Introduction to Grating Analysis

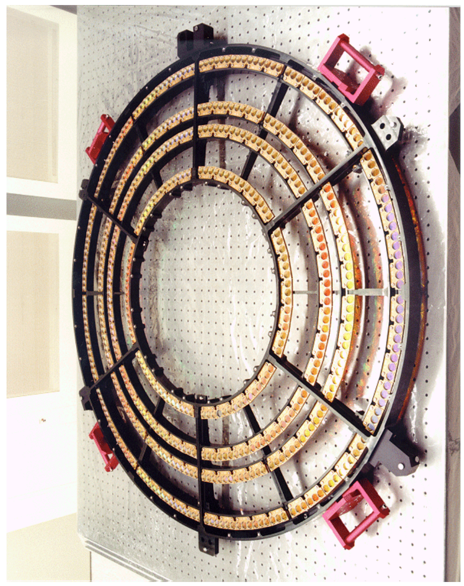
Randall Smith
Chandra X-ray Center

The text of this talk is available at
http://asc.harvard.edu/ciao/wrkshp.html

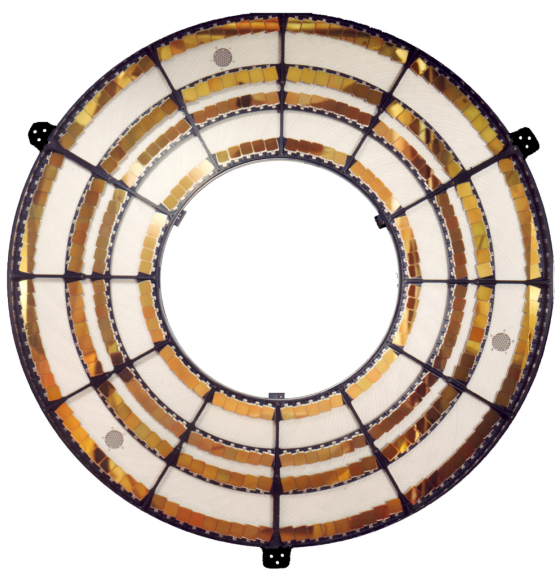
Thanks to David Huenemoerder and his spectroscopy page
http://space.mit.edu/ASC/analysis/AGfCHRS/AGfCHRS.html

Chandra has either two or three gratings, depending on how you count.

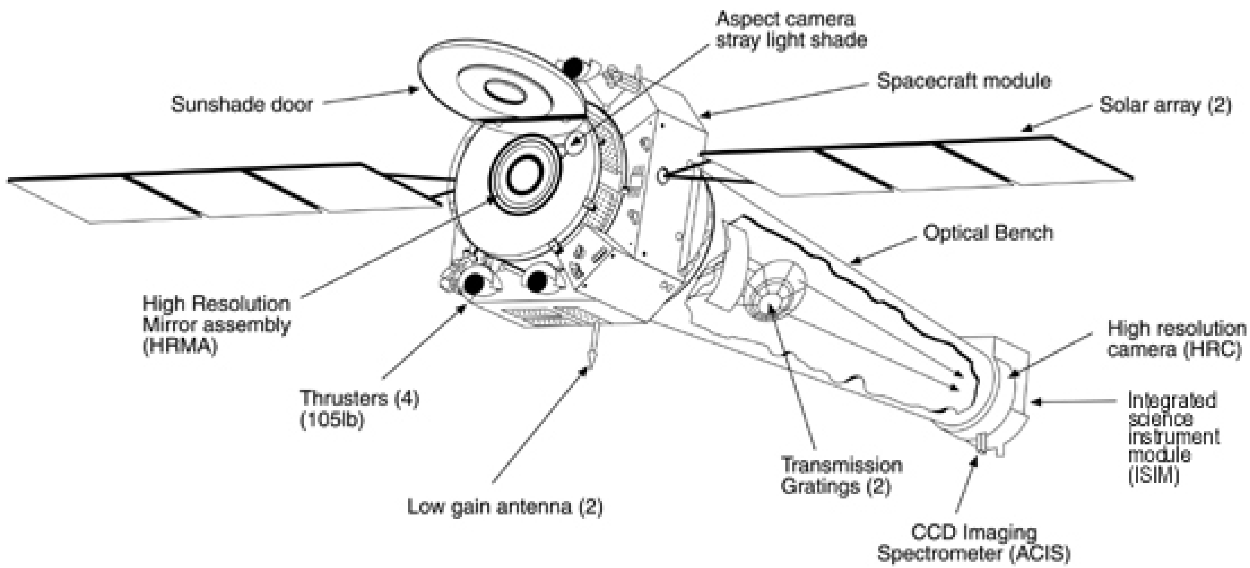
The LETG: Spacing = 1 μm



The HETG: Spacing = 0.2, 0.4 μm



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

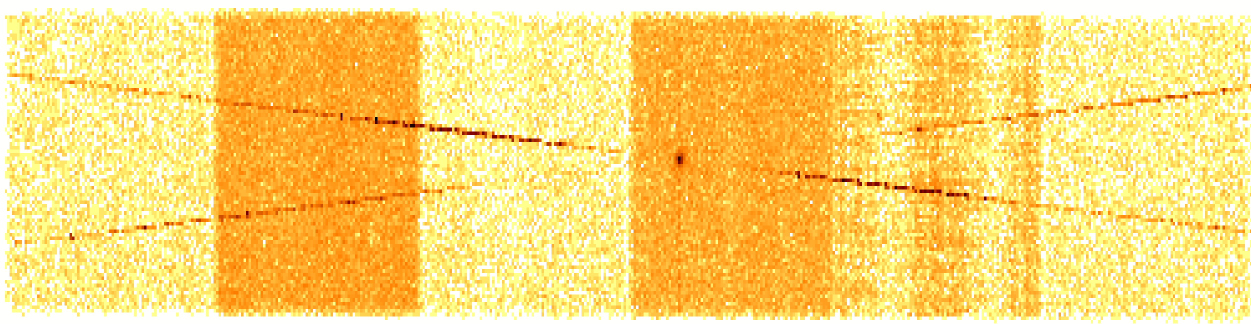


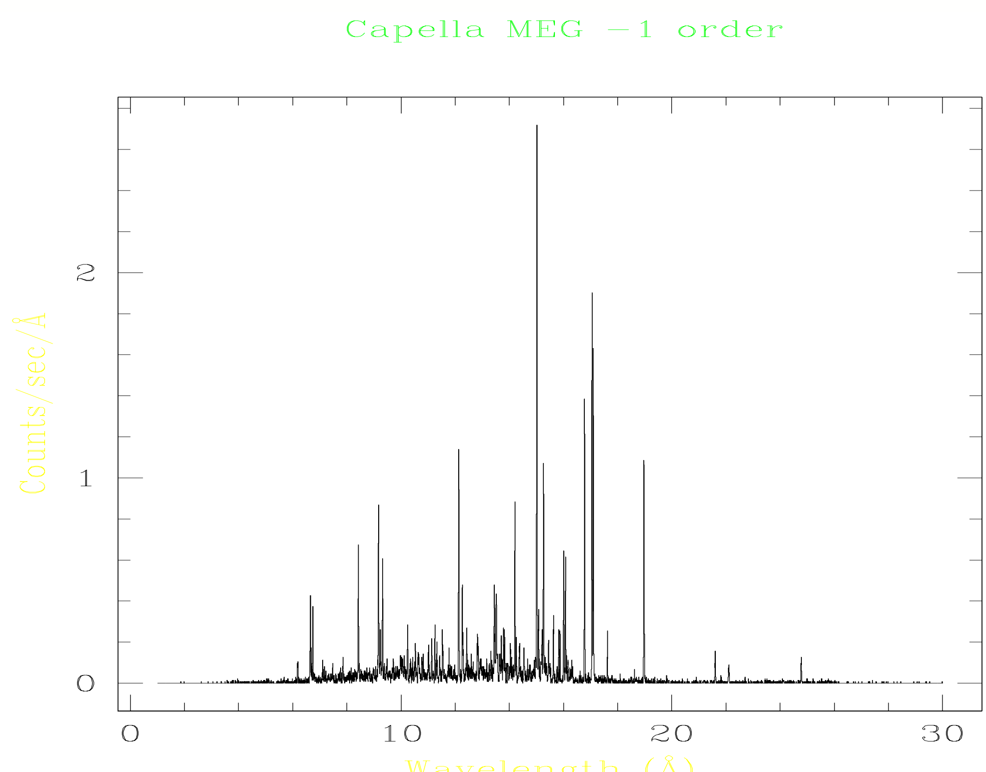
This is a manual process in the case of the LETG, and so LETG observations are bunched together to save time.

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

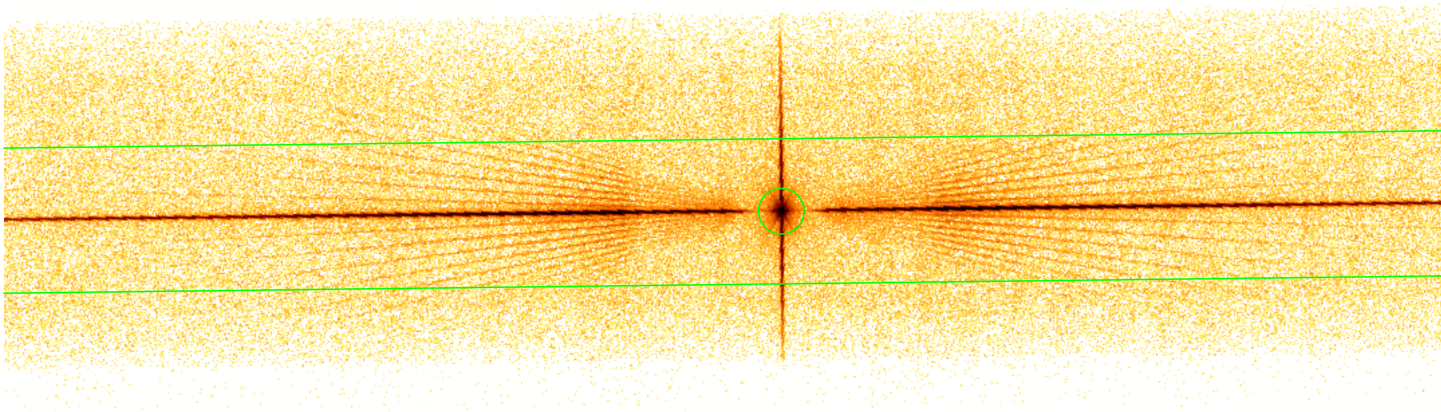
Capella with the HETG/ACIS-S detector:





Spectrum from the MEG -1 order

High-resolution (grating) spectra on Chandra cover a huge range of wavelengths: from 1.2-170Å, over two orders of magnitude. Note that wavelength is the natural unit, since all the high-resolution data are from gratings.



LETG/HRC-S Observation of NGC6624

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

Clearly, the spatial and spectral elements are tightly coupled. If the zero-order image is slightly displaced (as can easily happen with heavily piled-up sources), the ± order wavelengths will be offset from each other. (If this occurs, you may wish to reprocess with a new position measured by hand.)

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:

$$\sin\beta = m\lambda/p \tag{1}$$

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.

So, 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

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=hrc_evt1.fits outfile=hrc_evt1_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=")stdlev1_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_sf,!av1,!av2,!av3,!au1,!au2,!au3,!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`

So, what **are** the standard outputs?

ACIS/HETG By default 12 spectra are created ($\pm 1, 2, 3$ orders for both the HEG and MEG).

ACIS/LETG By default 6 spectra are created ($\pm 1, 2, 3$ orders for the LEG)

HRC/LETG By default 2 spectra are created ($\pm \sum_n i$ orders).

HRC/HETG Not a recommended configuration.

In each case, a single PHA file (called a PHA Type II) is output. 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**, and has a relatively simple format. Other standard outputs are the grating arf ("garf") and grating rmf ("grmf"); these are also FITS files.

In Sherpa, grating spectra can be jointly fit to a model. Or, each PHA can be extracted and divided by the ARF to create a fluxed spectrum, which can be fit using any fitting program.

Know your Data: The Event File is your Friend

```
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	-400.0:400.0	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

XMM RGS data reduction uses the same concepts as Chandra, but the SAS software bundles the commands more than the CIAO software. For example, here is a thread to re-reduce an RGS observation:

Make lightcurve to check for flares

```
evselect table=rgs1_evt1.fits:EVENTS withrateset=yes
rateset=rgs1_ltcrv.fits maketimecolumn=yes timecolumn=TIME
timebinsize=10
```

Examine lightcurve; assume here we use the entire dataset. So, rerun standard processing to pick up the latest calibration data:

odfingest odfdir=$SAS\_ODFoutdir$ =SAS_ODF
rgsproc orders='1 2' withgtiset=no

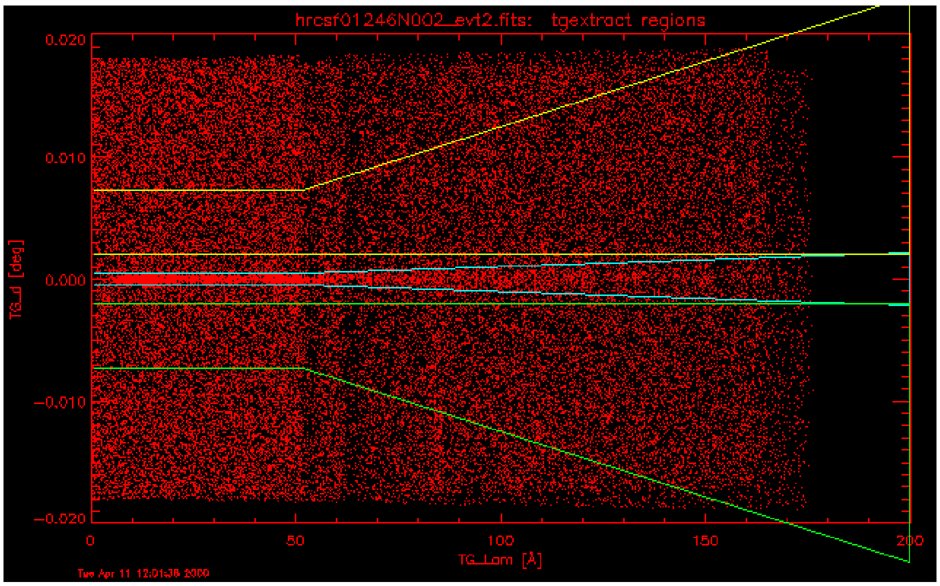
Now make the RMF

```
rgsrmfgen file=rgs1_o1.rmf set=rgs1_evt1.fits

withspectrum=yes spectrumset=0226_0021750101_R1S00700_net1o1.pha

sourceset=0226_0021750101_R1S00700_sources.ds emin=0.3 emax=2.8 ebins=4000
```

A side note: Because of the design of the RGS, the line profile has substantial wings. As a result, proper RGS analysis **requires** that an RMF be used. Not using an RMF will lead to systematically smaller line flux measurements.

Backgrounds

For bright sources on ACIS-S, the background is likely negligible. However, in the HRC-S it is usually large, and a faint source on the ACIS-S can have a significant background.



Source/Background Regions for the LETG/HRC

The background is extracted in two regions: above the grating arm (background_up) and below it (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.

It is up to the user to decide how (and whether) to combine and apply these background arrays; by default in Sherpa they are averaged, although this may not be the best method for all wavelengths.

The area in the background extraction region is usually larger than that in the source region, so 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.

ACIS Continuous Clocking

ACIS can be run in Continuous-Clocking (CC) mode for high time resolution. Spatial information in the cross-dispersion direction is lost in this mode.

We can still process HETGS data, however, into binned MEG and HEG spectra. In this mode, orders still separate according to pulse-height.

The odd-orders' pulse-height regions are unambiguously from MEG. If even, we assume to be HEG since MEG even order efficiency is low (e.g., MEG "2nd" order is really mostly HEG 1st; MEG "4th" is really HEG 2nd, and so on).

The pipeline applies an iterative step in processing CC-mode, first assuming events are from MEG, and guessing the CHIPY position given the zero-order position and CHIPX, then if the order is odd, it re-resolves it assuming HEG.

Relatively few observations have been done using ACIS-CC with gratings; as a result, calibration of the line shape function and effective area in this mode is not as developed as other modes.

Unfortunately, not every X-ray object as bright as Capella, NGC6624. In these cases, you might wish to co-add the grating data to increase the number of counts per bin. This will, of course, increase the number of calibration issues with the data.

There are four choices:

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 obs and instruments. *All of the above*

In many cases, however, the calibration issues are either not a problem or are an "acceptable risk." In this case, CIAO provides a number of tools:

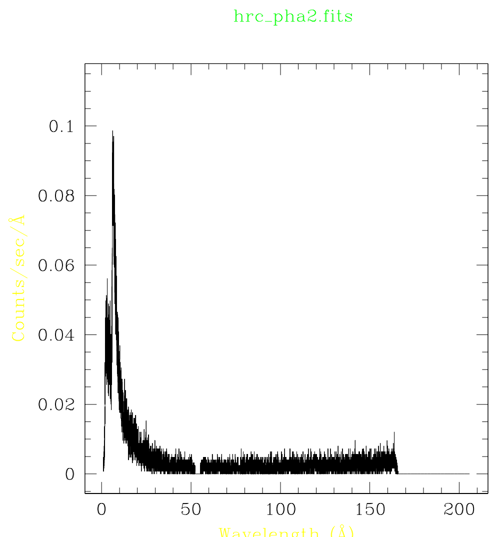
Adding together plus, minus orders

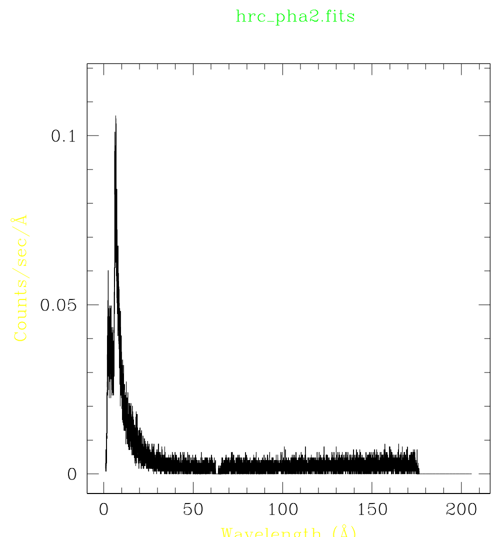
```
add_grating_orders pha2=acisf00459N002_pha2.fits
  order=1 garm=MEG garfm=acisf00459MEG_-1_garf.fits

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

Adding together same orders, different observations

```
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
```

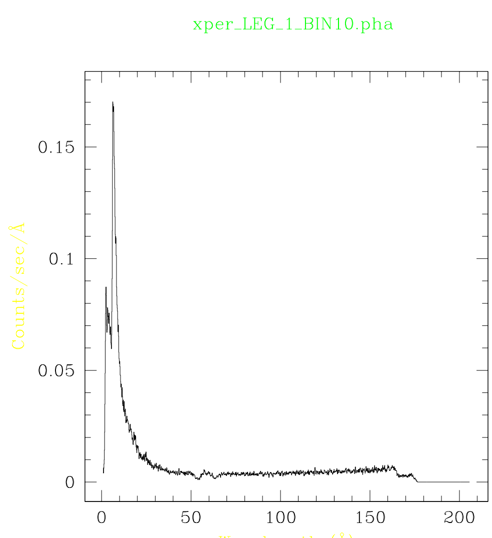
Consider the HMXB X Per, observed for 50 ksec with the HRC/LETG. The raw data looks as follows (*without* error bars!) :

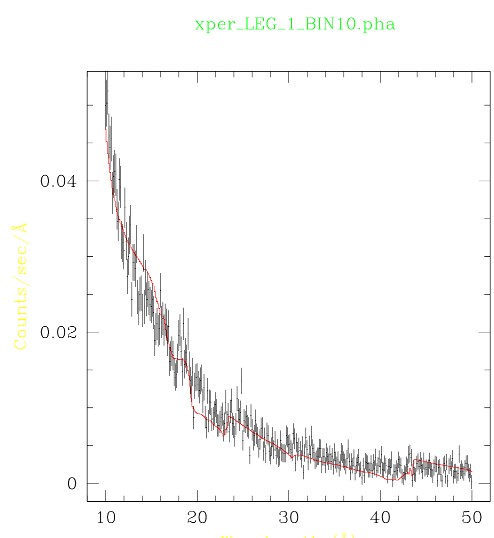




We can co-add and bin this data with **add_grating_orders** to increase the number of counts/bin:

```
add_grating_orders pha2=hrc_pha2.fits order=1 garm=LEG \
  garfm=x_perLEG_-1_garf.fits garfp=x_perLEG_1_garf.fits \
  gtype=BIN gspec=10 root=xper
```





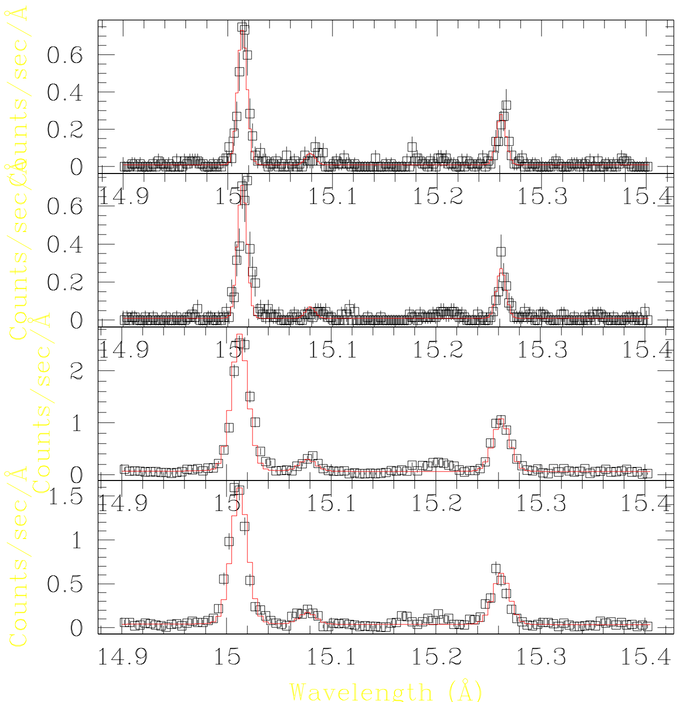
With low or moderate resolution data, forward-folding models and comparing to the data is the only analysis possible. With grating data, this becomes optional depending on the analysis needs. If the inherent resolution of the gratings is kept in mind (HEG: 0.012Å, MEG: 0.023Å, LEG: 0.05Å), analysis of a fluxed spectrum using any tool is entirely reasonable.

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 = acisheg1D1999-07-22rmfN0004.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

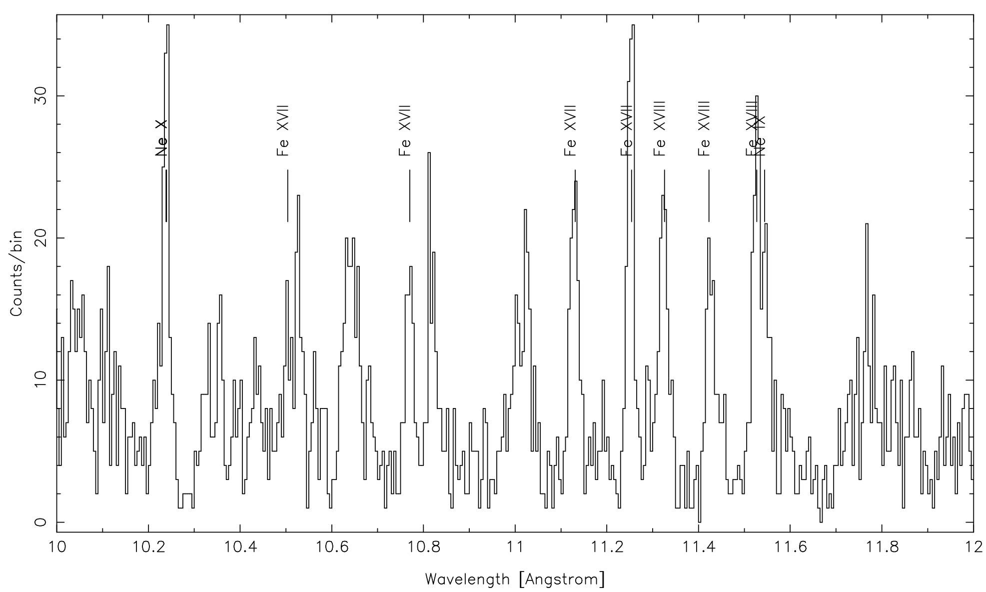


while the `mdl2latex` command gives the table:

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	

Alternatively (or in conjunction), ISIS can be used in Sherpa or standalone. ISIS was developed by the MIT grating team, and is particularly good for thermal plasma analysis:

```
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);
```



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));
  return Result;
}
() = 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
```

Some details: Sherpa allows models to be run either “integrated” or not integrated; this means that either single points or a bin range may be passed to the S-lang function, depending on the data in use and the user’s choice. So we must allow for either 3 or 4 arguments here.

Also, although the *ISIS* code can be run stand-alone, as of CIAO 2.2, it can also be incorporated into Sherpa directly (import(”isis”)). Using a routine similar to the above, we can combine ISIS’s ability to make thermal plasma models for any ion or set of ions (at any resolution) with Sherpa’s sophisticated statistics and fitting algorithms, to fit arbitrarily complex models.

GUIDE is a collection of S-lang scripts whose purpose is to simplify access to the atomic database ATOMDB, which is itself a combination of the astrophysical plasma emission code (APEC) spectral calculations and the astrophysical plasma emission database (APED). GUIDE provides almost entirely 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

And of course 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 $\rightarrow$ 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..66..586D
Wavelength (theory) reference	:	1983ADNDT..29..467S
Transition rate reference	:	1987JPhB...20.6457F

Given a “base” temperature, what lines should be strong?

```
sherpa> strong(1.e7,5.e-17,5,25)
The listed "Approximate Emissivity" is scaled from the peak value
using the ratio of the ionization balance at the requested temperature
and the peak temperature for the line.

                                   Approximate
  Lambda  --  Ion      UL -  LL Emissivity@   kT  RelInt  For More Info
 Angstrom                         ph cm^3/s   keV
   6.1804    Si XIV      4-   1  5.21e-17 @ 0.862 0.104 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  6.99e-17 @ 0.862 0.140 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  9.14e-17 @ 0.862 0.183 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)
  12.9650     Fe XX     48-   1  8.77e-17 @ 0.862 0.175 describe(26,20,48,1)
  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)
  14.0080    Fe XXI     28-   7  9.31e-17 @ 0.862 0.186 describe(26,21,28,7)
  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  1.22e-16 @ 0.862 0.244 describe(8,8,4,1)
  18.9725    O VIII      3-   1  5.88e-17 @ 0.862 0.118 describe(8,8,3,1)
```

- Reprocessing grating data is no longer absolutely required, but has gotten far easier and provides a sense of confidence about the data.
- 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 is handled in 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 for Sherpa and ISIS (and are in the new version of XSPEC as well). However, remember to check the caveats on this data before trusting it totally! For the ATOMDB, they are at

  http://asc.harvard.edu/atomdb/doc/caveats.html