and key information. On completion files and some figures may be produced.

4.3.1 In the Matlab workspace

- The final reduction result, `final_data`, is a structure array with the first layer being the objectname(s) that was set. The format will depend on the options set.
- The variable, `objectname` is what objects were asked to be reduced. In the case of a singular target this is a character array. If more than one target was set then this is a structure array.
- The structure array `star_database` containing the sections (`star_database.filename`), exposure times (`star_database.exptime`), calendar date (`star_database.date`), flux-weighted mid-exposure Julian date (`star_database.mjd`) and observing folder (`star_database.months`).

4.3.2 Saved files

Megara will save reduced data in the `Reduced_Data` directory where the `pointer_reduced_data_directory` file is located. It will automatically generate a folder with the objectname that was set.

- `file_information.txt` is a handy log of the files in each `Raw_Data` directory. It is saved in the `Raw_Data` directory. A corresponding Matlab version, `file_info.mat` is also saved.
- Matlab files record all rejected files from the file check routines. `badfiles_general.mat` records all automatically removed files, mostly those that are too small and/or corrupted. `badfiles_calibration.mat` and `badfiles_(objectname).mat` record the calibration files (ThAr and Flats) and science object files respectively rejected by the vertical traces- either automatically or by the user. All these files are moved into the `removed_files` subdirectory.

- For each raw data directory a summed flat is produced. This is saved as flat_info_blue_X.mat where X is the blue data chop value used in producing the flat.

- For each raw data directory the wavelength solution for the thoriums is produced. This is saved as ThAr_info_blue_X.mat where X is the blue data chop value used in reducing the thoriums.

- Each J*.fit stellar file will be reduced into a J*.mat file and a J*_prc.mat file. The former is the calibrated extracted spectra order by order in a structure file. Each order has a intensity and wavelength component. In addition the Julian Date and the barycentric correction is written in this file (although not yet applied) along with the signal-to-noise of the frame measured at approximately 5777 Angstroms. The J*_prc.mat file is a record of the reduction settings. J*.mat files are located in the Reduced_Data directory in a subdirectory named by the objectname. The J*_prc.mat files are saved in the subdirectory processing_files.

- A file star_database_(objectname).mat is produced in a sub-directory Observation Summaries in the Reduced_Data directory. This is a structure array containing the sections (star_database.filename), exposure times (star_database.exptime), calendar date (star_database.date), flux-weighted mid-exposure Julian date (star_database.jd) and observing folder (star_database.months). If star_census is selected then this is automatically overwritten, otherwise it is loaded from a previous session. In the case none exists then this file is created.

- The final reduction result, final_data_(objectname), is saved in the reduced data directory for each object. The format will depend on the options set. For a typical run with order_merge then this will be a structure array with fields fullwave, fullint and jd. If rv_measurement is selected then there will also be fields systemic_velocity, systemic_velocity_gauss radial_velocity, radial_velocity_error, vsini and vsini_error, which all have units of kms^{-1}. For a run where order_merge is not selected then final_data_unmerged_(objectname) will be written.

- In the J*.mat files and in the final_data files the signal-to-noise of the stellar frames is recorded. This is calculated at approximately mid-chip and mid-order at 5777 Å using equation 4.5 in Gray [2005]. The background value is the sum in quadrature of the shot noise, dark current and bias. The shot noise comes from the root of the image sum minus the dark and bias. The dark frame signal is calculated from the exposure time with fit to a series of standard dark frames in the file dark_exposure_fit.mat. The bias is defined from a master in readout_noise_value.mat. The counts for both the image and the background are converted from ADU to photons. This conversion is calculated from the flat fields where the signal-to-noise is defined from the extraction of order 100. This value is approximately 278 photons per ADU. Should this conversion factor need to be modified it can be found in photon_ADU_conversion.mat .

- If cross_correlation is selected the cross-correlation profile for each star is generated. The cross-correlation data are saved as ccf_(objectname).mat in the corresponding object name directory. This is a structure array with fields coarse_ccf.velocity, coarse_ccf.intensity and coarse_ccf.jd.

- Supplementary reduction results for the least-squares cross-correlation profile, suplementary_data_(objectname), is saved in the reduced data directory for each object if the radial velocities are measured. This is a structure array with fields systemic_velocity, systemic_velocity_gauss radial_velocity, radial_velocity_error, vsini and vsini_error, which all have units of kms^{-1}.

4.3.3 Figures

- If order_merge is selected then a plot of the full order-merged spectra for each star is produced.

- If cross_correlation is selected the cross-correlation profile for each star is generated. The cross-correlation data are saved as ccf_(objectname).mat in the corresponding object name directory.

- If rv_measurement is selected figures showing the radial velocities and $v\sin i$s are produced. The data are saved as part of the final_data_(objectname).mat in the corresponding object name directory.

The final reduction result, final_data, is saved in the folder with the objectname that was set. The format will depend on the options set.

4.3.4 Other file formats

- **Fits formats**
  If fits_output=1 then each observation will have additional *.fits files written in their object reduced_data subdirectory. These are J*_reduced.fits .
  - If order_merge=1 then the J*_reduced.fits files have two columns in the image- wavelength in Å and intensity.
  - If order_merge=0 then the J*_reduced.fits files have four columns in the image- wavelength in Å, intensity, relative weight and order number.
  - In either case the fits files will also contain the following keywords:
    * The name of the original J*.fit file, Filename.
    * The truncated, helocentric, mid-exposure Julian date, JD.
    * The observation date, Date.
    * The UT time exposure started, Exp_Start.
    * The exposure duration in seconds, Exp_Time.
    * The UT flux-weighted mid-time of exposure, FWMT.
    * The barycentric correction in kms^{-1}, BCorr.
    * A flag to say if the barycentric correction has been applied (0=No, 1=Yes), BCorr_App.
    * The signal-to-noise of the spectrum as measured at an approximate wavelength of 5777 Angstroms, S/N.
      If rv_measurement is selected then there will also be
    * The systemic velocity in kms^{-1}, Syst_Vel.
    * Radial velocity measurements in kms^{-1} , RV.
    * The error in the radial velocity measurements in kms^{-1} , RV_err.
    * $v\sin i$ measurements in kms^{-1} , Vsini.
    * The error in the $v\sin i$ measurements in kms^{-1} , Vsini_err.

  If a cross-correlation profile is produced in the reduction then this is saved as ccf_(objectname).dat. It has the format of the first column being the velocities in kms^{-1} and then one column per observation in JD order.

- **Ascii formats**
  If ascii_output=1 then each target will have additional *.dat and *.txt files written in their object reduced_data subdirectory. These are J*_reduced.dat and summary_file_(objectname).txt.
  - If order_merge=1 then the J*_reduced.dat files have two columns- wavelength in Å and intensity.
  - If order_merge=0 then the J*_reduced.dat files have four columns- wavelength in Å, intensity, relative weight and order number.
  - In either case a summary_file_(objectname).txt is created that lists:
    * The name of the original J*.fit file, Filename.
    * The truncated, helocentric, mid-exposure Julian date, JD.
    * The observation date, Date.
    * The UT time exposure started, Exp_Start.
    * The exposure duration in seconds, Exp_Time.
    * The UT flux-weighted mid-time of exposure, FWMT.
    * The barycentric correction in kms^{-1}, BCorr.
    * A flag to say if the barycentric correction has been applied (0=No, 1=Yes), BCorr_App.
    * The signal-to-noise of the spectrum as measured at an approximate wavelength of 5777 Angstroms, S/N.
      If rv_measurement is selected then there will also be
    * The systemic velocity in kms^{-1}, Syst_Vel.
    * Radial velocity measurements in kms^{-1} , RV.

* The error in the radial velocity measurements in kms^{-1} , RV_err.
* $v\sin i$ measurements in kms^{-1} , Vsini.
* The error in the $v\sin i$ measurements in kms^{-1} , Vsini_err.

If a cross-correlation profile is produced in the reduction then this is saved as `ccf_(objectname).fits`. It has an image format of the first column being the velocities in kms^{-1} and then one column per observation in JD order.

- **FAMIAS formats**
  If `FAMIAS_output` is selected (and `cross_correlation` is selected) then the line profiles for both the Coarse CCF and LSF CCF are output as .dat files ready for import into FAMIAS. The files are placed in two folders within the `reduced_data` directory for each target. The two folders are labelled as the two CCF types and include a `times*.dat` file that imports all the individual observation files into FAMIAS.

4.4 Other Useful Code

- `darks` folder contains `make_new_dark_exposure_fit` which can be modified if a new dark exposure fit is needed. This dark exposure fit is a function of photon count versus exposure time and is used in the calculation of the signal-to-noise.

- `photon_ADU_conversion` folder contains `make_new_photon_ADU_conversion` which is a calculation of the conversion for the signal-to-noise calculation. The conversion uses the signal-to-noise as measuresd from a series of flat field frames as described in Gray [2005]. It can be modified if a new conversion is needed.

- `calculate_resolving_power` takes a given thorium image and calculates the spectral resolving power for each order. A usage example is `[resolving_power,wave_loc,number_lines]= calculate_resolving_power('J7731016.fit','flat_info_blue_500.mat',500,'ThAr_info_blue_500.mat')` with inuts of thorium filename, relevant flat file, blue data chop value and thorium information file. Note this requires a standard reduction to have run for the relevant run in order to generate the above files. The outputs are the weighted mean resolving powers, weighted mean wavelengths and number of lines used for each order. A plot of resolving power against order number is also produced. Central orders should have values around 41000.

- `display_directory_file_information` produces a matlab screenprint of the fits files in a directory with some useful information. A usage example is `info=display_directory_file_information`. A list of fits files in the directory is printed with headings Filename, HERCEXPT (frame type from the header file), JDmid, FIBRE, Object and S/N.

- `fix_wonky_shoulders` is a small code to correct continuum problems in cross-correlated line profiles. The user selects a few points on each side of a line profile to adjust the continuum level. Be careful doing this if precise measurements of the line are needed in future.

- `hercules_fitsread` loads and formats the header and the image from a given HERCULES fits file. A usage example is `[image,header] = hercules_fitsread('J7731001.fit')`. The header is a cell array and the image is a 4k by 4k matrix.

- `make_new_thardat` makes a new `thardat_x` file which is used in the thorium line calibration. New thardats are generally needed after the HERCULES tank has been opened or other mechanical change to the optical path. After generating a new thardat it must be named and placed in the `thar_processing` folder. The file `process_thar_frames` will need to be updated for the new date ranges for the thardat to be used.

- `manual_CCF` is an example of how to do a manual cross-correlation modifying the regions of the spectrum to be used and/or the species being cross-correlated. Modify the script as needed.

- `Mus_known_alias_names.mat` is a file which has known alternative names which have been used for MUSICIAN stars. For example 'hd_27290' is sometimes labelled as 'Gam_Dor'. This file can be updated as needed and is checked in the reduction.

- plot_fits_image plots a fits image with appropriate scaling. A usage example is plot_fits_image('J7733017.fit') which generates a plot of the fits image. This code accepts inputs as filenames in *.fits formats or pre-loaded data matrices in matlab.
- radial_velocity_calculation_with_smoothing is an alternative radial velocity calculation method using a smoothed version of the cross-correlated line profile. It can produce better radial velocities for noisy profiles. An example usage is [radial_velocity,rv_error,systemic_velocity_direct, systemic_velocity_gauss,vsini,vsini_error]=radial_velocity_calculation_with_smoothing(coarse_ccf) where coarse_ccf is the cross-correlation as saved in the ccf_hd_xxxxx.mat file after reduction and post reduction.

4.5 Notes on Times

There are some subtle but sometimes important differences in the times recorded by HERCULES and those used in MEGARA and hence written in files.

The header in the fits files MJD-OBS is used generally as the JD. This is the truncated, heliocentric, mid-exposure Julian date. Despite the name it is NOT the Modified Julian Date (with a subtraction of 0.5 days). It includes the mid-exposure time, not the flux-weighted mid-exposure time. This value is directly output as the JD of the observation in all output types.

The barycentric correction is calculated using the UT flux-weighted mid-time of the exposure (not heliocentric corrected). The latest version of the HRSP barycorr code includes leap seconds correct to January 2020 but still contains some approximations. From tests the barycentric correction is accurate to approximately 10 ms^{-1}.

5 Common errors and Tips

- If there are too many input argument in `cd` command then check that the path from the home directory to Megara code or the data directories does not have any directories with spaces in the titles. If directory names change then the set path directories may need to be updated in Matlab.
- If there are too few lines in multiple thorium images a good place to check first is the flat-field data. Inspect very carefully the vertical traces of the flats or thars in the file-check routine summary window. if some are shifted horizontally then this indicates motion of the spectrum on the chip (e.g. from changing fibre or opening the tank). Reduce sections of the run which have the same shifts in separate directories.
- If new data, raw or reduced is added to the directories, it is best practice to update the paths in matlab.
- If the cross-correlation profiles seem to have unbalanced shoulders then this may be a problem with the synthetic spectrum not matching the star well. Check there were no errors with synspec when the code ran, otherwise input the stellar parameters manually when running. If nothing solves the problem try `fix_wonky_shoulders` (see 4.4).

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