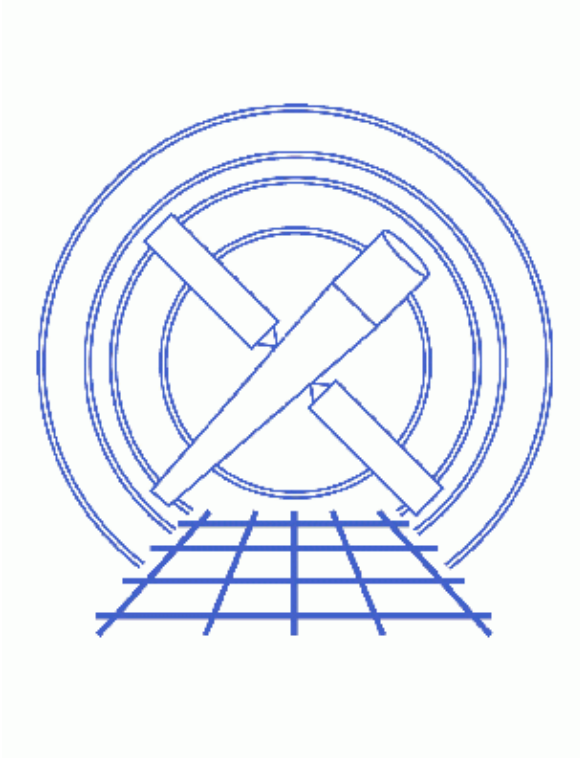
GUIDE: Fitting and Identifying Spectral Lines



Sherpa Threads (CIAO 3.4)

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GUIDE: Fitting and Identifying Spectral Lines

Sherpa Threads

Overview

Last Update: 1 Dec 2006 − updated for CIAO 3.4: *Sherpa* version

Synopsis:

GUIDE is a command line interpreted language that functions, essentially, as an extension of *Sherpa*. One of its more advanced applications is in identifying spectral lines to derive physical conditions and differential emmision measures.

Purpose:

To determine the flux and identity (ion and transition) of an emission line, and to write the results to a Model Descriptor List (MDL) file.

Related Links:

- WebGUIDE: an interactive GUIDE interface for ATOMDB v1.3. It provides a web interface for the Identify, Describe, and Strong commands.
- GUIDE Users Manual (PS, 23pp): full details on using the GUIDE package with *Sherpa*.
- Analysis Guide for Chandra High Resolution Spectroscopy: an in−depth discussion of grating analysis.

Proceed to the HTML or hardcopy (PDF: A4 | letter) version of the thread.

Get Started

Sample ObsID used: 1318 (HETG/ACIS−S, Capella)

In order to complete this thread, you will need grating ARFs for your dataset:

```
1318HEG_−1_garf.fits
1318HEG_1_garf.fits
1318MEG_−1_garf.fits
1318MEG_1_garf.fits

acis_1318_pha2.fits
```

The Create an HETG/ACIS−S Grating ARF thread shows you how to do so (there are similar threads if you are working with LETG/ACIS−S, LETG/HRC−S, or LETG/HRC−I data). We are using only the 1st order spectra, which correspond to data elements 3 and 4 (−1, +1 for HEG) and 9 and 10 (−1, +1 for MEG) in the standard Level II PHA file. The Examining PHA2 Files thread has more information on identifying gratings

and orders.

Loading GUIDE

Start *Sherpa* and load the GUIDE package:

```
unix% sherpa

-------------------------------------------------------
Welcome to Sherpa: CXC's Modeling and Fitting Program
-------------------------------------------------------
Version: CIAO 3.4

Type AHELP SHERPA for overview.
Type EXIT, QUIT, or BYE to leave the program.

Notes:
    Temporary files for visualization will be written to the directory:
    /tmp
    To change this so that these files are not deleted when you exit Sherpa,
    edit $ASCDS_WORK_PATH in your 'ciao' setup script.

    Abundances set to Anders & Grevesse

sherpa> import("guide")
GUIDE Initialized using ATOMDB v1.3.0
```

If a series of messages is printed here indicating that various files are not found, then it is likely that the ATOMDB is not correctly installed on your system. Please see your system manager or the CIAO download page and the ATOMDB webpage.

Read the Spectrum File and Build Responses

```
sherpa> paramprompt off
Model parameter prompting is off

sherpa> data acis_1318_pha2.fits
The inferred file type is PHA Type II.  If this is not what you want, please
specify the type explicitly in the data command.
Warning: could not find SYS_ERR column
WARNING: statistical errors specified in the PHA file.
         These are currently IGNORED.  To use them, type:
         READ ERRORS "<filename>[cols CHANNEL,STAT_ERR]" fitsbin
WARNING: backgrounds UP and DOWN are being read from this file,
         and are being combined into a single background dataset.
Warning: could not find SYS_ERR column
WARNING: multiple datasets have been input.
         The next available dataset number is 13.

sherpa> analysis
Analysis Space for Dataset 1: Wavelength
Analysis Space for Dataset 2: Wavelength
Analysis Space for Dataset 3: Wavelength
Analysis Space for Dataset 4: Wavelength
Analysis Space for Dataset 5: Wavelength
Analysis Space for Dataset 6: Wavelength
Analysis Space for Dataset 7: Wavelength
Analysis Space for Dataset 8: Wavelength
```

```
Analysis Space for Dataset 9: Wavelength
Analysis Space for Dataset 10: Wavelength
Analysis Space for Dataset 11: Wavelength
Analysis Space for Dataset 12: Wavelength
```

By default, the analysis mode is set to wavelength when reading in a type II PHA file. For analysis in wavelength space to make any sense, however, a wavelength grid must be created; this is done when the instrument response (either ARF, RMF, or both) is defined.

```
sherpa> instrument 3 = rsp[hegm1](,1318HEG_−1_garf.fits,)
The inferred file type is ARF.  If this is not what you want, please
specify the type explicitly in the data command.

sherpa> instrument 4 = rsp[hegp1](,1318HEG_1_garf.fits,)
The inferred file type is ARF.  If this is not what you want, please
specify the type explicitly in the data command.

sherpa> instrument 9 = rsp[megm1](,1318MEG_−1_garf.fits,)
The inferred file type is ARF.  If this is not what you want, please
specify the type explicitly in the data command.

sherpa> instrument 10 = rsp[megp1](,1318MEG_1_garf.fits,)
The inferred file type is ARF.  If this is not what you want, please
specify the type explicitly in the data command.

sherpa> # turn off Y errorbars
sherpa> sherpa.dataplot.y_errorbars=0
sherpa> sherpa.dataplot.curvestyle="histo"
sherpa> sherpa.dataplot.symbolstyle="none"

sherpa> lp 4 data 3 data 4 data 9 data 10
sherpa> ignore allsets all
sherpa> notice allsets wave 8.2:8.6
sherpa> lp 4 data 3 data 4 data 9 data 10
```

For this thread, we are not using a grating RMF (which acts as a line shape function for grating data), and are therefore assuming that the line profile is gaussian.

Figure 1 shows the resulting plot which highlights a feature that is present in all four orders of the observation.

Defining the Source Model

We model this source with a 1−D normalized Gaussian (`ngauss1d`) combined with a 1−D polynomial function (`polynom1d`). Separate source models are used for the HEG and MEG datasets.

```
sherpa> source 3,4 = ngauss[hg1] + poly[hp1]
sherpa> source 9,10 = ngauss[mg1] + poly[mp1]

sherpa> mg1.ampl => hg1.ampl

sherpa> show source 10
Source 10: (mg1 + mp1)
ngauss1d[mg1]  (integrate: on)
    Param   Type      Value        Min        Max                Units
    -----   ----      -----        ---        ---                -----
 1   fwhm thawed 9.9987e−02 9.9987e−04     9.9987
 2    pos thawed     8.4225     8.1975     8.5975
 3   ampl   link 1.7195e−03     expression: hg1.ampl
poly1d[mp1]  (integrate: on)
    Param   Type      Value        Min        Max                Units
```

```
    -----   ----      -----        ---        ---                  -----
 1     c0 thawed  4.681e-03 -1.022e-04 9.2599e-03
 2     c1 frozen          0    -2.2894     2.2894
 3     c2 frozen          0    -5.7236     5.7236
 4     c3 frozen          0 -1.022e-04 9.2599e-03
 5     c4 frozen          0 -1.022e-04 9.2599e-03
 6     c5 frozen          0 -1.022e-04 9.2599e-03
 7     c6 frozen          0 -1.022e-04 9.2599e-03
 8     c7 frozen          0 -1.022e-04 9.2599e-03
 9     c8 frozen          0 -1.022e-04 9.2599e-03
10 offset frozen          0    -8.1975     8.5975
```

We choose to link the amplitudes for the models (`mg1.ampl => hg1.ampl`). This forces *Sherpa* to find the best−fit amplitude for all four datasets.

Fitting

Fit all four datasets simultaneously:

```
sherpa> fit 3,4,9,10
WARNING (Sets 3,4,9,10): background data have been entered,
        but they have not been subtracted, nor have background models been set.
 LVMQT: V2.0
 LVMQT: initial statistic value = 118084
 LVMQT: final statistic value = 138.672 at iteration 14
           hg1.fwhm  0.0118774
           hg1.pos  8.42135
           hg1.ampl  0.000177587
           hp1.c0  0.000341403
           mg1.fwhm  0.0176838
           mg1.pos  8.42178
           mp1.c0  0.000421502
```

The fit gives us a line position and flux (for a normalized gaussian, the flux is simply the amplitude [`hg1.ampl`]: 1.81e−4 photons/cm^2/s). The `mg1.ampl` is not listed because it was linked to `hg1.ampl`, and so has the same best−fit value.

Identify the Line

The next step is to use the `identify` command to determine the source of the line; it takes a given wavelength and searches the APEC line list for strong lines with wavelengths close to it (within 0.01 Å by default). An optional second parameter allows a search range to be set (i.e. `identify(8.42, 0.02)` prints all lines with wavelengths between 8.40 and 8.44 Å):

```
sherpa> identify(8.42, 0.02)
  Lambda  --  Ion     UL -  LL Emissivity@   kT  RelInt  For More Info
 Angstrom                      ph cm^3/s   keV
   8.4053   Fe XXII   177-   8  1.28e-18 @ 1.085 0.019 describe(26,22,177,8)
   8.4192    Mg XII     4-   1  6.89e-17 @ 0.862 1.000 describe(12,12,4,1)
   8.4246    Mg XII     3-   1  3.45e-17 @ 0.862 0.500 describe(12,12,3,1)
```

The fifth and sixth columns give the peak emissivity and temperature, respectively. The best identification is usually the strongest line in the list; if the peak emissivities are similar, the line could be a blend. In this case, the strongest lines are the 4−>1 and 3−>1 transitions of Mg XII (hydrogen−like magnesium).

We can find out more about some of the lines with the `describe` command; this command gets its

information from APED. The syntax is `describe(element, ion, upperlevel, lowerlevel)`: `element` is the number of protons (i.e. Mg = 12), `ion` is the ion stage in astronomical usage (i.e. XII = 12), and the upper and lower energy levels are given in the identify list. Note that the appropriate `describe` syntax is provided by the `identify` command. To find out about the strongest line in the previous list:

```
sherpa> describe(12,12,4,1)
Ion Mg XII, energy level 1 ---
electron configuration      : 1s~^2S_{1/2}
energy above ground (eV)    : 0.000000
Quantum state               : n=1, l=N/A, s=2, degeneracy=2
Energy level data source    : 1983ADNDT..29..467S
Photoionization data source : 1964ApJS....9..185B
----------------------------------------
Ion Mg XII, energy level 4 ---
electron configuration      : 2p~^2P_{3/2}
energy above ground (eV)    : 1469.430054
Quantum state               : n=2, l=1, s=2, degeneracy=4
Energy level data source    : 1983ADNDT..29..467S
Photoionization data source : 1964ApJS....9..185B
----------------------------------------
Ion Mg XII, 1 - 4 interactions ---
Electron collision rate from    1 ->    4  : nonzero.
Reference bibcode                          : 1983ADNDT..29..467S
Wavelength (lab/observed) (Angstrom)       : 8.419209 +/- 0.000040
Wavelength (theory) (Angstrom)             : 8.438330
Transition rate/Einstein A (s^-1)          : 1.278220e+13
Wavelength (lab/observed) reference        : 1977JPCRD...6...3E
Wavelength (theory) reference              : 1983ADNDT..29..467S
Transition rate reference                  : 1987JPhB...20.6457F
```

This tells us that the 4−>1 transition in Mg XII is in fact an n=2−>1 hydrogen−like transition, or one component of the hydrogen−like Mg XII Lyman alpha line. Using `describe(12,12,3,1)` shows that it is the other transition in the n=2−>1 doublet. This identification information (along with the current filter) can then be associated with a particular model element (in this case, the gaussian model `hg1` used to fit the HEG +/−1 orders) using the `lineid` and `filter` commands:

```
sherpa> hg1 lineid "APECline(12,12,4,1)+APECline(12,12,3,1)"
sherpa> hg1 filter "ignore allsets all; notice allsets wave 8.2:8.6"
```

Write an MDL File

Finally, the results are written to an MDL file which stores the data, the model, and the identification. This formatted FITS file can be read back into *Sherpa* (using `read mdl "MgXII_MDL.fits"`) and can also be used for more sophisticated projects, such as fitting a differential emission measure (DEM) model.

```
sherpa> write mdl "MgXII_MDL.fits"
WARNING (Sets 3,4,9,10): background data have been entered,
        but they have not been subtracted, nor have background models been set.
```

Use `prism` to examine the file that was just created:

```
sherpa> prism MgXII_MDL.fits
```

Figure 2 shows the resulting display; the modeling information is saved in the `MDL_Models` block.

History

14 Jan 2005	reviewed for CIAO 3.2: no changes
21 Dec 2005	reviewed for CIAO 3.3: no changes
09 Feb 2006	minor change to filenames; organized thread into sections
01 Dec 2006	updated for CIAO 3.4: *Sherpa* version

URL: http://cxc.harvard.edu/sherpa/threads/guide/ Last modified: 1 Dec 2006

Image 1: Plot of 8.2−8.6 Å HEG/MEG +/−1 orders

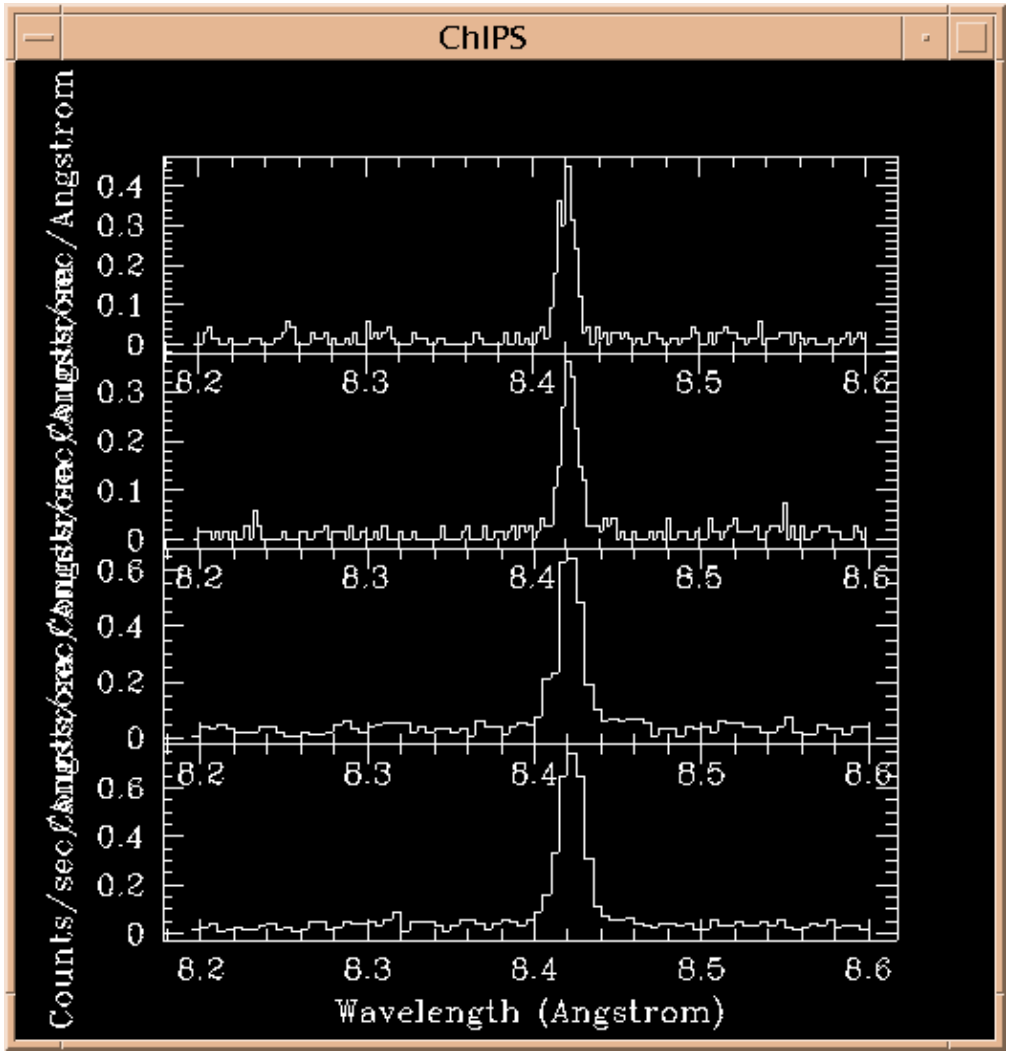
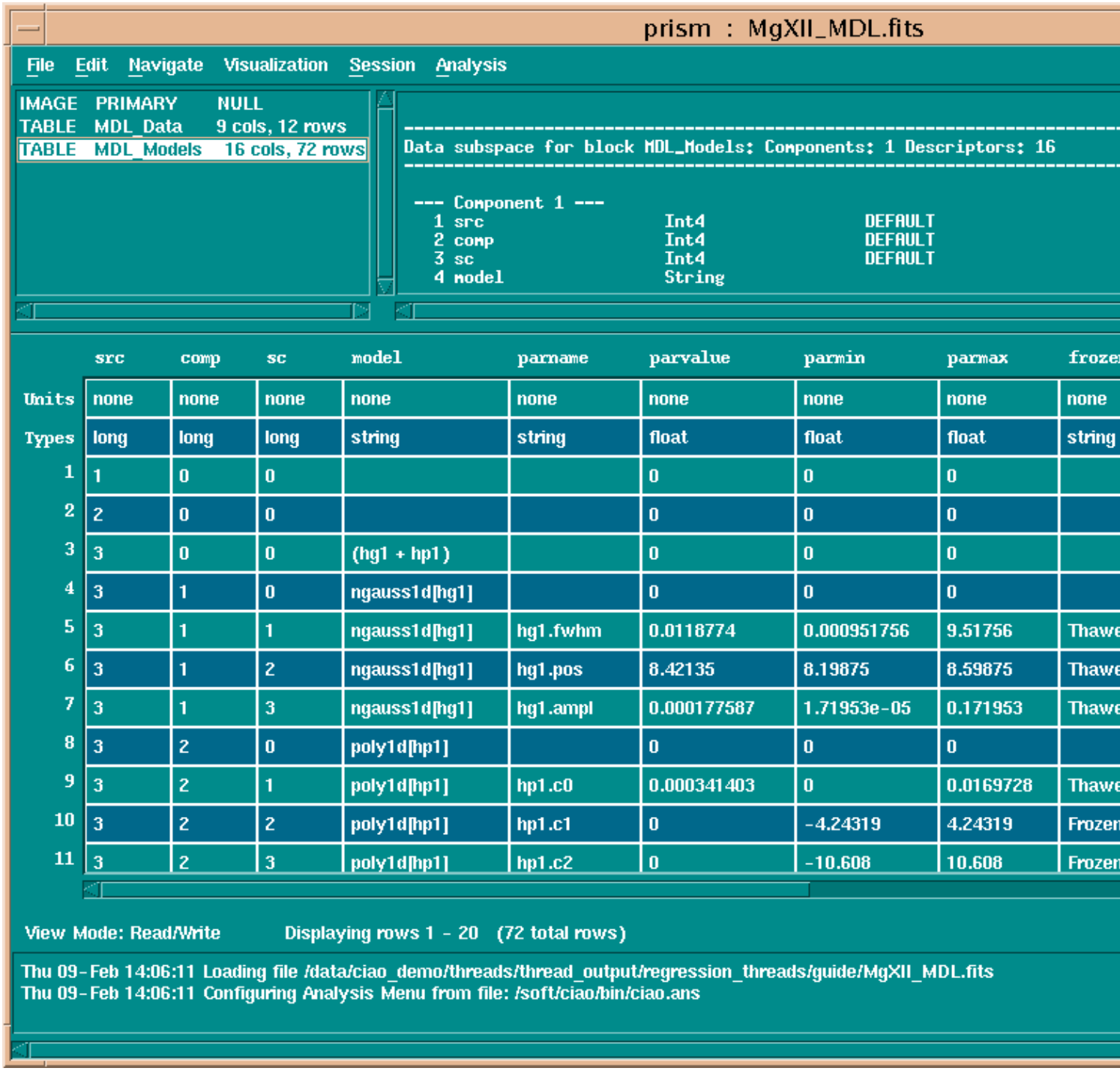
Image 2: Viewing the MDL file with Prism