Instructions for use of “molly” to prepare files for Doppler or Modmap

In the following instructions, computer output is in small type**, prompts end with “:” or “>”, comments are in boldface and that which the user should type is in** *italics***:**

Preparation to use 'molly'

To use molly, you will need two input files in addition to ascii files that contain wavelength, flux, and errors for each of your spectra. The first input file, to be named 'molly.in', should contain a line for each spectrum used, as follows:

lasc spectralfile1.asc 1 1 2 3 \ \ \
lasc spectralfile2.asc 2 1 2 3 \ \ \

The 3rd column lists the file number and '1 2 3' refers to the three columns of data - wavelength, flux and error. If no errors are given, the '3' in each line should be replaced by '-3', so that modmap can still process the data.

The second input file, named 'molly.info', should contain two initial lines for column headings and, once again, a line for each spectrum, giving the information shown below:

Object	UTC	RA	Dec	Equinox	Dwell	Day	Month	Year
C	D	D	D	D	R	I	I	I
V616Mon	5.0000000	6.3771111	-0.3165000	2000	900.000	14	12	2006
V616Mon	5.3075000	6.3771111	-0.3162500	2000	900.000	14	12	2006

All of these data should be in the image headers of the spectra: Object Name (Object), UTC time at mid of exposure in decimal hours (UTC), RA of telescope in decimal hours (RA), Declination in decimal degrees (Dec), Equinox of coordinates (Equinox), Exposure time in seconds (Dwell) and UTC date of observations split into Day, Month and Year. The first line of the file contains the name of the header items, the second line whether they are strings (C), integers (I), reals (R) or double precision entries (D).

Trimming for Doppler
Unlike Modmap, Doppler requires the spectra to be trimmed around the desired line. Whilst masking is possible in molly, the 'wdopp' command required for for output usable by Doppler ignores this and saves the entire spectrum. For this reason, it is necessary to trim the spectra before input into molly. As the input files are simple files, this only requires a simple program to create a new set of files containing only the desired wavelength range. A python program (trimmer.py) that does this is provided. Note: the number of data points must be the same for all files being imported into molly, or molly will not be able to process them together.

Starting molly

To access molly routines, source the following in the directory in which you want to work:

: *source /data/saku10/software/setup.csh*

Then type 'molly' in the prompt:

: *molly*

You will then see the following start-up text:

molly -- spectrum analysis. If you are new to molly type 'help molly' for
information about the program. Type 'help' or '?' for a command list.

This version was linked at 10:29:07, 10/08/2010

Startup file found.

Opened1: /data.saku/software/F77/molly/startup
Maximum spectrum length set = 4000
Maximum number of spectra = 7500
Files will be written even if a file of the same name exists.
Closed1: /data.saku/software/F77/molly/startup

No local startup file found

To exit molly, simply type 'q', then 'y' to confirm

Setting up files to edit in molly

To load the ascii files, type the following in molly:

molly> *@molly.in*

Opened1: molly.in
*lasc m06053c2.txt 1 1 2 -3 \ \ *
Slot 1 , NPOLY = 2 , Max dev = 0.0006360767 pixels.
Acceptable fit found
Spectrum data range: 257.5366 446.8187
Constant added to make data positive: 44.68187
Mean photons per data number: 0.898266170058243
Median filtering 1798 points.
*lasc m06054c2.txt 2 1 2 -3 \ \ *
Slot 2 , NPOLY = 2 , Max dev = 0.00063941866 pixels.
Acceptable fit found
Spectrum data range: 229.5087 400.58
Constant added to make data positive: 40.058
Mean photons per data number: 0.8765018851187771
Median filtering 1798 points.
*lasc m06055c2.txt 3 1 2 -3 \ \ *
Closed1: molly.in

As you can see above, the spectra will be loaded into numbered 'slots', corresponding to the file numbers allocated in the 'molly.in' file. These numbers will be used to refer to individual files. Newly created, edited spectra can be assigned new slots of your choice. Be aware, though, that slots are overwritten without warning if you reuse numbers! When using commands, default entries will be shown in [square brackets] and are automatically assigned if no value is given.

To assign the data in 'molly.info' to your spectra, use the 'edit' command:

molly> *edit* **Open files for editing**
First slot to edit [1]: *1*
Last slot to edit [1]: *2* **(Where 1 & 2 are the first and last file numbers to edit)**

Commands:

clear -- Clear headers
file -- Read in headers from special file
any -- Read in a column from a file
term -- Entry from terminal.
del -- Delete header item.
ren -- Rename header item.
quit -- Quit

edit> *file* **Assign the data**

Enter filename [header]: *molly.info* **Enter the data file name**

Variable 1 name: Object , type: C
Variable 2 name: UTC , type: D
Variable 3 name: RA , type: D
Variable 4 name: Dec , type: D
Variable 5 name: Equinox , type: D
Variable 6 name: Dwell , type: R
Variable 7 name: Day , type: I
Variable 8 name: Month , type: I
Variable 9 name: Year , type: I

edit> *Quit* **Return to the main program**

To adjust the heliocentric correction for telescope location enter the following:

molly> *hfix*
First slot to fix [1]:
Last slot to fix [1]: *48*
Telescope ('list' for list, 'skip' to ignore) [Campanas]: *list* **Enter 'list' to see the available options, or enter the name, if known**
Please identify the telescope
Palomar 200in
Wilson
Campanas
Lemmon
WHT
INT
JKT
UKIRT
Kitt Peak
AAT
CTIO
McDonald
MMT
VLT
ANU 2.3m
SAAO 1.9m
NTT

```
      or 'elsewhere'
telescope> Campanas
  Telescope:Campanas
      Site:Campanas
  Longitude:  70 42  9       70.70250
   Latitude: -29  0 11      -29.00306
  Elevation:              2280.00000
    1, obj: V616Mon        , run:       1 exp:   900.0    time: 14/12/06, 05:00:00
    2, obj: V616Mon        , run:       2 exp:   900.0    time: 14/12/06, 05:18:27
    3, obj: V616Mon        , run:       3 exp:   900.0    time: 14/12/06, 05:34:09
```

If choosing 'elsewhere', you will need to give the name of the telescope, name of the observing site, the Longitude and Latitude in hours, minutes, seconds, and the altitude. You must use integers.

Averaging and Plotting Spectra

Averaging

The easiest may to check how a set of spectra look is to average them and plot the result. Spectra can be average using the 'av' command:

```
molly> av
First spectrum to average [       1]:
Last spectrum to average [       2]:3
Slot for average spectrum [      3]:4
What method of averaging (U,D,R,V) [U]:
File of weights [ ]:
 Added in slot  1 , mean weight  1.
 Added in slot  2 , mean weight  1.
 Added in slot  3 , mean weight  1.
 Number of spectra averaged =  3
 WARNING: Arc scales of spectra are not the same. Averaging will go ahead though
 Result stored in:
4, obj: V616Mon         , run:       1 exp:   660.6    time: 15/12/06, 07:25:13
```

Using slot after the last spectrum you averaged makes it easy to remember where your average spectrum is

Plotting

The default method of plotting allows you to plot spectra which are adjacent to one another, using the 'plot' command:

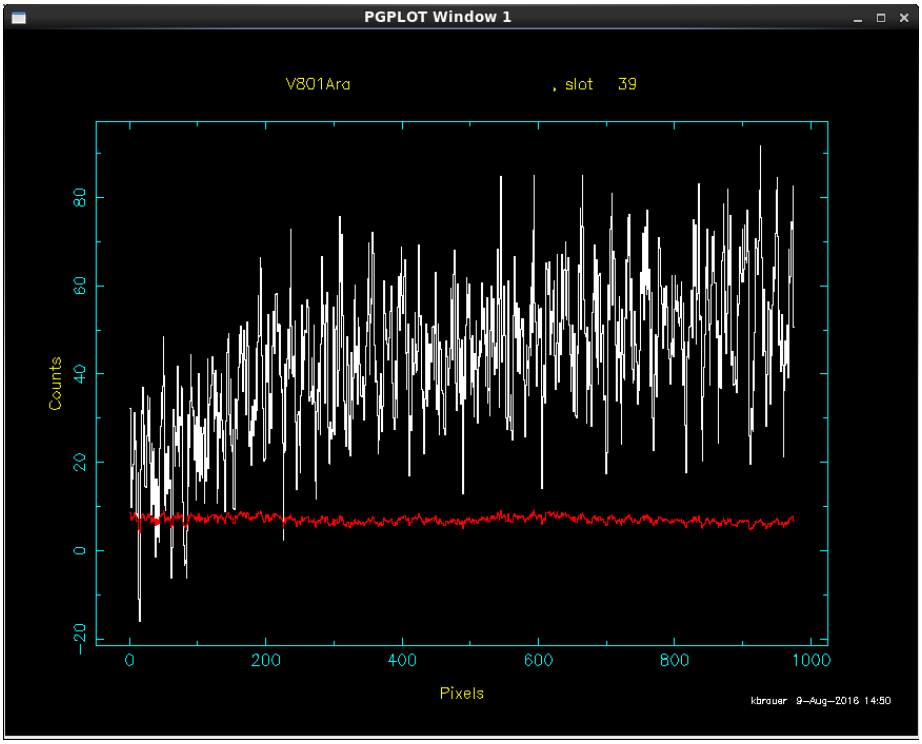
```
molly> plot
First slot to plot [      49]:
Last slot to plot [      49]:

Enter plot limits (Left,Right, Bottom,Top) :
  -200.1       4201.     -1.9844E+05  1.7876E+04
 0, 0 for old pair, A(bort), <CR> to proceed
300. 1300. -1.e4 2.e4

 Enter plot limits (Left,Right, Bottom,Top) :
   300.0       1300.     -1.0000E+04  2.0000E+04
 0, 0 for old pair, A(bort), <CR> to proceed

49, obj: V616Mon         , run:       1 exp:   660.6    time: 15/12/06, 07:25:13
```

Limits are chosen automatically to include the whole curve. Press enter to use these, 'a' to abort, or enter your own in the same format.



A plot of the spectrum in slot 39. Note that the x-axis is pixels, not wavelength.

If you want the plot axis to be in wavelength(angstroms):
molly> axes a

Alternatively, if you would like to plot spectra which are NOT next to one another, entering 0 into both the first and last slots to plot will take you to a subroutine in which you can pick the spectra you want to plot together:

molly> *plot*
First slot to plot [1]: *0* **Enter zero in both!**
Last slot to plot [1]: *0*
Enter list of spectra to plot
No slots chosen at present
Enter series of slot ranges
N,-M for M copies of spectrum N; 0,0 to stop

At this point, spectra can be chosen by typing the slot number, followed by a comma and the negative of the number of copies you want, then typing 0,0 to end your choice, e.g.:

234, -1
N,-M for M copies of spectrum N; 0,0 to stop
325,-1
N,-M for M copies of spectrum N; 0,0 to stop
0,0
Entry finished

This will select slots 234 and 325 for plotting once each. When you have finished your entry, you will still be in 'pick' mode - here you can type 's' to show the selected slots, 'c' to clear your choice, 'p' to pick more slots or 'q' to exit picking, choose axes and plot.

Note: if you want to plot your continuum fit together with your data you can put the average of the fits in a slot immediately adjacent to the average of your data.

Finally, if you would like to plot graphs in several windows, use the command 'device' before plotting and type successive numbers for each new window you want to plot in, followed by /xs (for an xserve window). Alternatively, you can save graphs by typing the file name, followed by /ps:

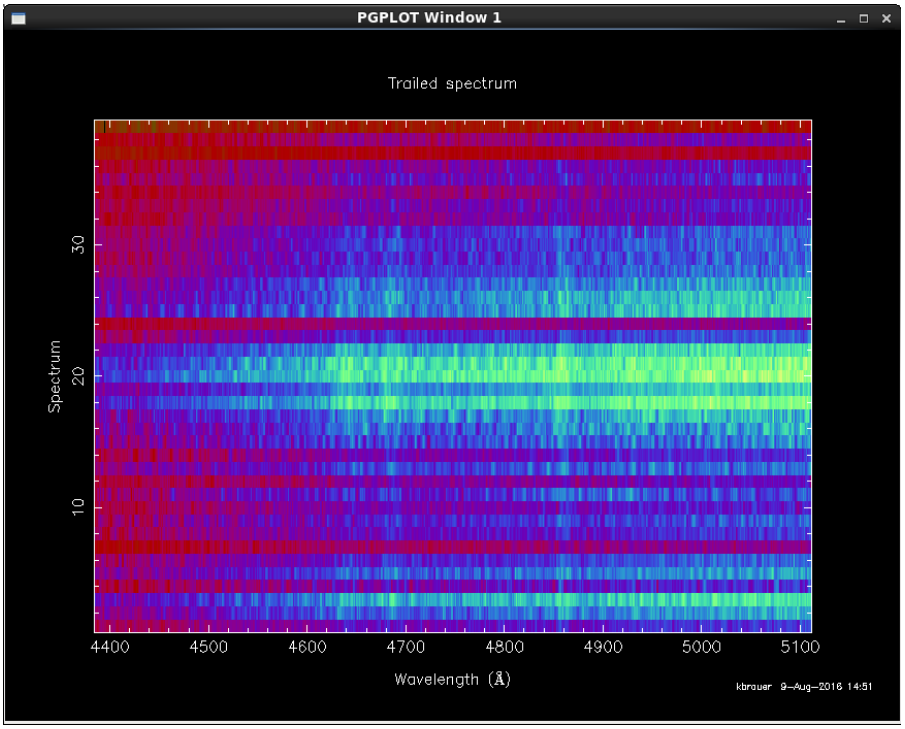
molly> *device*
Plot device [/xserve]: *1/xs*

molly> *device*
Plot device [/xserve]: file.ps*/ps*

Creating a trail

A trail composed of your spectra can be created using the 'trail' command:

molly> *trail*
First slot for trail [1]:
Last slot for trail [1]: *48*
Level for lowest colour index [0.000000]: *100* **These indexes must be adjusted to get a good**
Level for highest colour index [0.000000]: 2000 **trail - lower the values if it is mostly black.**
Enter X axis type [W]: **Wavelength (W) should be chosen**
Start wavelength [5964.839]: **The wavelength range of your spectra**
End wavelength [6653.628]:
Number of pixels [1798]: **The number of pixels for each spectrum**



An example of trailed spectra.

Preparing spectra for modmap

In order to optimise the output from modmap, several steps are required in molly:

Vbin

Firstly, the spectra should be rebinned on the velocity scale into a heliocentric frame, to account for the earth's velocity. This is done using the 'vbin' command:

molly> *vbin*
First spectrum to rebin [1]: *1*
Last spectrum to rebin [1]: *3*
First valid spectrum covers 5964.84 to 6653.63
Using 1798 pixels at 18.22 km/s/pixel.
Velocity centre is at 6299.826927247331
First spectrum for output [2]: *101* **Using a round starting number (101, 201 etc.) for a new set of spectra makes things less confusing later**
Central wavelength [6299.8269272473]: **The default parameters should fine to use here**
Number of km/s/pixel [18.221555592700]:
Number of pixels [1798]:
Interpolation method (L,Q,S) [Q]:
101, obj: V926sco , run: 1 exp: 420.0 time: 06/06/10, 00:39:20
102, obj: V926sco , run: 2 exp: 420.0 time: 06/06/10, 00:47:53
103, obj: V926sco , run: 3 exp: 420.0 time: 06/06/10, 00:56:29

Phase Assignment

To allow the orbital modulation to be fitted in modmap, the orbital phases of the spectra must next be assigned using the 'phase' command:

molly> *phase*
First slot to fix [1]: *1*
Last slot to fix [1]: *3*
Enter phase to compute [Orbital phase]:
Zero (Heliocentric Julian date) [2440000.0000000]: *2556782.027* **The Julian date of the zero ephemeris**
Period (days) [0.10000000149012]: *0.19278* **The period, in days, of the system's orbit**
Quadratic term (days) [0.0000000000000]:

An ephemeris containing the Heliocentric Julian date of zero phase and the orbital period can usually be found in previous papers. If the period is incorrect, the tomography will fail completely, whilst an incorrect zero point will result in inaccurate positioning of the primary and secondary objects in relation to the emission.

Polynomial Fitting, masking and Subtraction

In order for the spectral feature which you are using for modmap to be as clear as possible, it is useful to fit a curve to the contimuum to subtract.

To fit a polynomial to the continuum, use the 'pfit' command. This will ask if you would like to set a mask before fitting, which is your chance to exclude features in the spectrum, to allow for a good fit. This mask will not be applied to the spectrum in general, only for the fit. It is

best to have an average spectrum on hand on which to choose the regions to be masked before you go into pfit:

molly> *pfit*
First spectrum to fit [1]: *1*
Last spectrum to fit [1]: *3*
First slot for fits [2]: *201*
Number of poly coeffs [3]: *10* **A higher number of coefficients should give a**
Lower reject threshold [-3.000000]: **better fit if spectral features are masked.**
Upper reject threshold [3.000000]:
Number of reject cycles [10]:
Weight factor (0=no change, 1=unit) [0.000000]:
Set mask? [YES]: **Set to NO if you do NOT want to mask**
Mask regions not wanted in fit.

No mask set

Masker options:

clear -- Clear the mask.
dump -- Dump mask to disk.
load -- Load mask from disk.
mask -- Mask.
unmask -- Unmask.
show -- Show mask.
plot -- Plot a spectrum for cursor.
quit -- Quit.

Masking

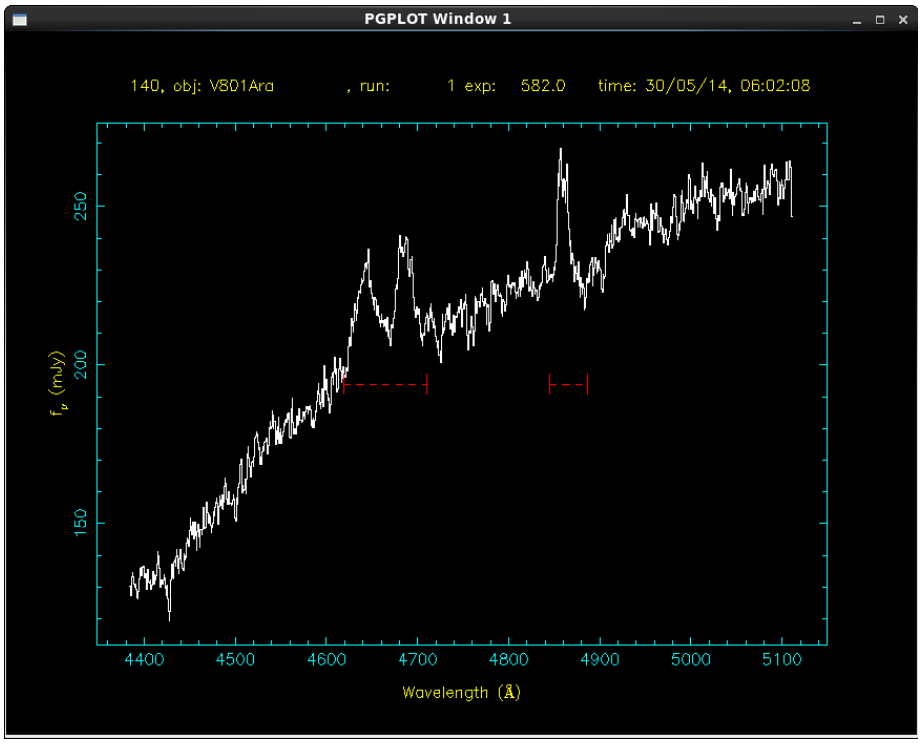
At this point you have entered 'mask' mode. Within this, the command 'mask' allows you to enter wavelength values of the areas of your spectrum which you would like to exclude. It is easier, however, to create an average spectrum of your spectra BEFORE starting pfit, then, once in 'mask' mode, to plot this average BEFORE typing 'mask'. If this plot is left open, option will be given to use a cursor on the graph to mask out regions. Selecting this option will activate the cursor on your pre-plotted graph. This will be a vertical red line, which can be positioned before hitting any key (except 'q') to select the start and end of regions around features to exclude. Hitting 'q' will return you to the 'mask' subroutine, which can also be exited using 'q'. This will process the spectra, create the fits in the chosen slots and return you to the main molly program.

mask> plot
Plot which slot? [1]: **Enter the location of your average spectrum and plot as above**
1, obj: V926sco , run: 1 exp: 420.0 time: 06/06/10, 00:39:20
Plot in P(ixels), W(avelength) or V(elocity)? [W]:

Enter plot limits (Left,Right, Bottom,Top) :
5951. 6269. -252.8 3922.
0, 0 for old pair, A(bort), <CR> to proceed

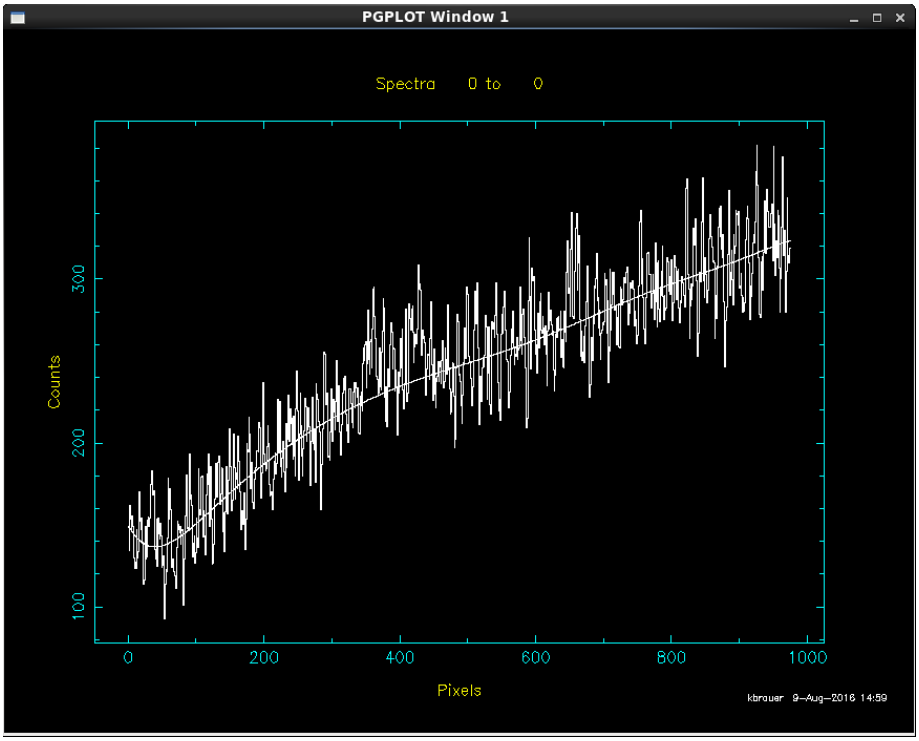
mask> mask **With the plot open, use the 'mask' command and**
Set mask via C(ursor) or T(erminal)? [C]: C **choose 'Cursor' to activate the masking cursor**
On plot, use any key to choose regions and 'q' to exit
Select ranges by positioning cursor and hitting any key except Q.
Hitting Q will exit immediately. **NOTE: don't type q in the command line. To quit,**

hit q while the plot is selected



The average spectrum plot with the emission features selected for masking.

At this point you will want to compare the fits to spectra, using the method for picking specific spectra shown above. This will allow you to make sure the fit is acceptable before subtraction.



An example of a spectrum plotted with its continuum fit. Make sure that the fit is good before subtracting it.

To subtract the fits simply use the 'sub' command and enter the spectra to subtract from and the fits to be subtracted:

molly> *sub*
First spectrum to process [1]: *1*
Last spectrum to process [1]: *3*
First spectrum to subtract [4]: *201*
Last spectrum to subtract [203]: *203*
First output slot [3]: 301
Slot 301 = 1 - 5
301, obj: V926sco , run: 1 exp: 420.0 time: 06/06/10, 00:39:20
Slot 302 = 2 - 6
302, obj: V926sco , run: 2 exp: 420.0 time: 06/06/10, 00:47:53
Slot 303 = 3 - 7
303, obj: V926sco , run: 3 exp: 420.0 time: 06/06/10, 00:56:29
Finished

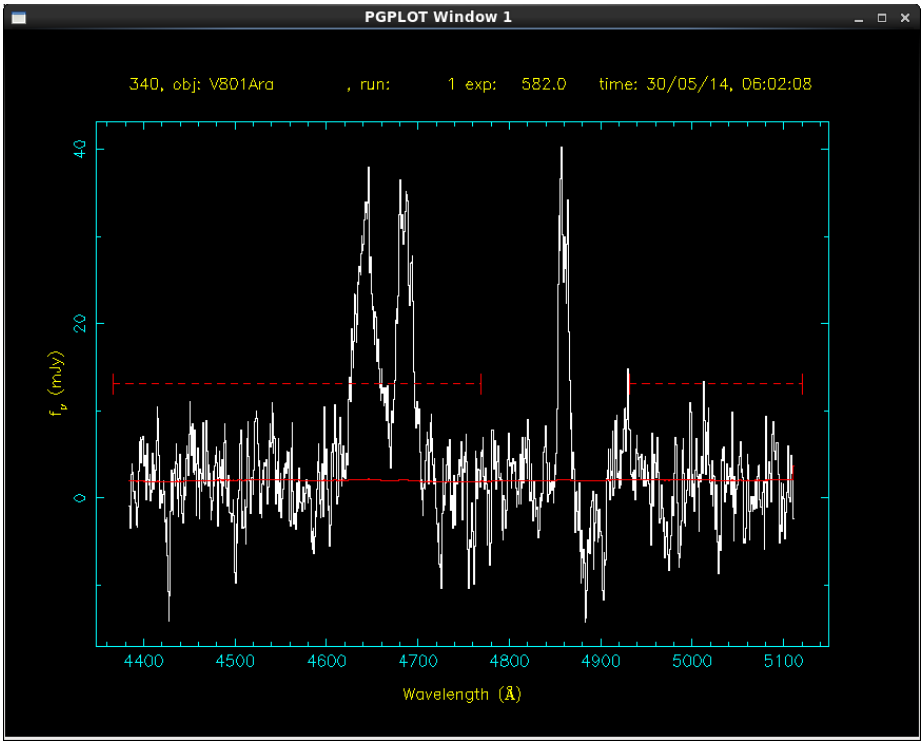
Finally, to trim the data to be used for modmap around the feature you wish to map, type 'mask' to enter the mask subroutine, selecting the slots you wish you to mask. You are then able to permanently mask all of the spectrum except the feature you wish to use:

molly> *mask*
First slot to mask [1]: *301*
Last slot to mask [301]: *303*
First output slot [2]: *401*
Mask (else unmask)? [y]: **If you make a mistake, reenter 'mask' mode and set this to no (n) to clear masks**
Set mask? [YES]:
Define regions to MASK

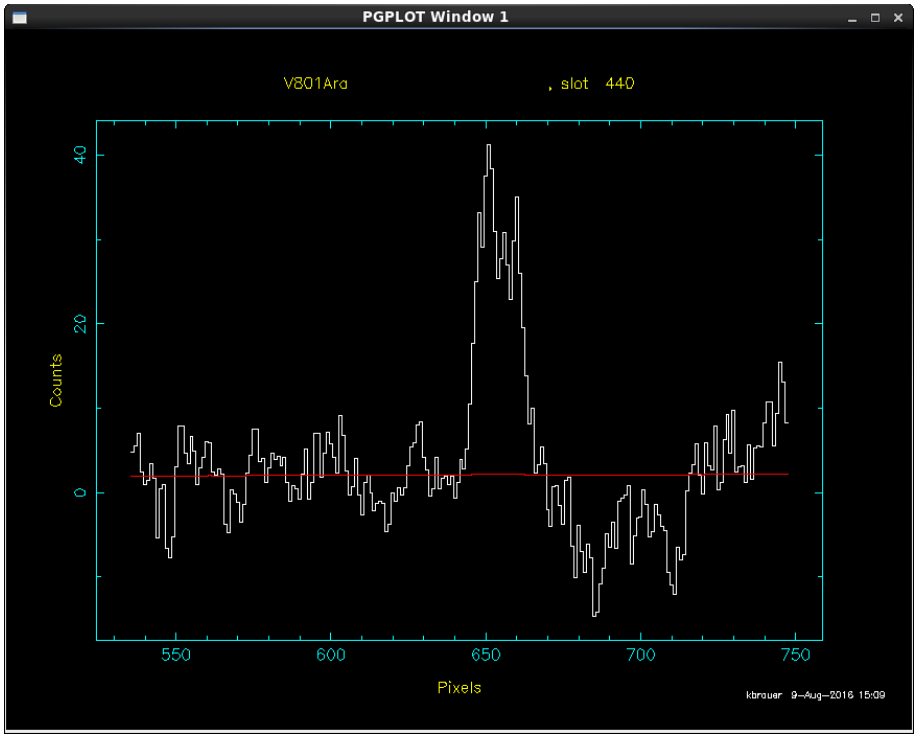
No mask set

Masker options:

clear -- Clear the mask.
dump -- Dump mask to disk.
load -- Load mask from disk.
mask -- Mask.
unmask -- Unmask.
show -- Show mask.
plot -- Plot a spectrum for cursor.
quit -- Quit.



The average continuum-subtracted spectrum within the mask subroutine. All of the spectrum except for the Hβ line and some continuum around it has been selected for masking.



The result of masking everything but the Hβ line and some continuum around it. This is the average spectrum.

Fitting a Gaussian to determine line center.

Use the routine mgfit to fit Gaussians to your lines. This requires an input file which contains basic information on the lines. Very important to input numbers as reals, eg 0. not 0, 1. not 1.

Molly> MGFIT N1 N2 N3 Infile Outfile THRLO THRHI NSPLIT FIT RESET SET

Parameters:

N1, N2 -- Range of slots to fit.
N3 -- First slot to store fits. Useful for comparing model with data, 0 to ignore.
Infile -- Input file defining the model to be used; see below.
Outfile -- Output file with fitted parameters.
THRLO, THRHI -- Lower and upper sigma reject thresholds. Pixels will be rejected and the fit repeated until no more are rejected. Thresholds measured in units of RMS of fit. See note above.
NSPLIT -- Number to split each exposure in as a means of accounting for binary motion during an exposure. In this case the model will consist of a trapezoidal integration over the exposure. Set = 1 for no account for smearing. This slows done the fits since every gaussian and derivatives have to computed NSPLIT times over.
FIT -- There are two fit methods:

'I' -- The variables are fitted separately for each spectrum.
'A' -- The variable parameters are fitted to all the spectra at once.

RESET -- Yes to reset to the starting values provided in the input file, No to use the previous spectrum's final fitted values.

SET -- yes to set bad pixel mask (if you know that some parts will not be fitted, it is better to reject them a priori than let the routine try to do it for you.)

For fitting a single gaussian plus a polynomial use a input file containing:

```
------------------------------
poly: 6500. $const $grad
gaussian: 6562.76 $off $fwhm 2.

$const = 1.
$grad  = 0.
$off   = 0.
$fwhm  = 25.
```

The polynomial is indicated by starting "poly:". This must be exactly this with no leading blanks. It is then defined by a pivot wavelength and coefficients. In this case 6500 is a fixed value whereas $const $grad are variables (the constant and gradient terms of the poly) or at least potentially variable -- see below for how they can be fixed.

The gaussian is similarly specified starting with "gaussian:". In this case the parameters are (1) the central wavelength (angstroms), (2) a velocity offset (km/s), (3) a full width half max (Angstroms) and (4) the peak height in mJy. In the example given, only the offset and FWHM are variable.

The variable names are case sensitive and must always begin with a $. Each variable must be given an initial value as in "$fwhm = 25.". The initial value lines can have no leading blanks. The names can be 8 characters at most, excluding the $.

FIXING "VARIABLES"

One often wants to switch which parameters vary or not. This can be done by adding an "F" for fixed at the end of its initialisation line, e.g.:

```
$fwhm =  25. F
```

In fact in complicated cases it is likely that you would want most of the

variables to be held fixed in this manner while you optimise subsets of them. This should be emphasized: the routine cannot magically find a solution if you give it too poor a start, and in complex cases you will need to "hold its hand".

Saving and Loading

To save spectra for use again in molly or for input into modmap, use the command 'write' and enter the file name and the slots of the spectra to save ('dump'). If you are overwriting an old file, select yes (y) when prompted:

```
molly> write
File name [spectrum]: filename.mol
First slot to dump [       1]: 1
Last slot to dump [ 1]: 3
Is this an old file? [N]:      Enter 'no' (n) for a new file, 'yes' (y) for an old file
    1, obj: V926sco        , run:      1 exp:   420.0    time: 06/06/10, 00:39:20
    2, obj: V926sco        , run:      2 exp:   420.0    time: 06/06/10, 00:47:53
    3, obj: V926sco        , run:      3 exp:   420.0    time: 06/06/10, 00:56:29
Dumped  3  spectra to 1.mol
```

To load saved spectra back into molly, use the command 'load', choose the slots into which to load the spectra and select the spectrum in the file with which to start:

```
molly> load
File name [file.mol]: filename.mol
First slot to read into [1]: 1
Last slot to read into [ 2]: 3
Start spectrum in file [ 1]: 1
    1, obj: V926sco        , run:      1 exp:   420.0    time: 06/06/10, 00:39:20
    2, obj: V926sco        , run:      2 exp:   420.0    time: 06/06/10, 00:47:53
    3, obj: V926sco        , run:      3 exp:   420.0    time: 06/06/10, 00:56:29
 Read  3  spectra from filename.mol
```

You should now be ready to enter your spectra into modmap!

Use wasc to write out a spectrum in ascii

Many details regards the routines available within Molly can be found at Tom Marsh's webiste: http://deneb.astro.warwick.ac.uk/phsaap/software/molly/html/CLASSES.html