Introduction to Grating Analysis

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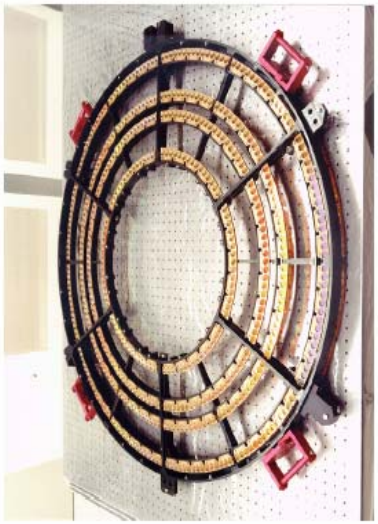
See also David Huenemoerder's spectroscopy page
http://space.mit.edu/ASC/analysis/AGfCHRS/AGfCHRS.html

Chandra has two transmission grating spectrometers.

The LETG: Spacing = 1μm

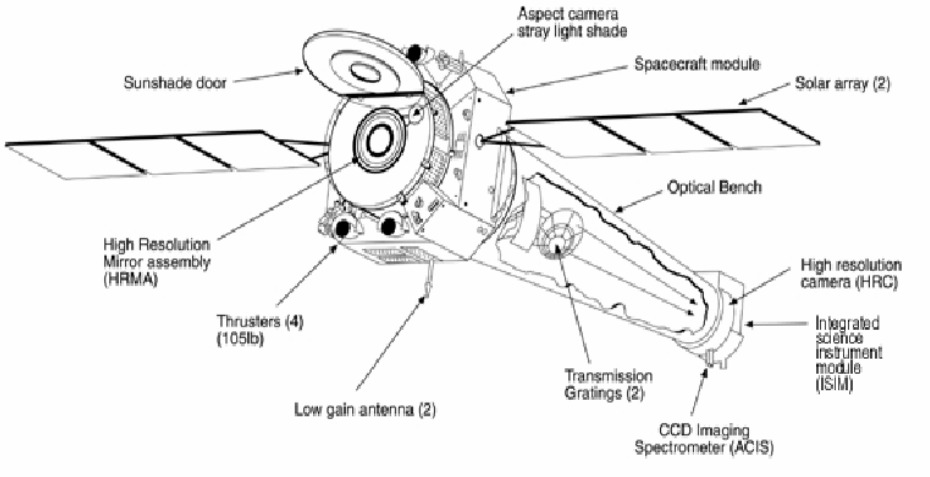
FWHM = .05 Å



The HETG: Spacing = 0.2, 0.4 μm

FWHM = .012, .024 Å

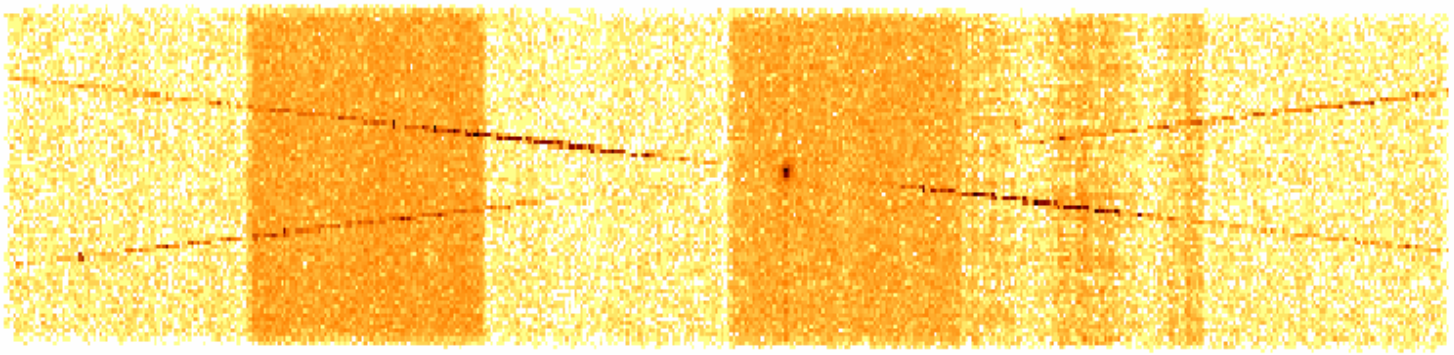
Either one of the two grating assemblies can be inserted at any time:

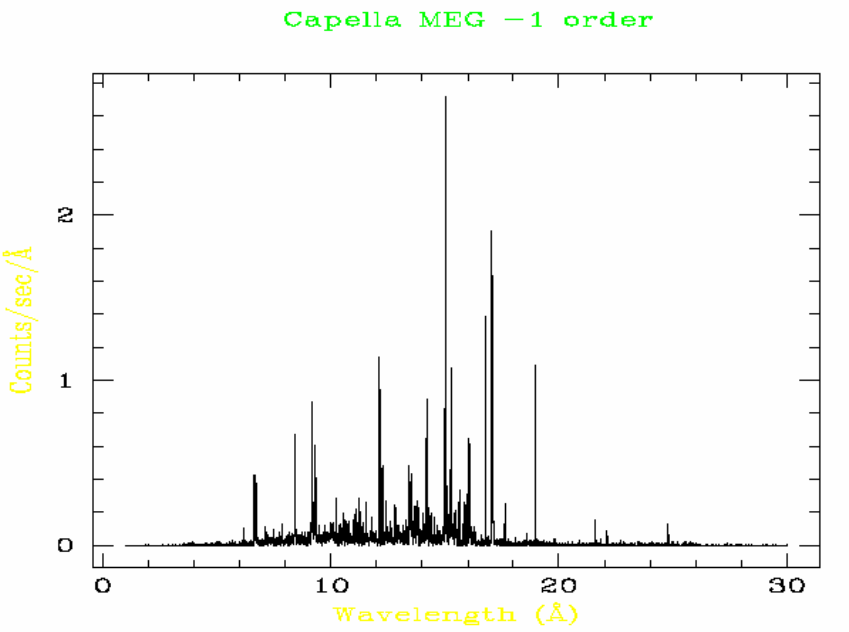


The gratings and the detectors are entirely independent, and so any combination may be selected (although some are less useful than others). The most common combinations are:

- HETG/ACIS-S
- LETG/ACIS-S
- LETG/HRC-S

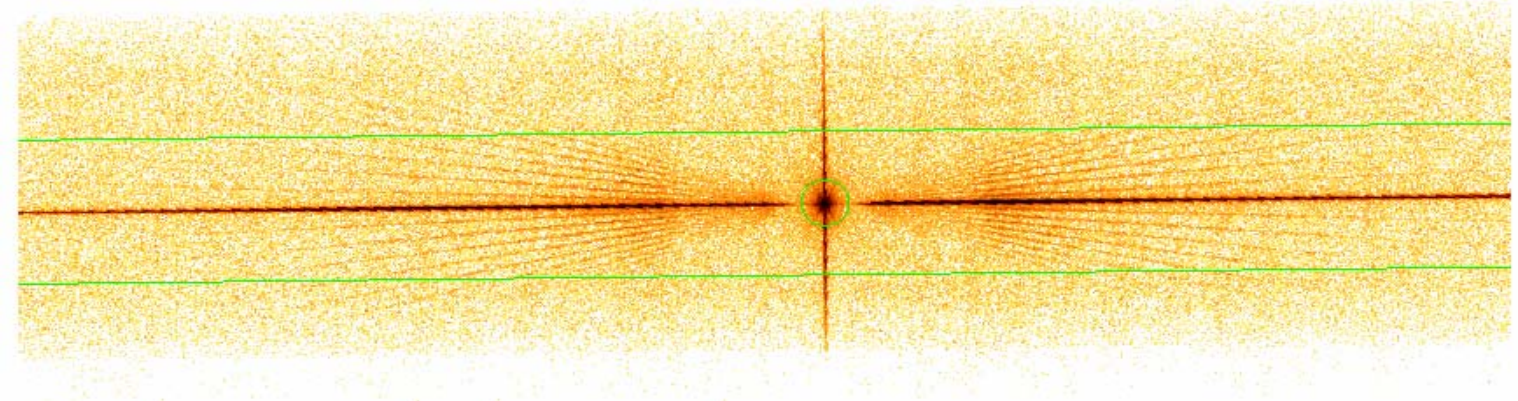
Capella with the HETG/ACIS-S detector:





Spectrum from the MEG-1 order

High-resolution (grating) spectra on Chandra cover a wide range of wavelengths: from 1.2-170Å. Note that wavelength is the natural unit.



LETG/HRC-S Observation of NGC6624

Grating Basics

X-ray gratings work exactly the same as optical gratings: the photons hit the gratings, and some are dispersed in a wavelength-dependent fashion, following the grating equation: $\sin \beta = m \lambda / p$

where λ is the wavelength, β is the dispersion angle (measured from the zero-order image), p is the spatial period of the grating lines, and m is the order number.

If ACIS is the detector, the CCD resolution can be used to distinguish between different orders; on the HRC, order separation must be modeled.

The goal of the grating pipeline is to:

- Select "good" X-ray events
- Identify the zero order and dispersed image
- Measure the dispersion angle for each event
- Create a binned spectrum
- Calculate the effective area and response matrix

Clearly, the spatial and spectral elements are tightly coupled. If the zero-order image is slightly displaced, the ± order wavelengths will be offset from each other.

Note: By default, pixel randomization is turned "on" in the *_process_events step. If you are not concerned about timing fluctuations on 1 ksec timescales, turning it off can increase the HEG resolution by 10%.

Identify zero-order, grating arms

```
tgdetect infile=hrc_evt1.fits outfile=hrc_evt1_src1a.fits OBI_srclist_file=NONE
```

Make mask for each grating arm (tg_create_mask)

```
tg_create_mask infile=frc_evt1.fits outfile=hrc_evt_L1a.fits
input_pos_tab=hrc_evt1_src1a.fits grating_obs=header_value
```

Measure dispersion angle for each event

```
tg_resolve_events infile=hrc_evt1.fits outfile=hrc_evt1a.fits regionfile=hrc_evt1_L1a.fits
acaofffile=hrc_aoff1.fits eventdef= ")stdlev_HRC"
```

Apply background filter (dmcopy)

```
dmcopy "hrc_evt1a.fits[EVENTS][pha=0:254, (tg_lam, pi)=region($CALDB/data/chandra/
hrc/bcf/tgmask2/letgD1999-07-22pireg062_N0001.fits]" hrc_back_evt1a.fits opt=all
```

Apply GTI filter (dmcopy) `dmcopy "hrc_back_evt1a.fits[EVENTS][@hrc_std_flt1.fits][cols !crsu,!crsv,!amp,!av1,!av2,!av3,!raw,!sumamps]" hrc_flt1_evt1a.fits opt=all`

Filter on status (dmcopy)

```
dmcopy "hrc_flt1-evt1a.fits[status=xxxxxx00xxxx0xxx0000x000x00000xx]" hrc_evt2.fits opt=all
```

Extract a Grating Spectrum (tgextract)

```
tgextract infile=hrc_evt2.fits outfile=hrc_pha2.fits inregion_file=CALDB
outfile_type=pha_typeII tg_srcid_list=all tg_part_list=header_value tg_order_list=default
ancrfile=none respfile=none
```

Make grating effective area

```
fullgarf phafile=hrc_pha2.fits pharow=1 evtfile=hrc_evt2.fits asol=pcad_asol1.fits
engrid="hrc_rmf.fits[cols ENERG_LO,ENERG_HI]" dtffile=hrc_dtf1.fits
badpix=hrc_bpix1.fits rootname=x_per
```

The standard output is a single PHA file (Type II PHA), containing

ACIS/HETG 12 spectra (±1, 2, 3 orders for both the HEG and MEG).

ACIS/LETG 6 spectra (±1, 2, 3 orders for the LEG).

HRC/LETG 2 spectra are created (± orders).

HRC/HETG Not a recommended configuration

This "PHA2" is a FITS format file that contains N rows of data, one for each spectral order. The file can be viewed with **prism**. Other standard FITS output files are the grating arf ("garf") and grating rmf ("grmf").

The pha spectrum is in counts vs bin edges; dividing by the effective area (garf) and exposure time creates a fluxed spectrum. The instrumental line profile is essentially the grmf.

In Sherpa, grating spectra can be jointly fit to a model.

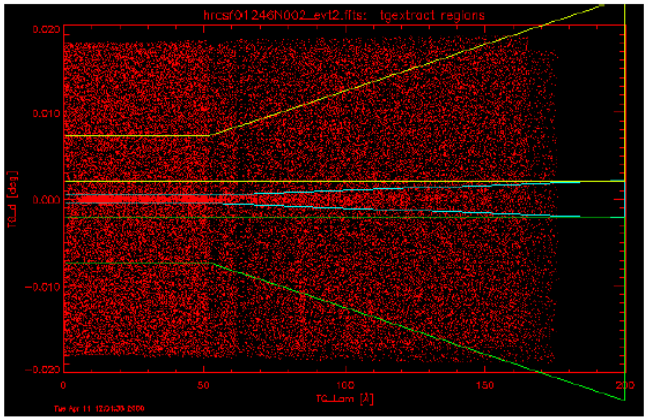
The Event File

unix% dmlist hrc_evt2.fits cols

Columns for Table Block EVENTS

Col	Name	Unit	Type	Range	Description
1	time	s	Real8	6.9e7:7.0e7	time tag of data record
2	rd(tg_r,tg_d)	deg	Real4	-2.0: 2.0	Grating angular coords
3	chip (chipx,chipy)	pixel	Int2	1:4096	Chip coords
4	tdet(tdetx,tdety)	pixel	Int4	1:49368	Tdet coords
5	det(detx,dety)	pixel	Real4	0.50:65536.50	Det coords
6	sky(x,y)	pixel	Real4	0.50:65536.50	Sky coords
7	chip_id	Int2	1:3		
8	pha	Int2	0:255		
9	pi	Int2	0:255		
10	tg_m	Int2	-62:62		Diffraction order (m)
11	tg_lam	angstrom	Real4	0: 400.0	wavelength (lambda)
12	tg_mlam	angstrom	Real4	-400.00:400.00	Order times wavelength (m*lambda)
13	tg_srcid		Int2	0:32767	source ID, index from detect table
14	tg_part		Int2	0:99	HEG, MEG, LEG, HESF regions
15	tg-smap		Int2	0:32767	source map; flags for up to 10 sources
16	status[4]		Bit(4)		event status bits

Background Regions



The background is extracted in two regions: above and below the grating arm (background_up) and (background_down). The default spectrum widths are given in the tgextract help file.

There are two backgrounds because the geometry is not necessarily symmetric, especially for HETGS near the zero-order, or if there are other sources in the field. By default in Sherpa they are averaged.

Each PHA2 file has three keywords BACKSCAL, BACKSCUP, BACKSCDN, which scale the background counts arrays to represent the expected background counts in each of the source, BACKGROUND_UP, and BACKGROUND_DOWN regions.

For bright sources on ACIS-S, the background is likely negligible. However, in the HRC-S it is usually large.

Faint Spectra

Most X-ray objects are not as bright as Capella or NGC6624. In these cases, you might wish to co-add the grating data to increase the number of counts per bin. There are four possibilities:

1. **Co-add plus/minus orders of the same grating.** *Can broaden lines if zero-order is offset.*

2. **Co-adding HEG and MEG data.** *Complicates line shape function.*

3. **Co-adding separate observations.** *Instrumental background can vary, plus same issues of zero-order offsets.*

4. **Co-adding separate observations and instruments**. *All of the above.*

These calibration issues are either not a problem or are an "acceptable risk." In this case, **CIAO** provides a number of tools:

Adding together plus, minus orders

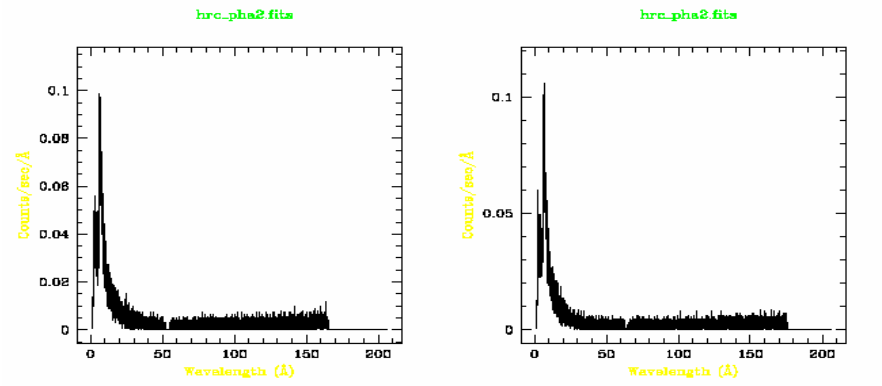
```
add_grating_orders pha2=acisf00459N002_pha2.fits
  order=1 garm=MEG garf=acisf00459MEG_-1_garf.fits

  garfp=acisf00459MEG_1_garf.fits gtype=BIN gspec=10 root=459
```

Adding together plus, minus orders

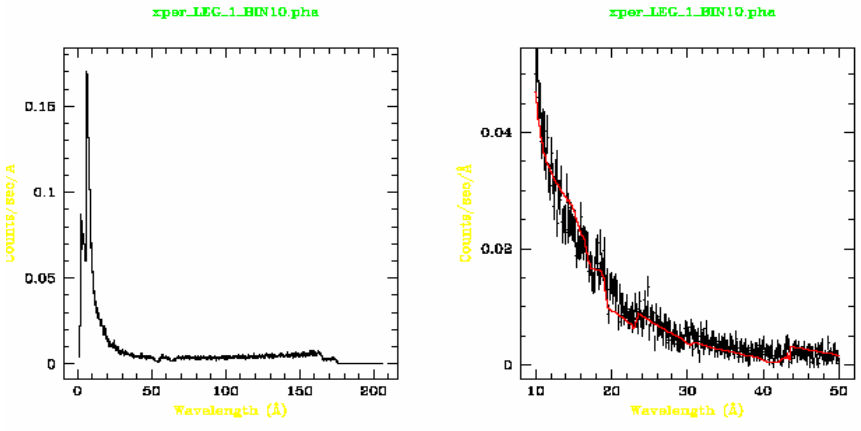
```
add_grating_spectra pha1=2463_MEG_1_BIN10.pha
  pha2=459_MEG_1_BIN10.pha garf1=2463_MEG_1.arf

  garf2=459_MEG_1.arf gtype=BIN gspec=10 root=3C273_summed
```



X Per, an HMXB observed for 50 ksec with the HRC/LETG.

```
add_grating_orders pha2=hrc_pha2.fits order=1 garm=LEG \
garfm=x_perLEG_-1_garf.fits garfp=x_perLEG_1garf.fits \
gtype=BIN gspec=1- root=xper
```



Co-add and bin this data with add_grating_orders to increase the number of counts/bin.

With low or moderate resolution data, one forward-folds models and compares to the data. With grating data, one can also measure line fluxes or equivalent widths directly.

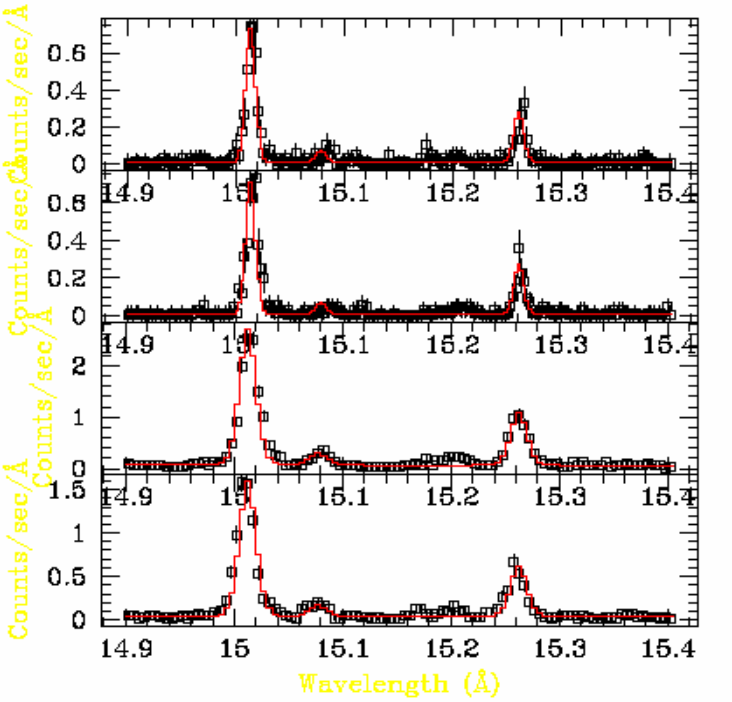
However, many standard X-ray models are available only in Sherpa, XSPEC, or ISIS and so using these programs for grating analysis is common. All that is needed is the spectral data (pha2) file and the grating arf (and possibly rmf) files:

A sample sherpa session:

```
unix% sherpa
sherpa> data acis_pha2.fits
sherpa> paramprompt off
sherpa> rsp[hm1]
sherpa> rsp[hp1]
sherpa> rsp[mm1]
sherpa> rsp[mp1]
sherpa> hm1.rmf = acisheg1D1999-07-22rmfN0004.fits
sherpa> hm1.arf = acisf01318HEG_-1_garf.fits
sherpa> hp1.rmf = acisheg1D1999-03-22rmfN0004.fits
sherpa> hp1.arf = acisf01318HEG_1_garf.fits
sherpa> mm1.rmf = acismeg1D1999-07-22rmfN0004.fits
sherpa> mm1.arf = acisf01318MEG_-1_garf.fits
sherpa> mp1.rmf = acismeg1D1999-07-22rmfN0004.fits
sherpa> mp1.arf = acisf01318MEG_1_garf.fits
sherpa> instrument 3 = hm1
sherpa> instrument 4 = hp1
sherpa> instrument 9 = mm1
sherpa> instrument 10= mp1
sherpa> ignore allsets all
sherpa> notice allsets wave 14.9:15.4
sherpa> source 3,4,9,10 = poly[b1] + delta1d[l1] + delta1d[l2] + delta1d[l3]
sherpa> l1.pos = 15.014
sherpa> l2.pos = 15.079
sherpa> l3.pos = 15.2610
sherpa> freeze l1.pos
sherpa> freeze l2.pos
sherpa> freeze l3.pos
```

```
sherpa> fit
sherpa> lp 4 fit 3 fit 4 fit 9 fit 10
sherpa> import ("guide")
sherpa> mdl2latex
\begin{tabular}{lllllll}
ModelName & Line Model & Position & Flux & Flux Error & Fit Data & Label \\
 &  & Angstrom & ph/cm$^2$/s & ph/cm$^2$/s & \\
l1 & delta1d & 15.014 & 0.00308923 & 6.7101e-05 & 3,4,9,10 & \\
l2 & delta1d & 15.079 & 0.000270431 & 2.81612e-05 & 3,4,9,10 \\
l3 & delta1d & 15.261 & 0.00125857 & 4.79625e-05 & 3,4,9,10 & \\
\end{tabular}
```

And the results are shown here. `lp 4 fit 3 fit 4 fit 9 fit 10` gives

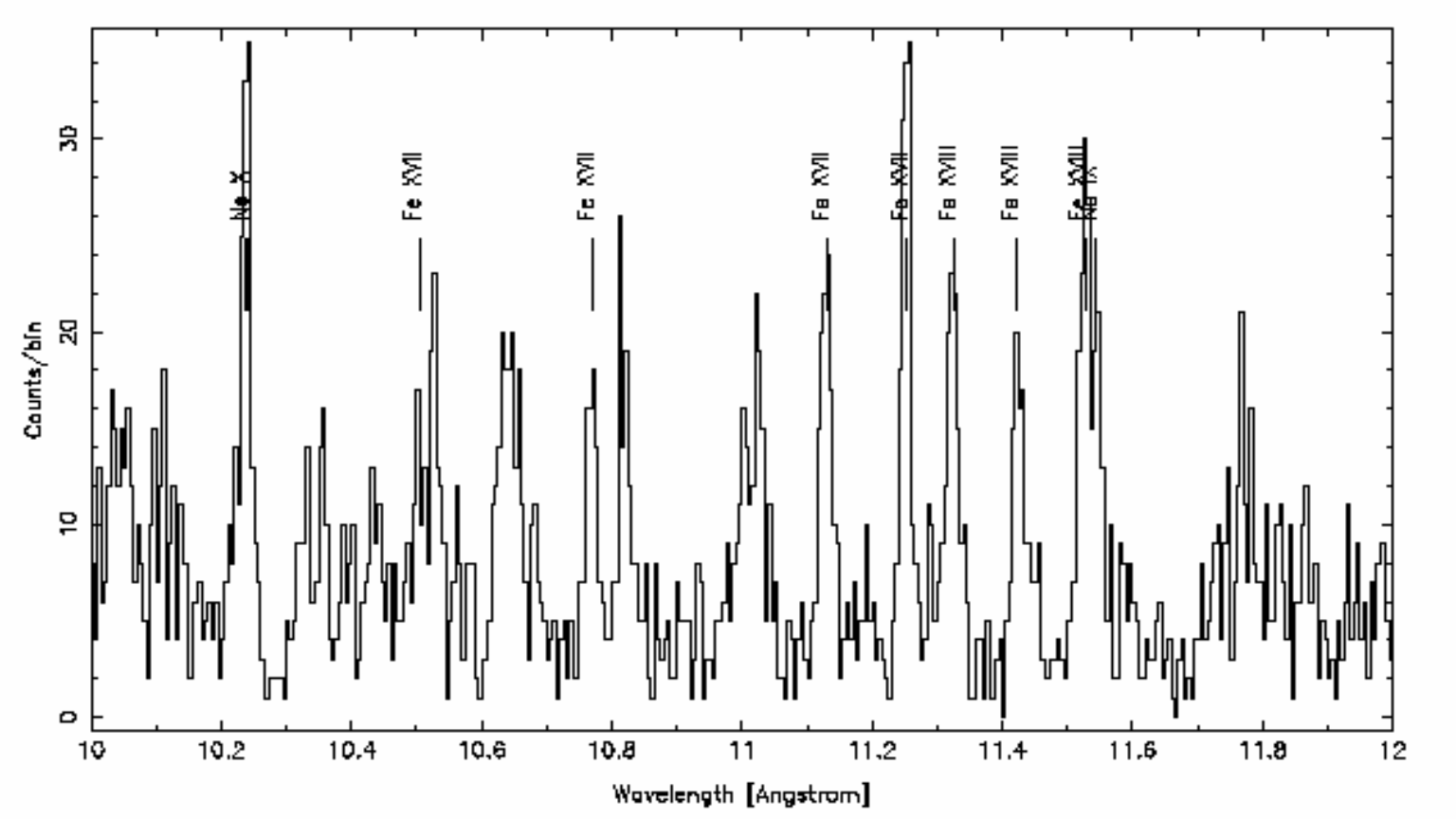


while the `md12latex` command gives the table:

ModelName	Line Model	Position Angstrom	Flux ph/cm²/s	Flux Error ph/cm²/s	Fit Data	Label
l1	delta1d	15.014	0.00308923	6.7101e-05	3,4,9,10	
l2	delta1d	15.079	0.000270431	2.81612e-05	3,4,9,10	
l3	delta1d	15.261	0.00125857	4.79625e-05	3,4,9,10	

Alternatively (or in conjunction), ISIS, developed by the MIT CXC team, can be used in Sherpa or stand-alone.

```
unix% sherpa
sherpa> import("isis");
sherpa> load_data("acis_pha2.fits");
sherpa> plasma(aped);
sherpa> load_arf("acisf01318MEG_-1_garf.fits")
sherpa> assign_arf(1,9);
sherpa> flux_corr(9,2);
sherpa> d = get_data_counts (9);
sherpa> load_model("model.dat");
sherpa> fl = model_spectrum (d.bin_lo, d.bin_hi);
sherpa> g = brightest(10, where (wl(10,12)));
sherpa> id = open_plot("isis_capella.ps/vcps");
sherpa> resize(15);
sherpa> xrange(10,12);
sherpa> plot_data_counts(9);
sherpa> plot_group(g);
sherpa> close_plot(id);
```


Ne X
Fe XVII
Fe XVII
Fe XVII
Fe XVII
Fe XVIII
Fe XVIII
Fe XVIII
Ne IX
Counts/bin
0
10
20
30
10
10.2
10.4
10.6
10.8
11
11.2
11.4
11.6
11.8
12
Wavelength [Angstrom]

S-lang, Sherpa, and ISIS: Easy user-defined models

Using *S-lang*, we can create a new power-law model quite easily:

```
define slang_pow() {
   variable p, norm, Emin, Emax, dE, Result;
   if (_NARGS == 3) (p, norm, Emin) = ()
   if (_NARGS == 4) {
      (p, norm, Emin, Emax) = ()
      dE = Emax - Emin;
   }
   if (_NARGS == 3) Result = norm*(E^(-p));
   if (_NARGS == 4) Result = norm*(E^(-p))*dE;
   Result = typecast(Result,_typeof(Emin));
}
() = sherpa_register_model("slang_pow", ["power","norm"], 1,
                           [1.0,1.e-2],   % default values
                           [-10,1.e-20],  % Minimum values
                           [10,1.e5],     % Maximum values
                           [1,1]);        % Both thawed by default
```

GUIDE is a collection of S-lang scripts whose purpose is to simplify access to the atomic database ATOMDB, which consists of the Astrophysical Plasma Emission Code (APEC) spectral calculations and the Astrophysical Plasma Emission Database (APED). GUIDE provides informational functions:

identify Print finding chart of wavelengths

strong List strong lines at a given temperature

describe Describe atomic parameters of a line

mdl2latex Convert fit parameters into a latex table

ionbal Output ionization balance values for a given ion

These routines can be found in the directory $ASCDS_BIN/interpreted/.

GUIDE can be run in either Sherpa or Chips, and is initialized in either case with the command

```
import("guide")
```

The GUIDE command `identify` outputs line lists over a user-specified spectral range, along with an expected emissivity for each:

λ(Å)	Ion	Upper	Lower	Emissivity	kT	RelInt
13.4403	Fe XX	158	9	2.23e-18	0.862	0.005
13.4440	Fe XX	116	8	8.75e-18	0.862	0.022
13.4440	Fe XXII	17	8	2.24e-17	1.085	0.055
13.4473	Ne IX	7	1	4.06e-16	0.343	1.000
13.4510	Fe XVIII	67	1	1.23e-17	0.685	0.030
13.4550	Ne IX	10205	19	1.74e-18	0.273	0.004
13.4550	Ne IX	10206	20	3.12e-18	0.273	0.008

More information on any given transition is available with the `describe` command:

Ion Ne IX, energy level 1 –

electron configuration	:	$1s^2\ ^1S_0$
energy above ground (eV)	:	0.000000
Quantum state	:	n=1, l=N/A, s=0, degeneracy=1
Energy level data source	:	1983ADNDT..29..467S
Photoionization data source	:	1986ADNDT..34..415C

Ion Ne IX, energy level 7 –

electron configuration	:	$1s2p\ ^1P_1$
energy above ground (eV)	:	922.609985
Quantum state	:	n=2, l=1, s=0, degeneracy=3
Energy level data source	:	1983ADNDT..29..467S
Photoionization data source	:	1986ADNDT..34..415C

Ion Ne IX, 1 – 7 interactions –

Electron collision rate from 1 → 7	:	nonzero
Reference bibcode	:	1983ADNDT..29..467S
Wavelength (lab/observed) (Angstrom)	:	13.447307 +/- 0.004000
Wavelength (theory) (Angstrom)	:	13.470000
Transition rate/Einstein A (s^{-1})	:	8.866670e+12
Wavelength (lab/observed) reference	:	1988CaJPh..6..586D
Wavelength (theory) reference	:	1983ADNDT..29..467S
Transition rate reference	:	1987JPhB..20.6457F

Given a "base" temperature, what lines should be so strong?

sherpa> strong(1.e7,5.e-17,5,25)

Lambda Angstrom	-- Ion	UL - LL	Approximate Emissivity@ ph cm^3/s	kT keV	RelInt	For More Info
6.1804	Si XIV	4- 1	5.14e-17 @	0.862	0.103	describe(14,14,4,1)
6.6479	Si XIII	7- 1	8.77e-17 @	0.862	0.175	describe(14,13,7,1)
8.4192	Mg XII	4- 1	6.89e-17 @	0.862	0.138	describe(12,12,4,1)
9.4797	Fe XXI	248- 1	5.47e-17 @	0.862	0.109	describe(26,21,248,1)
11.7360	Fe XXIII	20- 5	8.39e-17 @	0.862	0.168	describe(26,23,20,5)
11.7700	Fe XXII	21- 1	1.94e-16 @	0.862	0.388	describe(26,22,21,1)
12.1321	Ne X	4- 1	9.02e-17 @	0.862	0.180	describe(10,10,4,1)
12.2840	Fe XXI	40- 1	5.01e-16 @	0.862	1.000	describe(26,21,40,1)
12.3930	Fe XXI	40- 2	9.01e-17 @	0.862	0.180	describe(26,21,40,2)
12.7540	Fe XXII	23- 6	7.17e-17 @	0.862	0.143	describe(26,22,23,6)
12.8220	Fe XXI	83- 7	6.62e-17 @	0.862	0.132	describe(26,21,83,7)
12.8240	Fe XX	60- 1	1.16e-16 @	0.862	0.231	describe(26,20,60,1)
12.8460	Fe XX	58- 1	2.83e-16 @	0.862	0.565	describe(26,20,58,1)
12.8640	Fe XX	56- 1	2.36e-16 @	0.862	0.471	describe(26,20,56,1)
12.9120	Fe XX	51- 1	7.35e-17 @	0.862	0.147	describe(26,20,51,1)
12.9650	Fe XX	48- 1	8.77e-17 @	0.862	0.175	describe(26,20,48,1)

Approximate

Lambda Angstrom	-- Ion	UL - LL	Emissivity@ ph cm^3/s	kT keV	RelInt	For More Info
13.0610	Fe XX	42- 1	6.90e-17 @	0.862	0.138	describe(26,20,42,1)
13.3850	Fe XX	111- 6	6.57e-17 @	0.862	0.131	describe(26,20,111,6)
13.4970	Fe XIX	71- 1	8.00e-17 @	0.862	0.160	describe(26,19,71,1)
13.5070	Fe XXI	42- 7	1.16e-16 @	0.862	0.231	describe(26,21,42,7)
13.5180	Fe XIX	68- 1	1.76e-16 @	0.862	0.352	describe(26,19,68,1)
13.7670	Fe XX	19- 1	5.56e-17 @	0.862	0.111	describe(26,20,19,1)
13.7950	Fe XIX	53- 1	7.07e-17 @	0.862	0.141	describe(26,19,53,1)
14.2080	Fe XVIII	55- 1	7.00e-17 @	0.862	0.140	describe(26,18,55,1)
14.2080	Fe XVIII	56- 1	1.28e-16 @	0.862	0.256	describe(26,18,56,1)
14.2670	Fe XX	54- 6	8.93e-17 @	0.862	0.178	describe(26,20,54,6)
14.3730	Fe XVIII	49- 1	5.04e-17 @	0.862	0.101	describe(26,18,49,1)
14.6640	Fe XIX	15- 1	5.34e-17 @	0.862	0.107	describe(26,19,15,1)
14.7540	Fe XX	33- 6	5.26e-17 @	0.862	0.105	describe(26,20,33,6)
15.0140	Fe XVII	27- 1	1.00e-16 @	0.862	0.200	describe(26,17,27,1)
15.0790	Fe XIX	11- 1	6.02e-17 @	0.862	0.120	describe(26,19,11,1)
16.0710	Fe XVIII	4- 1	5.85e-17 @	0.862	0.117	describe(26,18,4,1)
16.1100	Fe XIX	37- 6	7.83e-17 @	0.862	0.156	describe(26,19,37,6)
17.0510	Fe XVII	3- 1	5.54e-17 @	0.862	0.111	describe(26,17,3,1)
17.0960	Fe XVII	2- 1	5.27e-17 @	0.862	0.105	describe(26,17,2,1)
18.9671	O VIII	4- 1	1.21e-16 @	0.862	0.241	describe(8,8,4,1)
18.9725	O VIII	3- 1	6.03e-17 @	0.862	0.120	describe(8,8,3,1)

The GUIDE *S-lang* functions can also be accessed via WebGUIDE:

http://obsvis.harvard.edu/WebGUIDE

More information on ATOMDB can be found at:

http://cxc.harvard.edu/atomdb

And, general questions about atomic rate calculations or line identifications can be posted on the new web forum AstroAtom:

http://cfa-www.harvard.edu/astroatom

- Reprocessing grating data is recommended for optimal quality control; however, pha2 files from the archive are usually reasonable for assessing the data analysis needs.

- Co-adding and/or binning grating data should be avoided when possible. Remember that, statistically, nothing is gained by it, although it may be much faster to fit it and easier to see the results.

- Background subtraction and/or modeling are handled by Sherpa in a reasonable fashion, but more complex, wavelength-dependent subtraction could be done as well. User experimentation is recommended if the data warrant it.

- A number of new facilities for atomic data analysis have been created, but the models still have limitations which should be kept in mind.