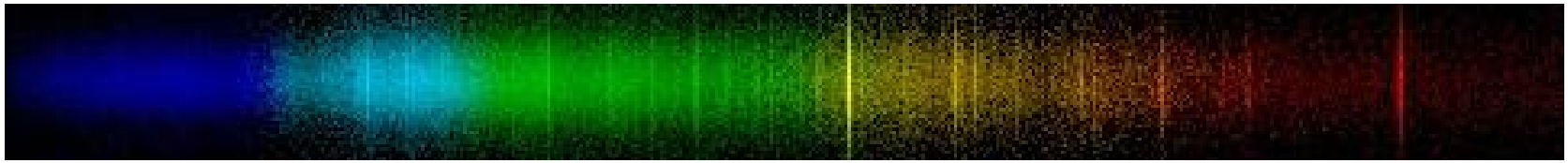


Chandra Grating Data Analysis

David P. Huenemoerder (MIT)

6^{th} Chandra/CIAO Workshop, 20-22 October, 2008

Figure 1: The Chandra LETG grating assembly

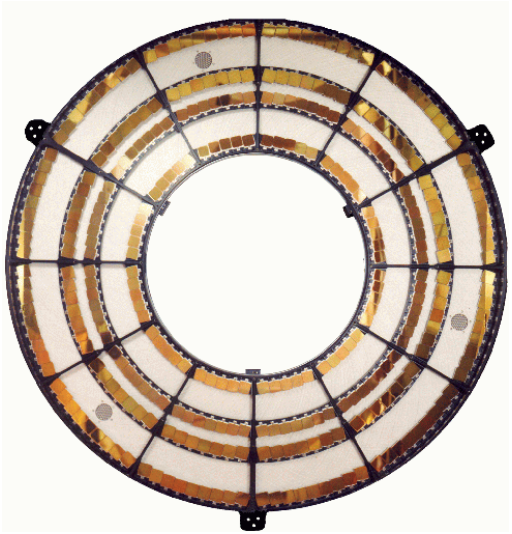


Figure 2: The Chandra HETG grating assembly

Contents

1 Why Use Gratings? For High Resolution!

The "Resolving Power" of a spectrometer is defined as

$$R = \frac{\lambda}{\Delta\lambda} = \frac{E}{\Delta E} \tag{1}$$

in which Δx is the Full-Width, Half-Maximum (FWHM). "High" is a relative term. In X-rays, $R \sim 1000$ is considered high, and that is what the HETGS and LETGS can deliver. The Chandra gratings are transmission gratings, whose diffraction is described by the simple grating equation:

$$m\,\lambda = P\,\sin(\theta). \tag{2}$$

The diffraction angle is small, and defined by $\theta = r/X_{\rm Rowland}$, where r is the linear distance along the spectrum. For the Chandra spectrometers we have periods P of 2000 Å (HEG), 4000 Å (MEG), or 9900 Å (LEG), a Rowland diameter (focal length), $X_{\rm Rowland}$, of about 8635 mm, and sensitivity to wavelengths from 1.5 to 15 Å for HEG, to 30 Å for MEG, and to about 180 Å for LEG in first order, m.

Note that m may be a positive or negative integer, or 0, and that for different values of m having the same sign, different wavelengths will appear at the same angle (and hence, same detector location) — these are "overlapping" orders.

Some pictures more clearly demonstrates what we obtain from high *resolution*:

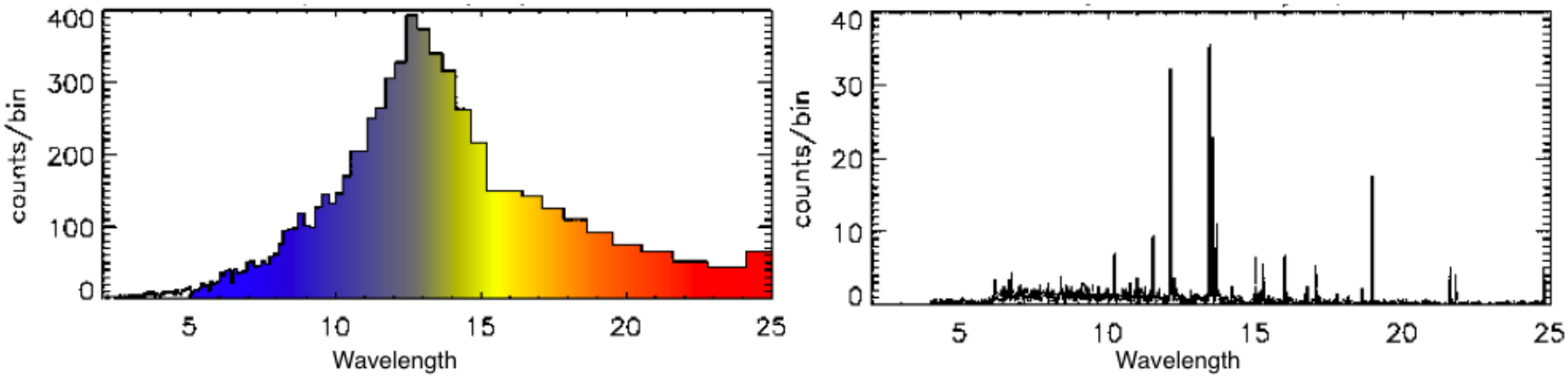


Figure 3: The low resolution (ASCA) spectrum of TW Hya (left), and the Chandra/HETGS spectrum (right). More counts cannot always compete with spectral resolution! (Adapted from Kastner et al. 2002, ApJ,567,434)

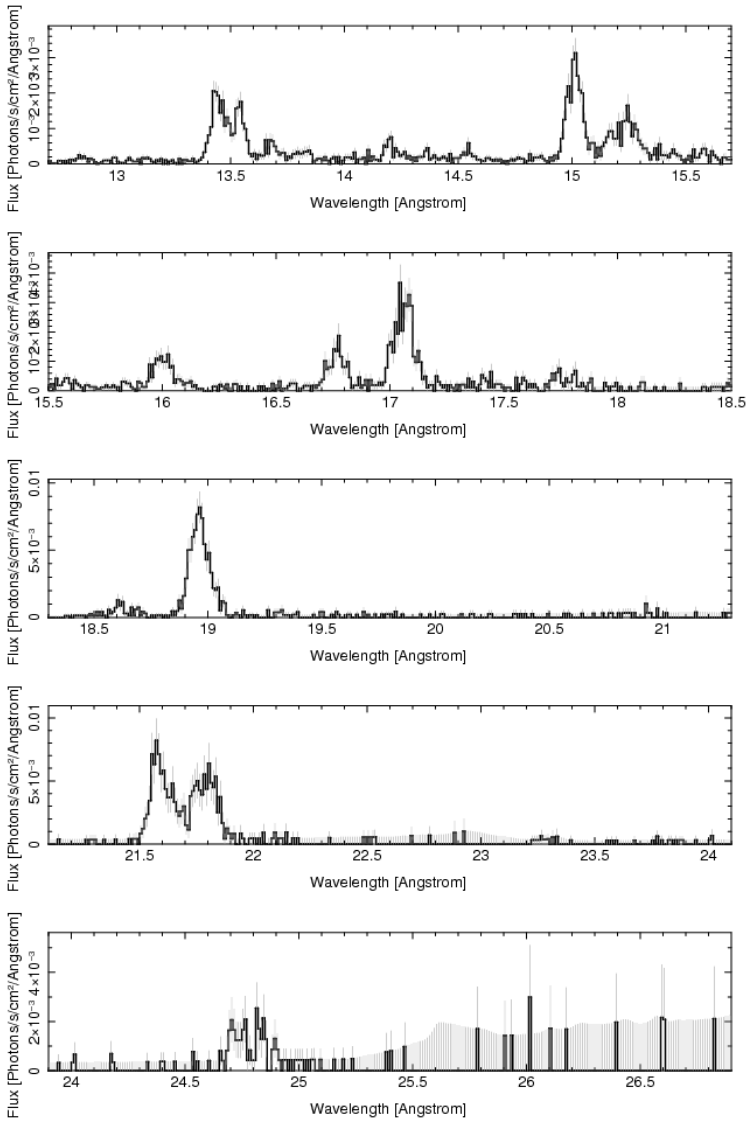


Figure 4: A portion of the HETGS flux-corrected spectrum of ϵ Ori. Note the broadened lines.

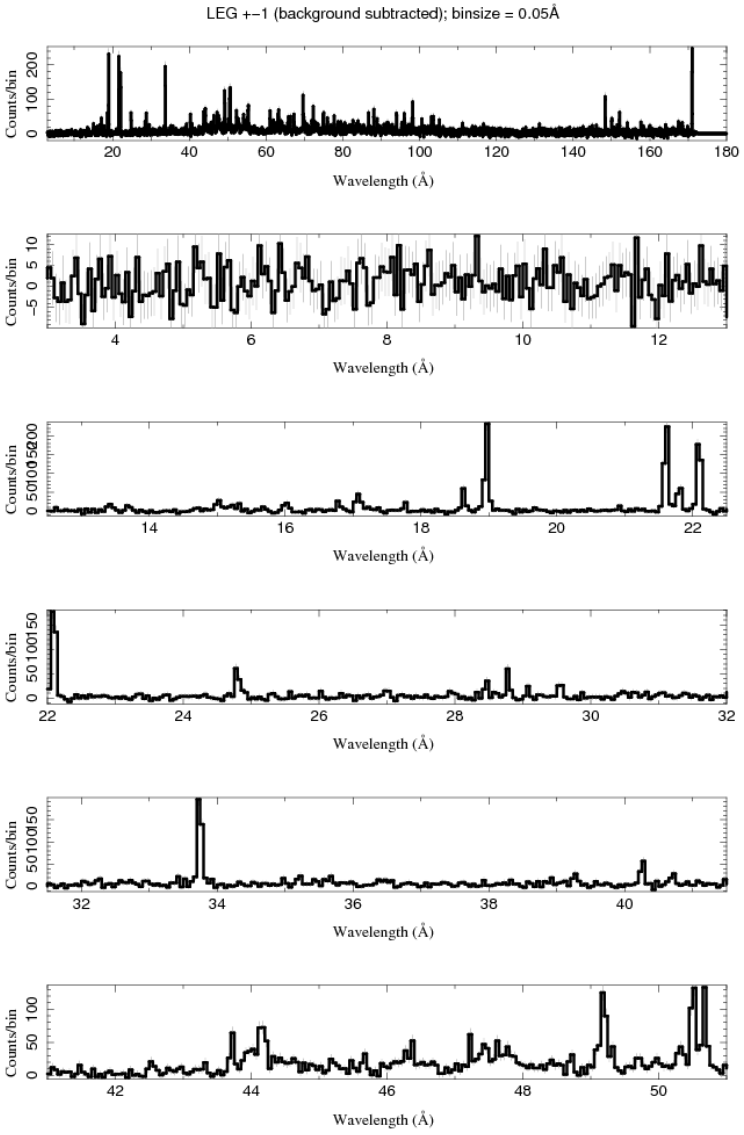


Figure 5: The LETGS counts spectrum of Procyon. Note the large wavelength coverage.

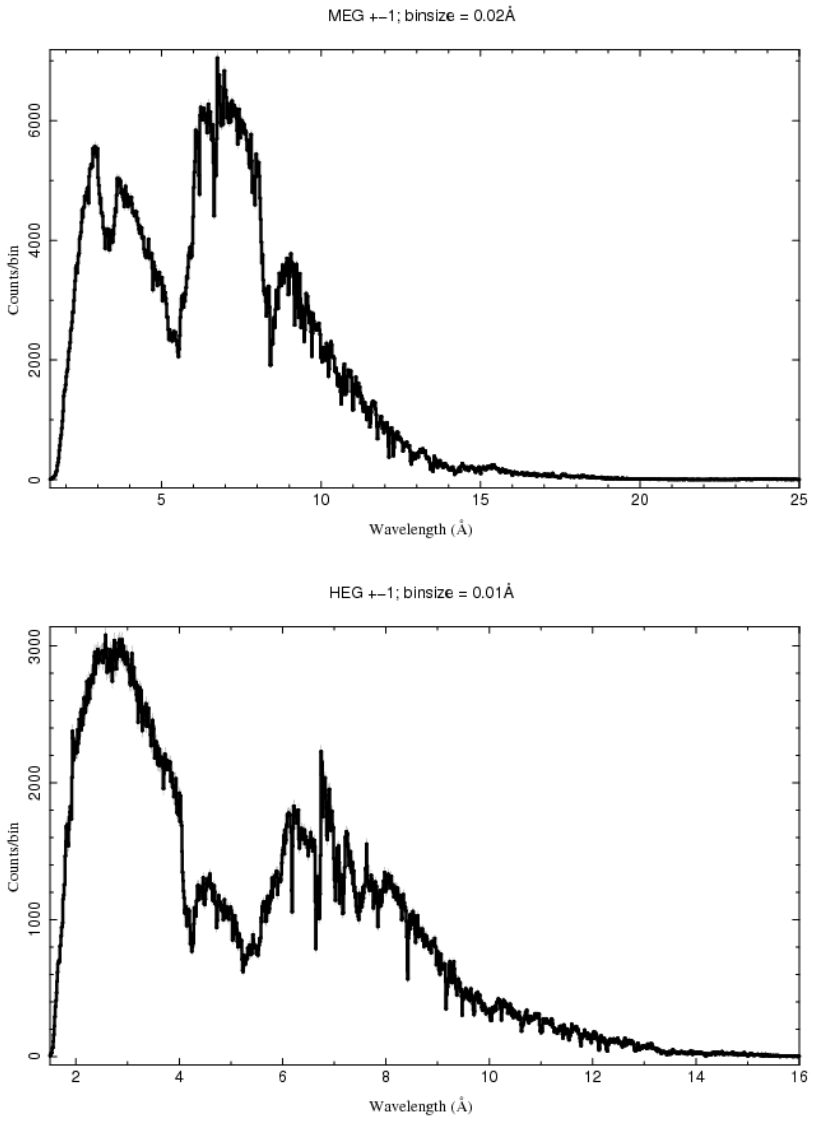


Figure 6: The HETGS counts spectrum of Cyg X-1, a strong continuum source with absorption lines.

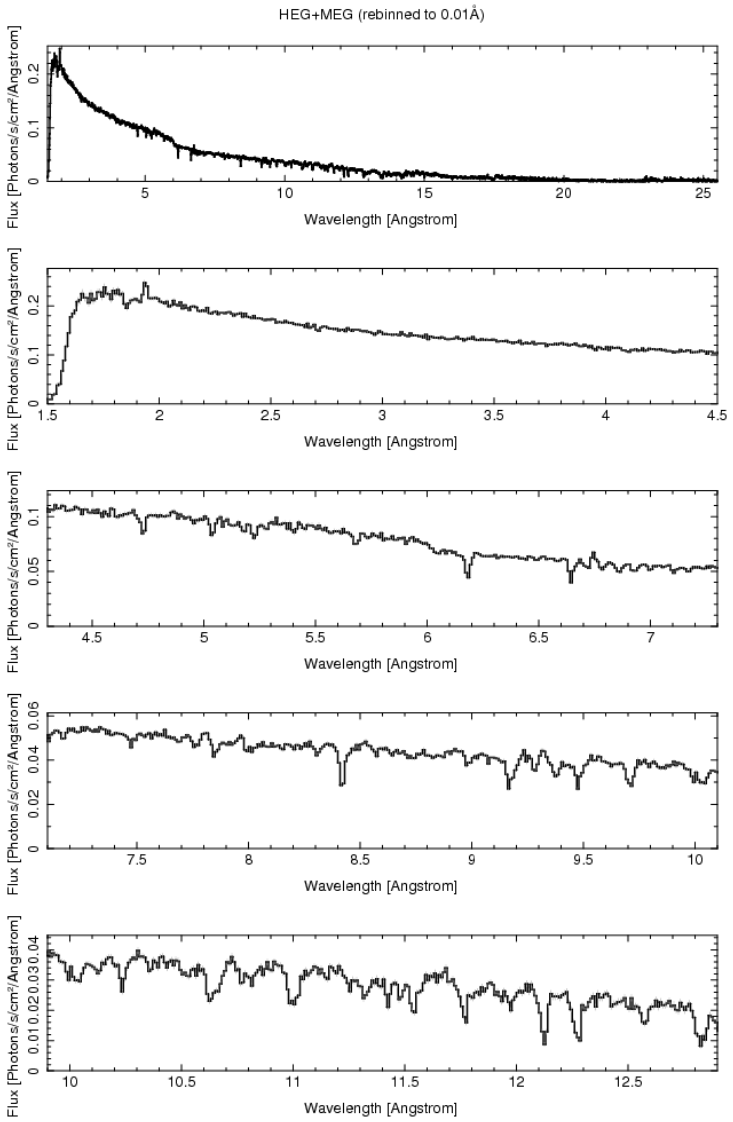
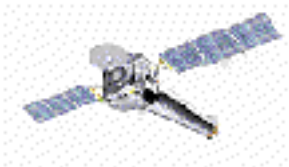


Figure 7: A portion of the flux-corrected HETGS spectrum of Cyg X-1



2 Fundamentals of the Gratings

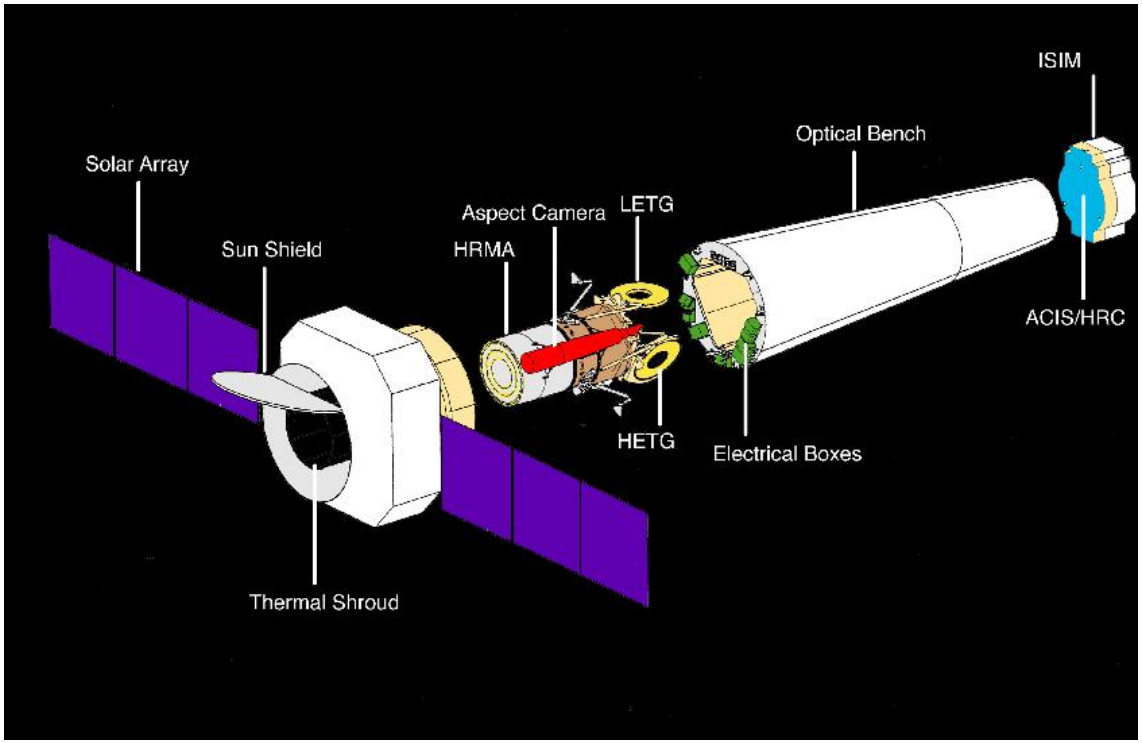


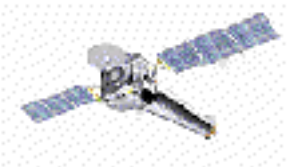
Figure 8: A Chandra diagram, showing the location of the two grating assemblies. Here they are both retracted. Either one can be inserted to disperse the light into the X-ray spectrum.

We have two grating assemblies on Chandra:

LETG Low Energy Transmission Grating, sensitive over about 2-180 Å (0.07 - 6 keV)

HETG High Energy Transmission Grating, sensitive over 1.5-30 Å (0.4 - 8 keV); The HETG itself has two types of grating facets:

HEG: High Energy Grating, which covers the inner two mirror shells;



MEG: Medium Energy Grating, which covers the outer two mirror shells.

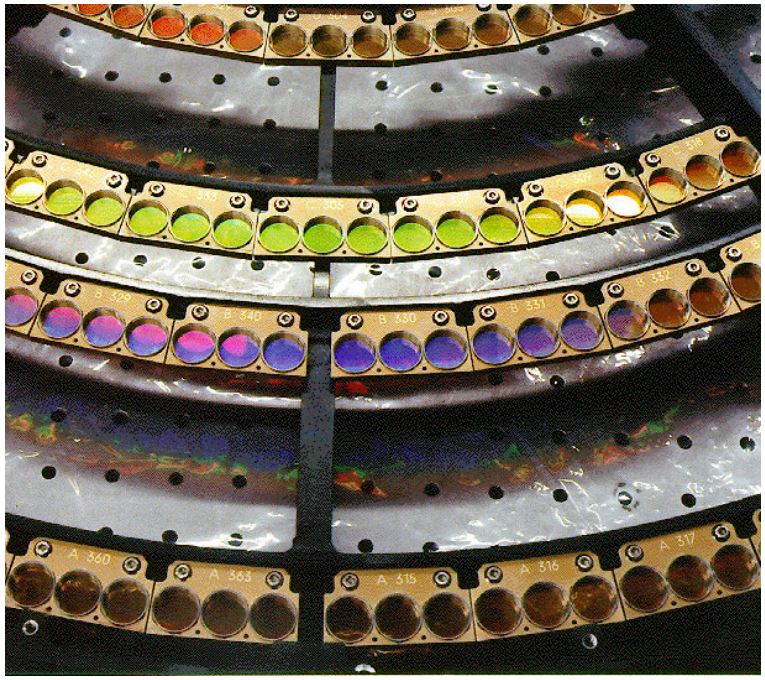


Figure 9: A closeup view of the LETG facets. The facets are the small disks. They are arranged on larger circles which fall behind the mirror shells.

Each grating instrument was designed for a particular detector array. The primary combination are:

HETG → ACIS-S (HETGS - the High Energy Transmission Grating Spectrometer)

LETG → HRC-S (LETGS - the Low Energy Transmission Grating Spectrometer)

Another useful configuration is LETG/ACIS-S

2.1 Detector Characteristics

- The ACIS-S CCDs have enough energy resolution to separate the spatially overlapping orders.

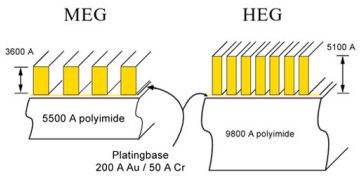


Figure 10: A schematic of the HEG and MEG facets. The HETG gratings are gold bars on a plastic substrate.

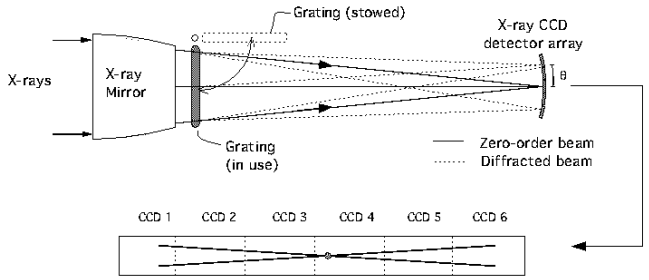


Figure 11: A schematic diagram of the inserted HETG and the focal plane image.

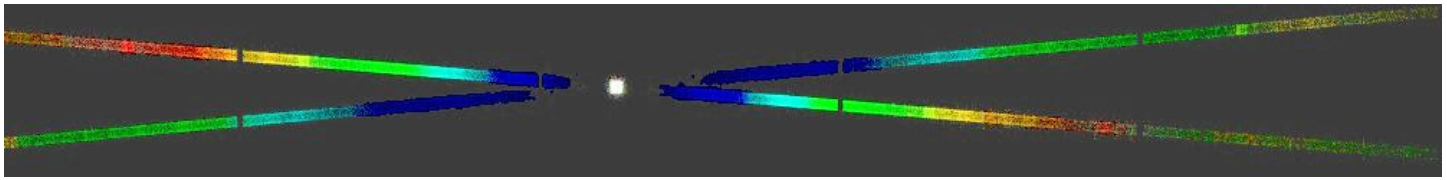
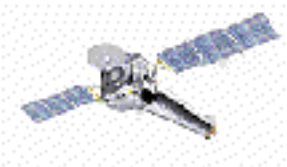


Figure 12: An image made from actual data, color-coded by energy. The positively sloped arm is from the HEG facets, and the other is from MEG. The white central spot is the zeroth order. MEG and HEG each disperse into both positive and negative orders, on opposite sides of the zeroth order.

- ACIS in timed-exposure mode (TE) has a relatively low time resolution (3 seconds). Bright sources can cause severe photon "pile-up" which can distort zeroth order image.
- ACIS can be run in continuous-clocking (CC) mode, but at the expense of spatial information in the cross-dispersion direction.
- The HRC-S detector has poor energy resolution and so *cannot resolve overlapping orders.* This characteristic must be handled in analysis by modeling.
- HRC-S has high internal background noise which must be incorporated into analysis.

See *The Proposers' Observatory Guide*[1] for more detail about Chandra's gratings and detectors.

[1] `http://cxc.harvard.edu/proposer/POG/`



2.2 A Gallery of Spectral Images

We will be more interested in the one-dimensional counts histograms, but first, a few more images may help you become more familiar with the spectrometer characteristics.

LETGS (LETG/HRC-S) Images

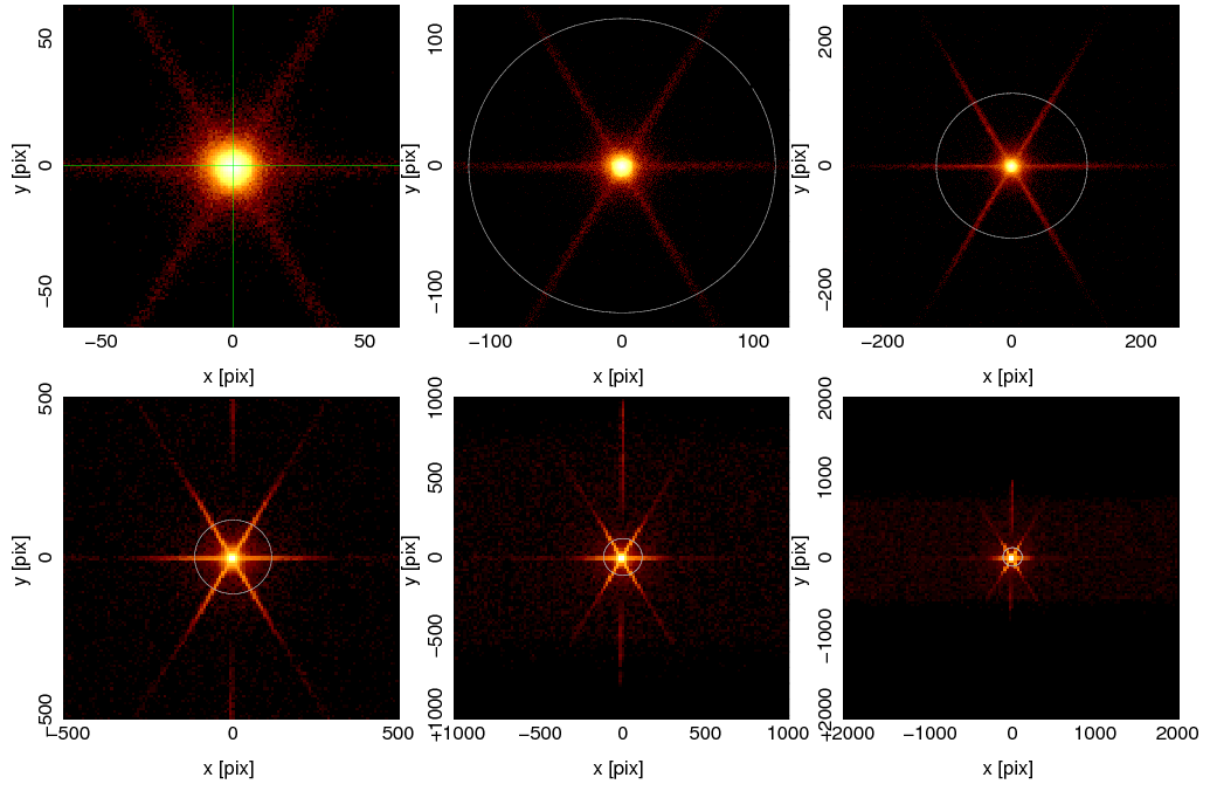


Figure 13: The zero order region of an LETGS spectrum. We step out by factors of two from upper-left to lower-right. The "star" pattern is diffraction from the grating coarse support structure. As we step out, you begin to see the detector boundary, and some "fine support" diffraction (vertical streak). (The green cross and circle were added as markers for the zero order position and region.)

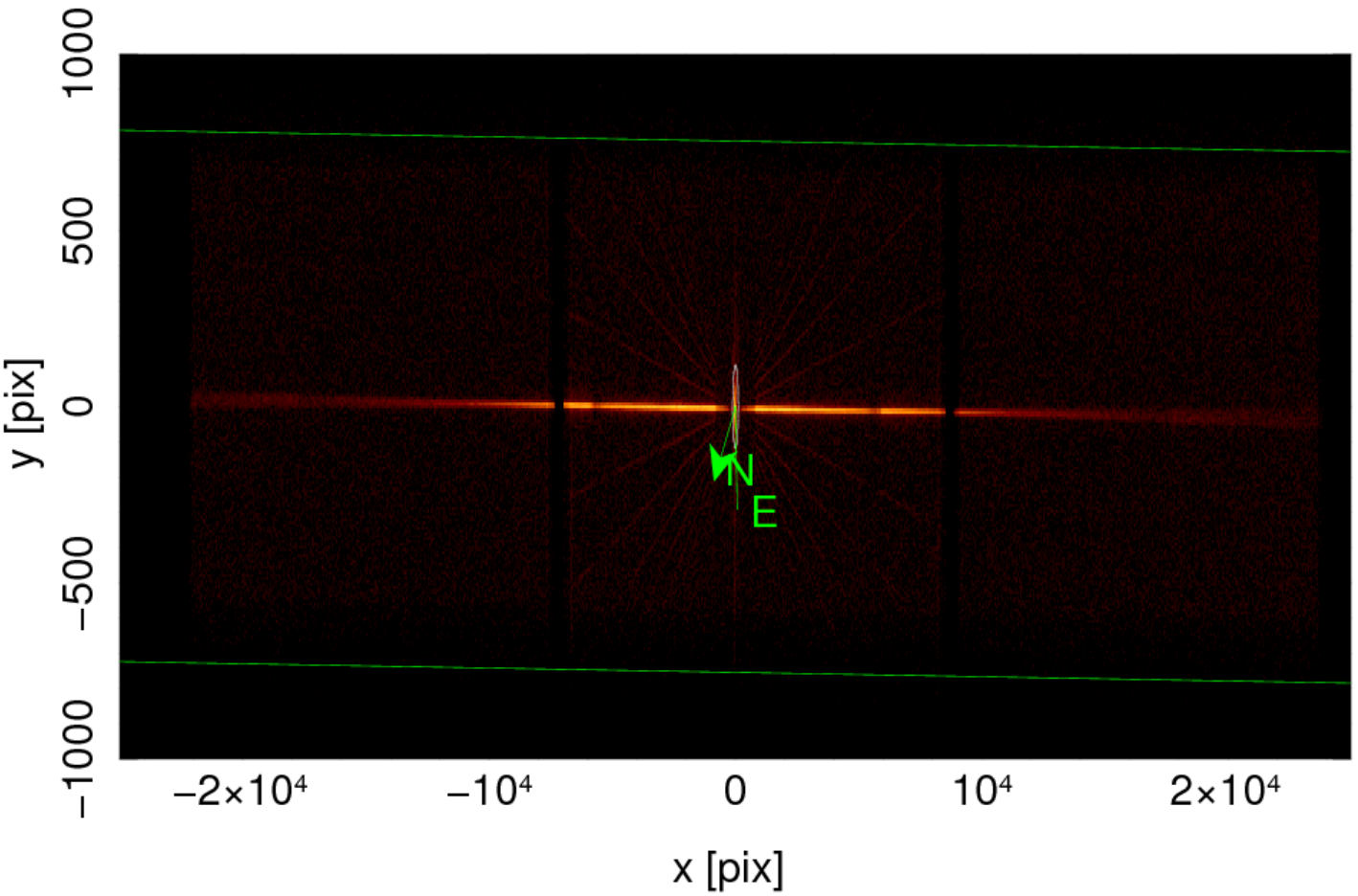
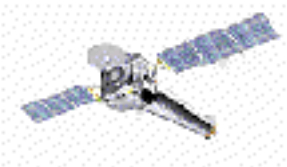


Figure 14: This is an image in sky coordinates, rotated to horizontal for better display. It shows the full HRC-S detector area with an LETGS spectrum. The source spectrum is the nearly horizontal bright streak, with positive orders on one side and negative on the other. The gaps between the 3 detector plates show as dark vertical lines. The faint radial features are from cross-dispersion from the grating bar support structure. North is marked by the green arrow, and east by a green line (they are not orthogonal in this view because of the non-square aspect ratio).



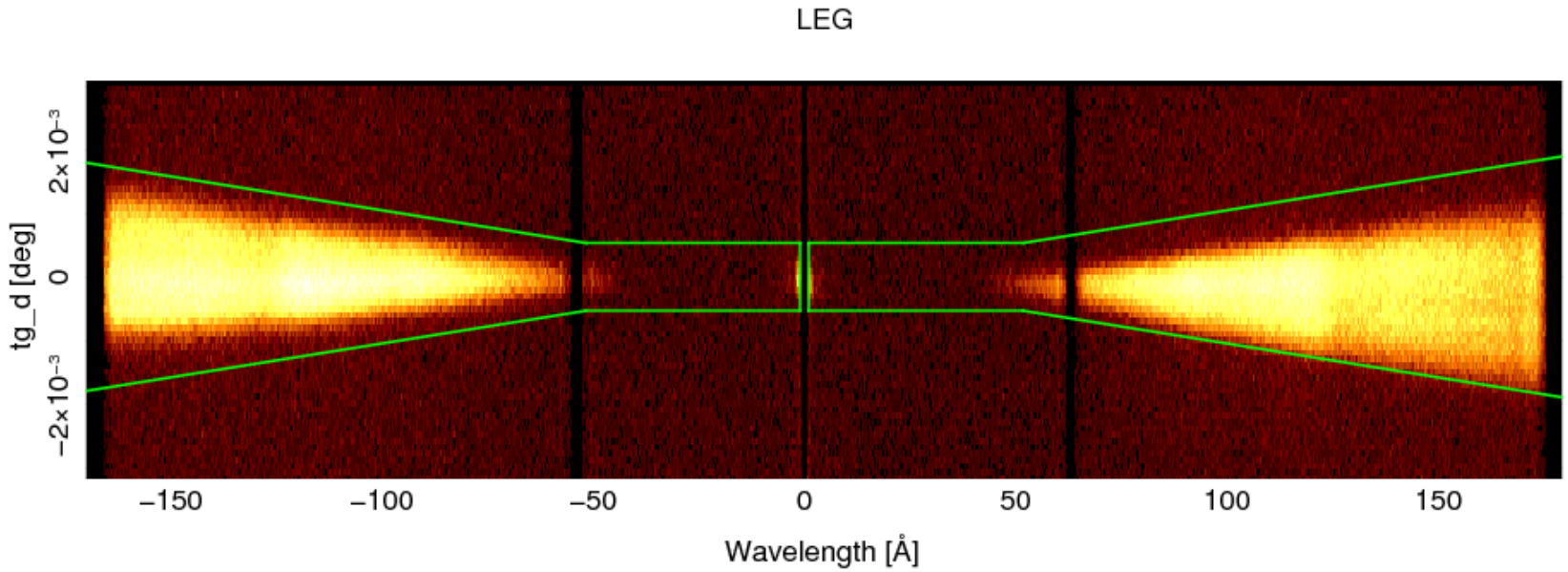
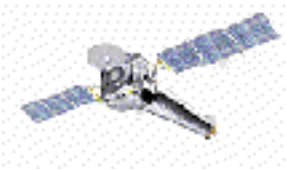


Figure 15: This is an LETG/HRC-S spectrum in grating diffraction coordinates. This shows another important characteristic of the LETGS: the spectrum gets wider at longer wavelengths. The green outline marks our default spectral extraction region.



HETGS (HETG/ACIS-S) Images

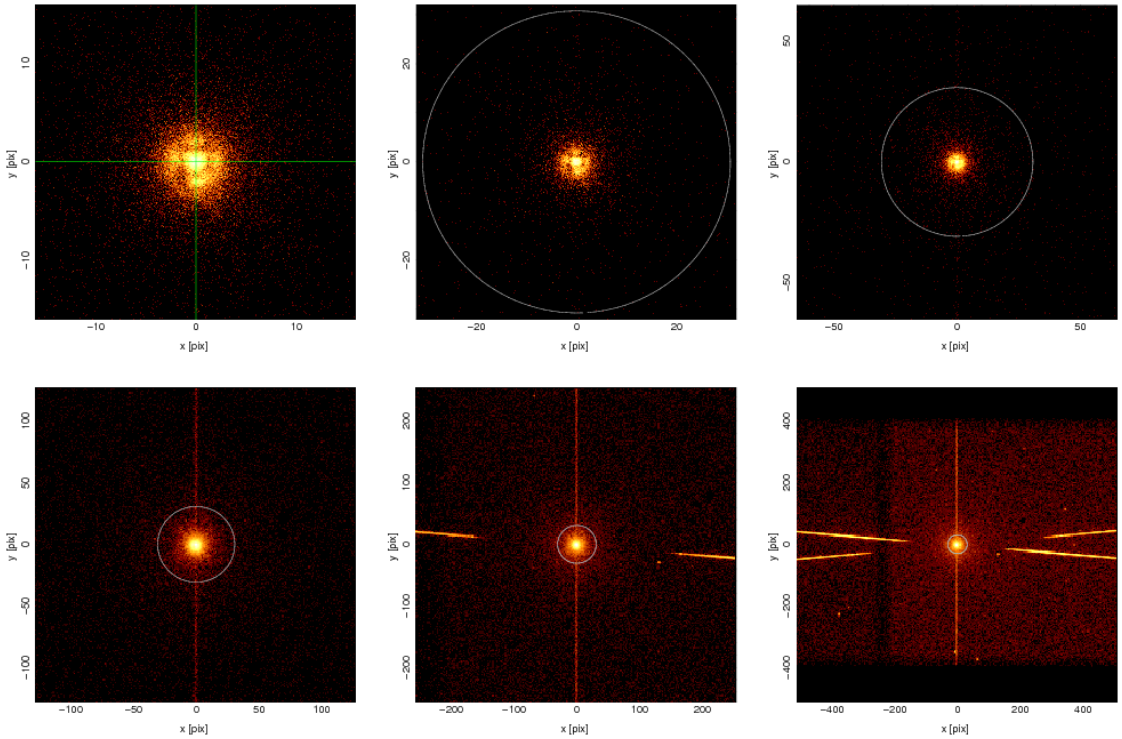
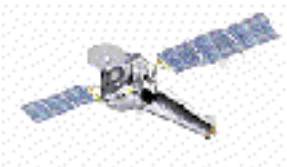


Figure 16: The zero order region of an HETGS spectrum. We step out by factors of two from upper-left to lower-right. As we step out, you begin to see the detector boundary, the "frame shift streak" (vertical feature) and the diffracted spectra. The dark vertical region is a chip gap. Bright points are perhaps other sources in the field. We can also see that the zeroth order is distorted and rather "boxy" — this is due to photon pile-up. (The green cross and circle were added as markers for the zero order position and region.)



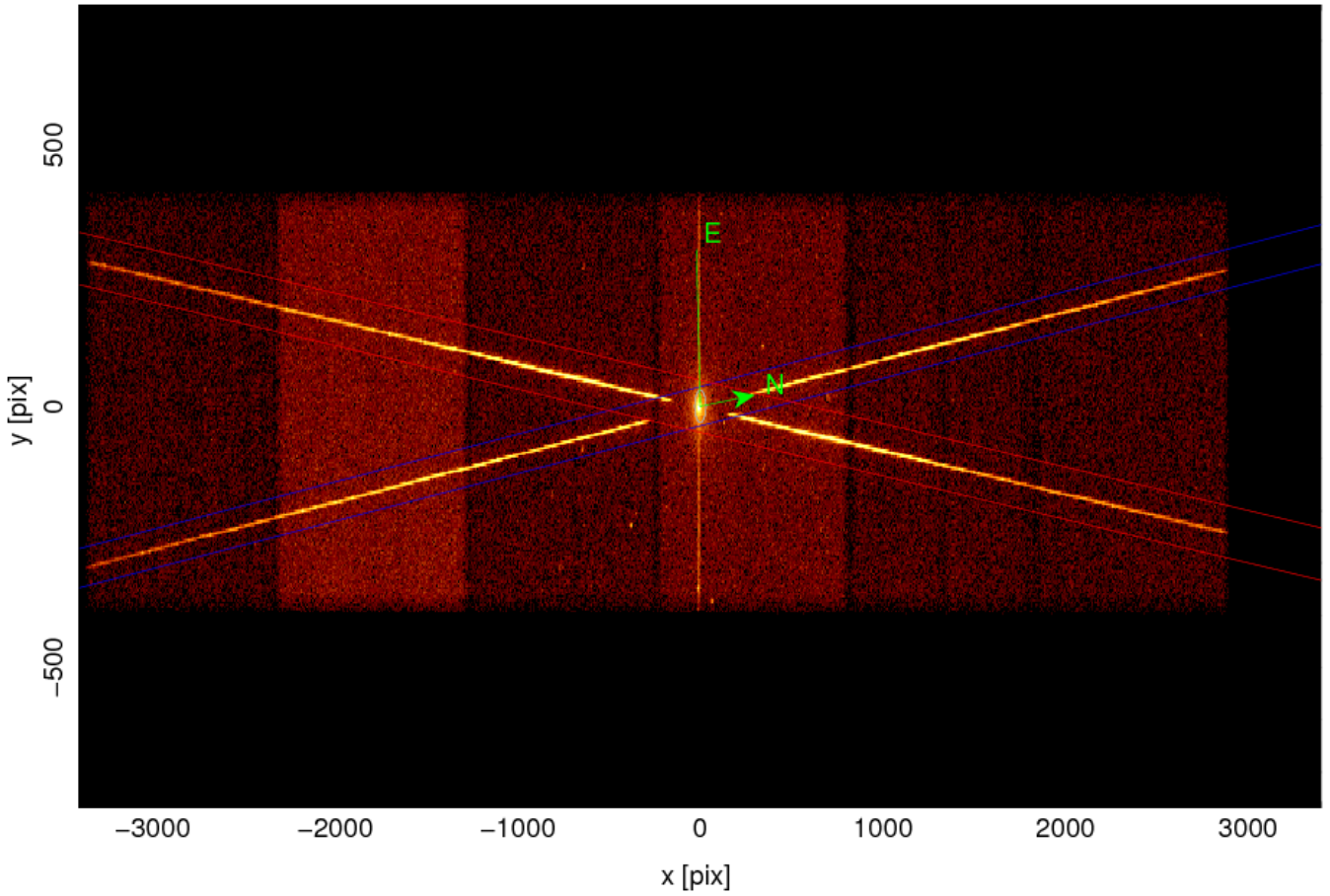
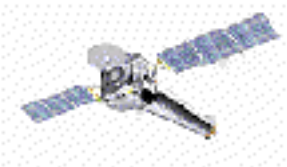


Figure 17: This is an image in sky coordinates, rotated to horizontal for better display. It shows the full ACIS-S detector area with an HETGS spectrum. The source spectrum is the "X". HEG positive orders are to upper right, negative to lower left (in blue box). MEG positive orders lie to lower right, and negative to upper left (in the red box). The gaps between the 6 CCDs show as darkest vertical lines. The chips with brighter background (2^{nd} and 4^{th} from the left) are back-illuminated (BI) devices. North is marked by the green arrow, and east by a green line (they are not orthogonal in this view because of the non-square aspect ratio).



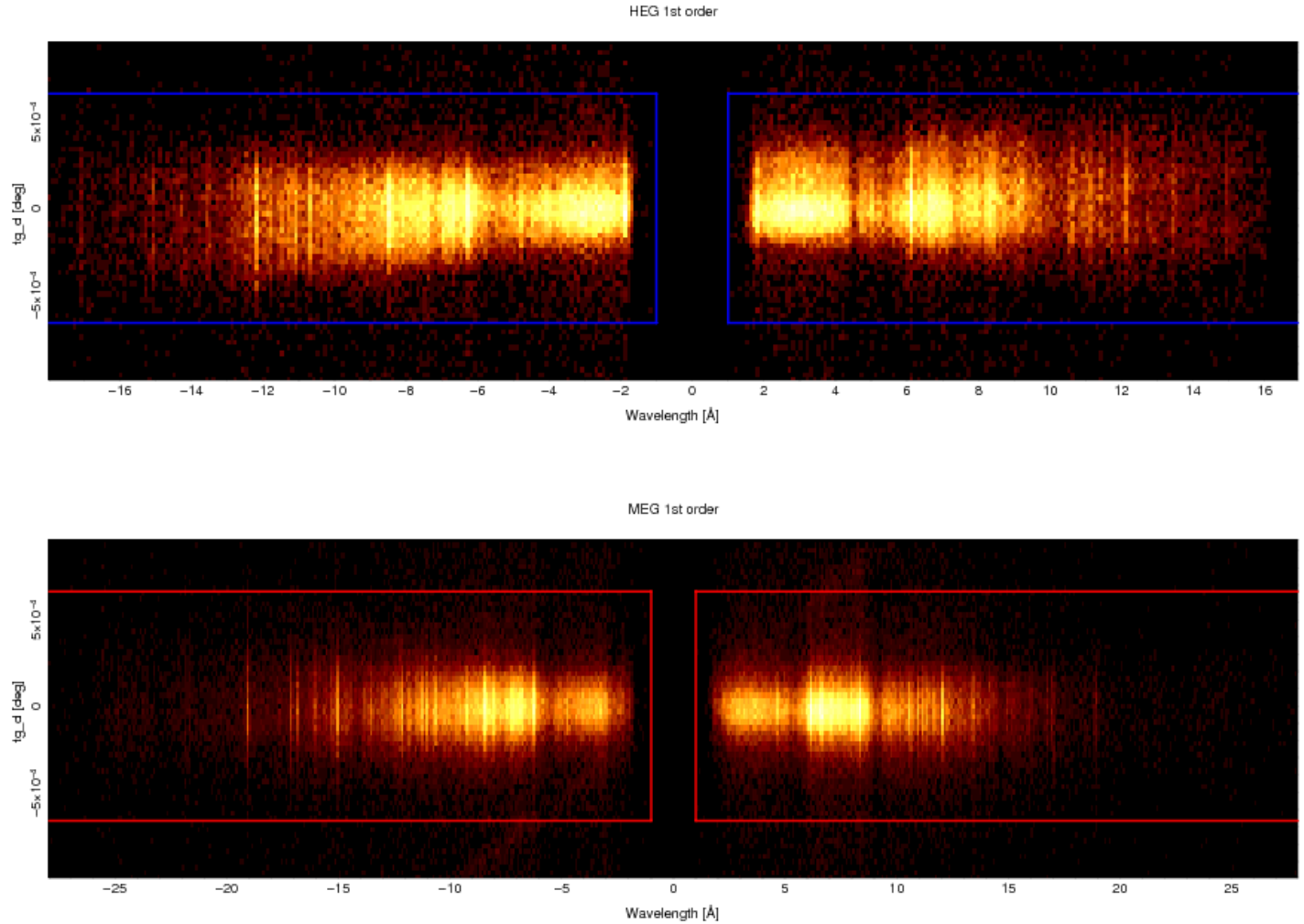
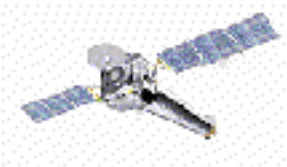


Figure 18: This is an HETG/ACIS-S spectrum in grating diffraction coordinates. The bright vertical streaks are emission lines in the source spectrum. The colored outlines mark our default spectral extraction regions.



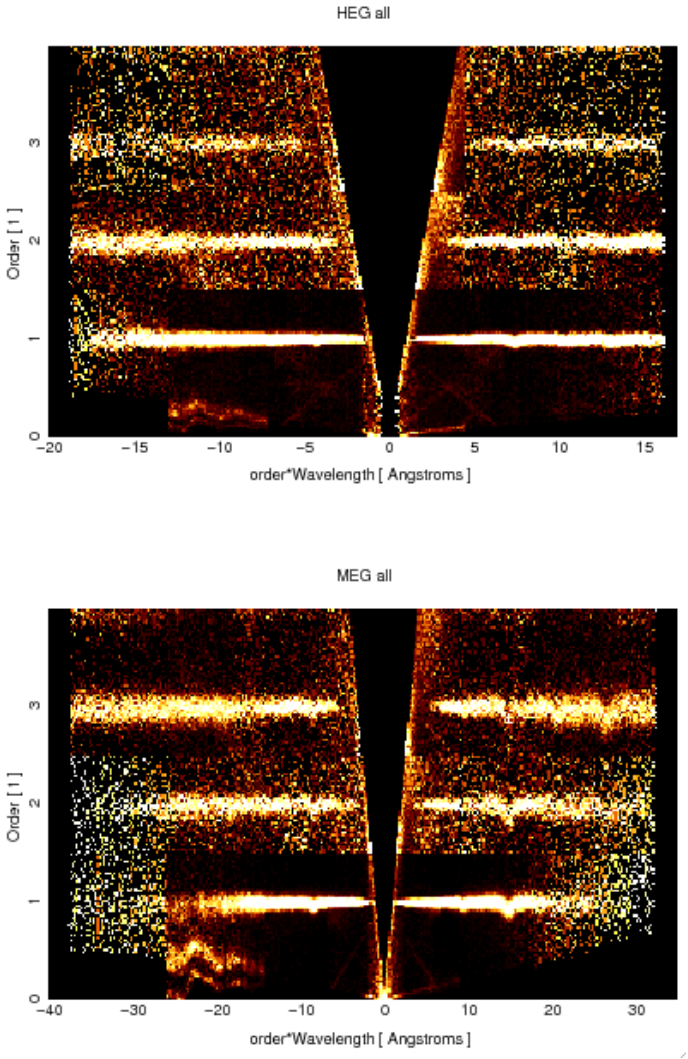


Figure 19: This is an HETG/ACIS-S "order sorting" image. The horizontal axis is $m\lambda$, and the diffraction order, m, is on the vertical axis. The distribution in the y-axis is characteristic of the intrinsic CCD energy resolution. Order-sorting selects the bright horizontal regions and excludes the background in between.

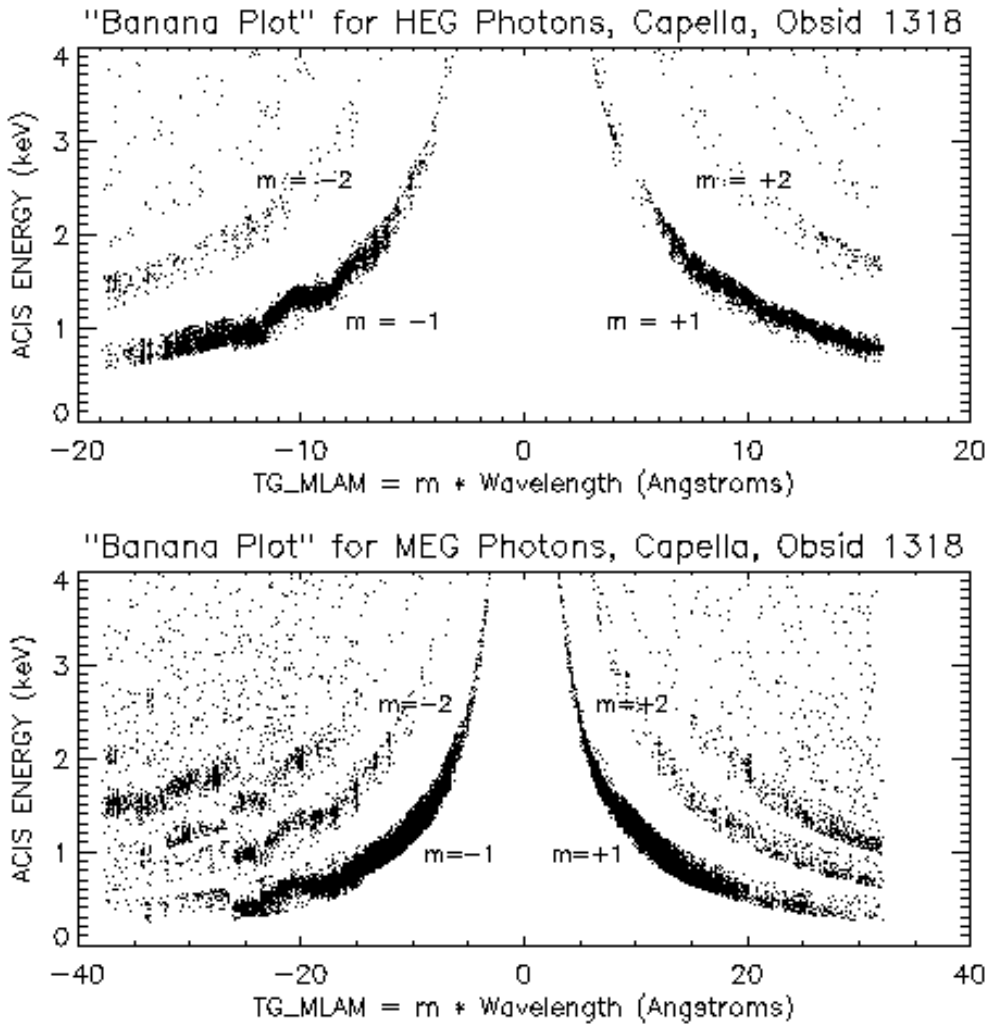


Figure 20: This another way to view the order-sorting. Here, the distributions in CCD energy have not been "flattened". The horizontal axis is still $m\lambda$, but now the vertical axis is the CCD blurred energy.

3 Practical Matters: Event Processing, Making Responses

What we really want in order to do data analysis are:

Grating PHA File: The binned counts vs wavelength (per order, per grating type);
Grating ARF: Ancillary Response File, the effective area;
Grating RMF: Response Matrix File, here, the line-spread function (but it also includes a correction factor on the effective area).

The forward folding equation is:

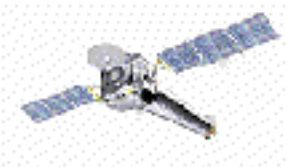
$$C(h) = T \int S(E)A(E)R(E,h)\,dE \tag{3}$$

$C(h)$ is the number of counts in spectral channel h;
T is the exposure time;
$S(E)$ is the source spectrum in [photons $\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$];
$A(E)$ is my effective area (ARF) in [cm^2] as a function of energy, E;
$R(E,h)$ (the RMF) defines the redistribution of photons of energy E into channel h.

3.1 The Grating Processing Steps

Here is a description of the processes and the primary CIAO tools for transforming your events into one-dimensional spectral counts arrays, and for computing the associated responses from observational and calibration information. The goals of the processing are to:

Reprocess the events to apply the most recent calibrations (optional);
Filter out the bad events (anytime *before* binning)
Determine an accurate zeroth order centroid;
Define the spatial regions which enclose the spectra and zeroth order;
Compute the dispersion coordinates for each event;
Resolve orders (if ACIS is the detector);
Bin the spectrum;
Compute the response matrices;
Compute the effective area files.



3.2 The Grating Processing Tools

The CIAO tool which need to be executed to go from the event file to PHA file and responses are:

***_process_events:** (optional) Re-run event processing to apply up-to-date calibration files. (Here "*" is to be replaced with `acis` or `hrc`.)

filter bad events: Filtering can be done at the start, or end of the processing. If done at the start, then files will be smaller. (But any filter requiring grating coordinates, such as a wavelength, will have to be done later.)

Example for ACIS: We filter on good grade, good status, and remove high energy (usually background) events:

```
dmcopy infile='evt1[events][grade=0,2,3,4,6,status=0,energy<12000]' outfile=evt1_filtered
```

In a separate step, we filter on the good-time-intervals in the "flt1" file.

```
dmcopy infile='evt1[events][@flt1]' outfile=evt1_filtered
```

Example for HRC: Here we select good `PHA` and `status` values and simultaneously apply the time filter.

```
dmcopy infile='evt1[events][pha=0:254,status=xxxxxx00xxxx0xxx0000x000x00000xx,@flt1]'\
       outfile=evt1_filtered
```

Note that this is not the only way to apply the filters. We can put the filters the input file specifications of other tools.

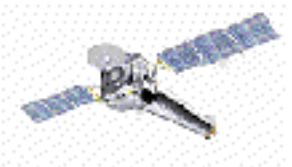
For ACIS we may also wish to apply the "destreak" filter. One CCD has artifacts, regions of spurious events in a horizontal streak. This removes artifacts from CCD S4:

```
destreak infile=evt1_filtered outfile=evt1_filtered_destreaked filter='yes'
```

tgdetect: Read the events; find the zeroth order's centroid, and write the "`src1a`" file.

tg_create_mask: Given the zero order position, write the "`reg1a`" file which defines spatial masks for the zeroth order region and for dispersed event regions. The spatial masks for the spectra are much wider than the spectrum so that they can also be used for local background spectra;

tg_resolve_events: using the regions and the aspect solution, compute diffraction coordinates for each event, given the zero order reference and spatial regions. If the detector is ACIS, also perform order-sorting to assign an order to each event, or flag it as background if it is outside the order-selection boundaries.



tgextract Bin the events into one-dimensional counts histograms.

Example for LETG/HRC-S: Note that the input file specification also includes a filter. This is a standard filter which reduces the HRC-S instrumental background. The other parameter shown indirectly refers to a default calibration database file which applies a spatial region filter appropriate for LETGS (a "bow-tie" shape which follows the outline of the spectrum; see Figure 15).

```
tgextract \
 infile="evt2[(tg_lam,pi)=region($CALDB/yadayada/letgD1999-07-22pireg075_N0001.fits)]"\
          inregionfle=CALDB outfile=pha2.fits
```

Example for HETG/ACIS:

```
tgextract infile=evt2 outfile=pha2.fits
```

tg_bkg This is a script which the background components in the PHA file output by `tgextract`. It is important for HRC-S, but may be omitted for ACIS data.

dmtype2split This is also for use with LETG/HRC-S to convert the background file output by `tg_bkg` from "Type II" to "Type I" PHA files (see below for definitions)

```
dmtype2split outfile='pha2_bg_-1[SPECTRUM],pha2_bg_1[SPECTRUM]'
```

mkgrmf: Makes a grating response matrix. We need one for each order of interest, typically ±1 for HETGS and LETG/ACIS-S, but up to ±8 for LETGS. These change very little, if at all, from observation to observation. If you wish, you may make a set once, then use it repeatedly. The only exception is if you use a non-standard region width (cross-dispersion) in `tgextract`. There is little cost to just make them for each observation, just to be safe.

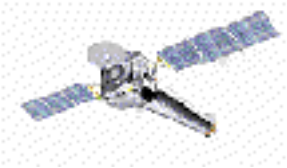
fullgarf: This is a script which packages several other tools which make the grating ARFS. ARFs are make for each chip, then summed, so running the individual steps can be tedious.

The subsidiary tools run by `fullgarf` are:

asphist: Make an "aspect histogram". This is a table of the exposure time for aspect offset bin

The aspect histogram for HRC-S requires specification of the "dead time factor" file:

```
dtffile='dtf1'
```



pset ardlib: There is a software library used by many response tools called "ardlib", in which "ARD" stands for Analysis Reference Data. Some parameters need to be set with observational values. For example, to set the observation-specific bad pixel files necessary for making responses (ACIS will have 6 such `psets` for bad pixels:

```
pset ardlib  AXAF_HRC-S_BADPIX_FILE='bpix1'
```

mkgarf: This actually constructs the grating ARF. It must be run for each detector element and order of interest.

dmarfadd: This combines all the per-chip files written by `mkgarf` into one "full" ARF per grating per order.

These tools are fully documented on the CIAO help pages and in threads. The ahelp files have many explicit examples of tool usage. (See Section 7 for relevant links.)

4 Description of the Important Files

4.1 The Event File: Your New Best Friend

Become familiar with the contents of the event file. You may need to to look for confusing sources, to inspect background, to verify zeroth order quality, to make pretty pictures. You can use `dmlist` to see the columns: `dmlist evt2 cols`

These are some the columns and definitions in a grating event file (as output by `tg_resolve_events` with the standard event definition. The galleries in Section 2.2 were made from binned counts in variations of these coordinates.

These are present in Level 1:

`time`	event time tag
`chipx,chipy`	chip pixel
`tdetx,tdety`	tiled detector coordinate
`x,y`	sky pixel
`ccd_id`	CCD index (ACIS)
`chip_id`	Chip index (HRC)
`energy`	"blurred" photon energy (ACIS)
`grade`	event geometry code (ACIS)

These are added by `tg_resolve_events`:

`tg_r`	grating angular coordinate, degrees in-dispersion
`tg_d`	grating angular coordinate, degrees cross-dispersion
`tg_srcid`	a source counter, starting at 1
`tg_part`	grating type; 1 → HEG; 2 → MEG; 3 →LEG; 99 → background; 0 → zeroth order
`tg_mlam`	order × wavelength
`tg_m`	order
`tg_lam`	wavelength [Å]

4.2 The PHA File

Now that you have obtained a PHA file, this is where your work will be centered. It helps to understand the file contents and types of PHA files.

Type II: This format has the counts spectra and associated data as array columns. Other information is also in the same row, such as the order and grating type, as well as other required field. This is the default format for CIAO. Using this format we can pack the spectra for 12 orders of HETGS (-3 to +3 for two gratings) into a single table.

Type I: This contains a single spectrum in a column oriented file. Some necessary information is in the header, such as order and grating type.

For Chandra data we also include wavelength coordinates in columns called `BIN_LO, BIN_HI`. These are not required by the spectral standard. The other "2" associated with the "`pha2`" file is not to be confused with "Type II". The digit "2" refers to a "Level 2" data product (see the CIAO dictionary). The CIAO tool `dmtype2split` (which breaks the rule of "2" vs "II") will convert from "Type II" to "Type I". Either Type can be read by most X-ray spectral analysis packages.

Here are the columns of a Chandra `pha2` file:

Column	Unit	Type	Description
`SPEC_NUM`		Int2	Spectrum Number
`TG_M`		Int2	Diffraction order
`TG_PART`		Int2	Spectral component (HEG, MEG, LEG)
`TG_SRCID`		Int2	Source ID, output by detect
`X`	pixel	Real4	X sky coord of source
`Y`	pixel	Real4	Y sky coord of source
`CHANNEL[16384]`		Int2(16384)	Vector of spectral bin numbers.
`COUNTS[16384]`	count	Int2(16384)	Counts array
`STAT_ERR[16384]`	count	Real4(16384)	Statistical error on counts
`BACKGROUND_UP[16384]`	count	Int2(16384)	Background count vector.
`BACKGROUND_DOWN[16384]`	count	Int2(16384)	Background count vector.
`BIN_LO[16384]`	angstrom	Real8(16384)	Bin boundry, left edge
`BIN_HI[16384]`	angstrom	Real8(16384)	Bin boundry, right edge

For LETGS, `TG_M` will be -1 or $+1$, and the file will have only 2 rows. For HETGS, the default product has orders -3 to $+3$ (excluding 0) for the two grating types, and will have 12 rows. The default array length for LETGS is 16384 bins, and half that for HETGS.

4.3 ARFs, RMFs, and all that.

The three most important things about data analysis are Calibration, *Calibration, and* **Calibration.** The ARFs combine the effective area and efficiency calibrations of the mirrors, gratings, filters, and detectors. They also incorporate the aspect dither - chip gaps will be bowl shaped depressions in the response. The ARFs also include bad pixels, which when dithered appear as cuspy depressions. The RMF contains the calibration of the instrumental profile, a combination of the mirror and grating blurs.

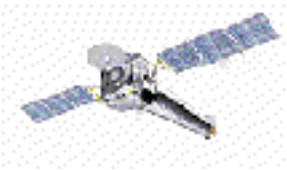
5 Analyzing Your Spectra

Now that you have the PHA file, the ARFs and RMFs, you can begin analysis. You need to choose an analysis system like ISIS or Sherpa. The procedure is usually something like:

Load data
Inspect data
Load ARFs
Load RMFs
Assign responses to data
Define a model
Notice/ignore spectra or regions
Group or combine data if necessary
Fit the model
Inspect the residuals
Determine confidence limits
Save results

As an elementary case, lets fit a single Gaussian to O VIII in the MEG -1 order. Here is an ISIS example:

```
isis> load_data("pha2", 9) ; % row 9 is MEG -1
isis> list_data; % see the data index (1 if new session)
isis> plot_data_counts( 1 ) ;
isis> load_arf( "meg_-1.arf" ) ;
isis> load_rmf( "meg_-1.rmf" ) ;
isis> list_arf;  % see what their indices are (1 if new session)
```



```
isis> list_rmf;
isis> assign_rsp( 1, 1, 1 ) ; % use indices from listings.
isis> fit_fun( "gauss(1)" );
isis> set_par( "gauss(1).area", 0.001, 0, 1.e-5, 0.1 ) ;
isis> set_par( "gauss(1).center", 18.97, 0, 18.9, 19.1 ) ;
isis> set_par( "gauss(1).sigma", 0.005, 0, 1.e-5, 0.1 ) ;
isis> ignore( all_data ) ; % in case other data are loaded
isis> xnotice( 1, 18.9, 19.1 );
isis> group_data( 1, 2 );
isis> fit_counts;
isis> rplot_counts( 1 ) ;
isis> conf( "gauss(1).center" );
isis> save_par("o8fit.par");
```

Sherpa steps are similar (CIAO 4.0.1 version, to be revised in 4.1):

```
unix>  slsh
slsh> require( "sherpa" ) ;
slsh> load_pha( "pha2" ) ;
slsh> load_arf( 9, "meg_-1.arf" ) ;
slsh> load_rmf( 9, "meg_-1.rmf" ) ;
slsh> show_all(  ) ;
slsh> get_data( 9).units="wavelength";
slsh> notice_id( 9, 18.9, 19.1 ) ;
slsh> plot_data( 9 ) ;
slsh> set_source( 9, normgauss1d.gauss1 ) ;
slsh> gauss1.pos = 12.398/18.97;
slsh> gauss1.fwhm = 0.001;
slsh> gauss1.ampl = 0.0002;
slsh> fit( 9 ) ;
slsh> plot_fit( 9 ) ;
slsh> print( get_fit_results( 9) ) ;
slsh> plot_fit_delchi( 9 ) ;
slsh> proj( 9 ) ;
slsh> show_all( ;filename="session.out" ) ;
```

Both ISIS and Sherpa are scriptable, extensible analysis packages. ISIS is based on S-Lang; Sherpa uses S-Lang and Python. They each provide access to low-level data and allow you to customize arbitrarily. For instance, in ISIS to define a new model:

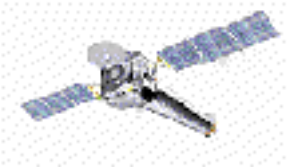
```
define my_function_fit( xlo, xhi, param )
{
  % insert code here to compute  y = f( xlo, xhi, param )
  return (y ) ;
}
add_slang_function( "my_function", param_names ) ;
fit_fun( "my_function( 1 )" );
```

See the CIAO/Sherpa threads or ISIS pages for more detailed examples.

5.1 Physical Models, Atomic Data

For many astrophysical models we rely on the `xspec` library. ISIS provides an interface to the Astrophysical Plasma Emission Database (APED) which allows evaluation of line or continuum emissivity functions and evaluation of model spectra for single ions, to pick two examples. Here is an ISIS example which lists model line fluxes for a multi-temperature plasma:

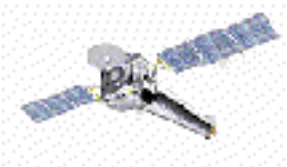
```
isis> plasma( aped ) ;   % load the database
isis> % Use the plasma variable to define a multi-thermal model:
isis> p = default_plasma_state;
isis> p.temperature = 10^[ 6.2, 6.8, 7.2 ] ;
isis> p.norm = [ 1, 2, 3] * 0.001 ; % guess the normalization.
isis> p.elem = [ Ne, Fe ] ;
isis> p.elem_abund = [ 1.0, 0.6 ] ; % use non-solar ratio of Ne, Fe
isis> create_aped_fun( "Aped_3T", p ) ;
isis> fit_fun( "Aped_3T(1)" );
isis> eval_fun( 13.5, 13.6 ) ;
isis> lines_in_region = where( wl( 13.5, 13.6 ) ) ; % get info from APED
isis> page_group( brightest(6, lines_in_region ) ); % list the brightest lines
#  index        ion   lambda    F (ph/cm^2/s)  A(s^-1)  upper lower   label
 129758 *    Fe XXI    13.507    6.468e-06   1.605e+12    42     7
  39128 *    Fe XIX    13.518    1.733e-05   1.868e+13    68     1
  77544 *     Fe XX    13.535    9.947e-07   4.121e+12   107     7
```



```
 38922 *    Fe XIX    13.551    1.143e-06   4.436e+12    65     1
  3946 *     Ne IX    13.553    5.048e-06   6.500e+09     5     1 1s2p~^3P_{1} - 1s^2~^1S_{0}
129754 *    Fe XXI    13.574    1.108e-06   3.866e+11    39     7
```

You can see that Fe XIX blends with Ne IX. To be thorough, you can search for other Fe XIX lines:

```
isis> eval_fun(10, 19);
isis> page_group( brightest(5, where( el_ion(Fe, 19) ) ) ) ;
#  index        ion   lambda    F (ph/cm^2/s)  A(s^-1)  upper lower   label
  38915 *    Fe XIX    13.497    7.867e-06   1.292e+13    71     1
  39128 *    Fe XIX    13.518    1.733e-05   1.868e+13    68     1
  39132 *    Fe XIX    13.795    6.989e-06   5.353e+12    53     1
  38901 *    Fe XIX    15.079    6.290e-06   9.785e+10    11     1
  40009 *    Fe XIX    16.110    8.035e-06   7.226e+10    37     6
```



Some examples of the plasma database use in ISIS, showing the model and line indentifications are in Figures 21 & 22.

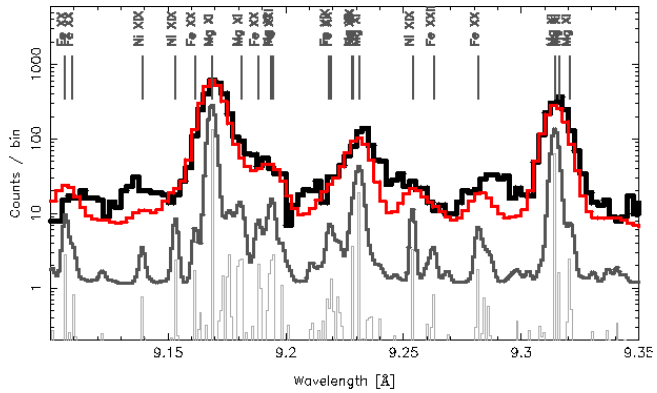


Figure 21: Capella and APED model in ISIS; observed–black; model counts–red; unconvolved thermal profiles – gray; unconvolved delta profiles – light gray.

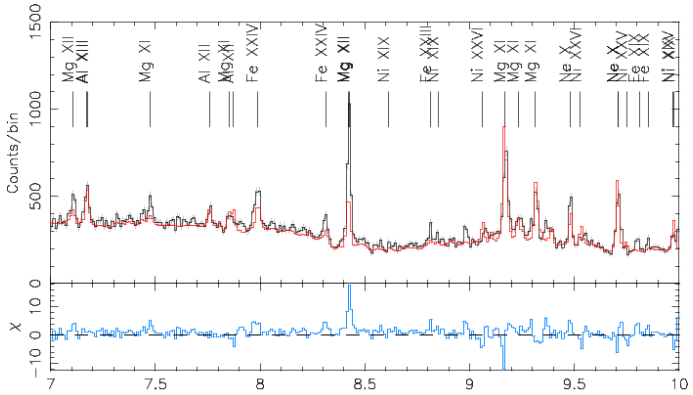
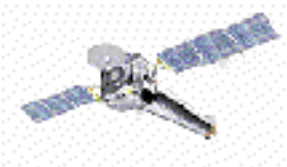


Figure 22: σ Gem and APED model in ISIS; observed–black; model counts–red.



`WebGuide` can also be a convenient interface to APED. It allows simple queries, and provides primary references to the data.

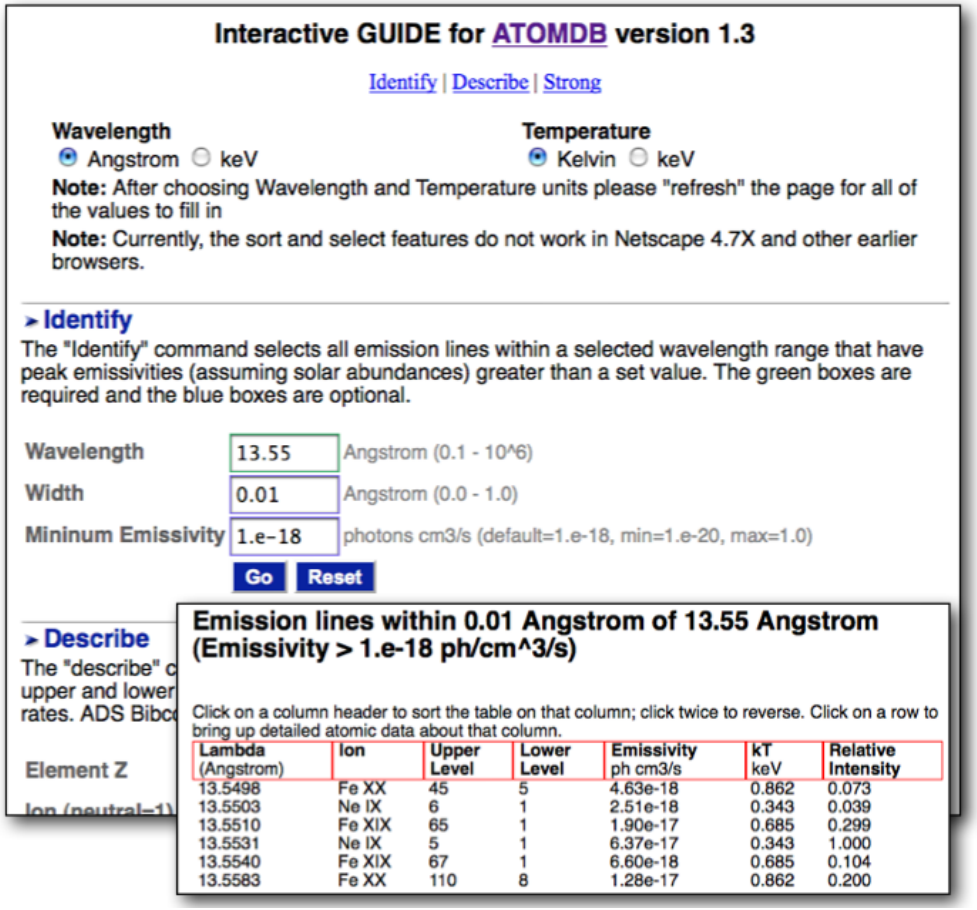
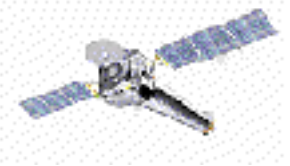


Figure 23: A portion of the WebGuide page output of "Identify" (`http://cxc.harvard.edu/atomdb/WebGUIDE/`).



5.2 Multiple orders, multiple gratings, multiple observations

Some common issues regarding grating data are:

1. I have an HETGS observation. How do I add plus and minus orders? How do I combine HEG and MEG? What about orders 2 and 3?
2. My observation was done in two parts, or, Object X was observed 5 times. How do I combine them?
3. How do I add RMFs?
4. Do I need to subtract background?
5. LETGS has overlapping orders. How do I fit a spectrum?

Items 1 & 2 are effectively identical.

There is no compelling reason to add multiple orders or observations into one file! Reasonable solutions use the high-level products – PHA, ARF, and RMF files; *DON'T* start by combining event files!

Advantages: Ability to include or exclude any spectrum during analysis; maintains unique responses and exposures.

Disadvantages: multiple files to handle; multiple datasets to manage.

It is ultimately a matter of *scientific judgement* about which path is appropriate. These are some of the techniques:

Joint analysis: Load the data of interest. Notice them all and fit jointly. Each spectrum can be binned appropriately within the analysis session. Choose a statistic appropriate to the counts. This will work for multiple orders or observations transparently.

Dynamically combined data: ISIS has a function, `combine_datasets`, which specifies that spectra and corresponding models are to be summed (in memory) *prior* to computing the statistic. This increases the signal-to-noise ratio (S/N) per bin. You can even combine HEG and MEG if you first regrid them and the responses to match (also possible within the session, in memory).

Separate analysis: If the S/N of your data is very high, systematic calibration errors could dominate, and it may be better to fit each spectrum separately, then decide later how to combine the results.

Add as files: If you really want to sum data on disk, use `add_pha` (an ISIS-based script with CIAO tool interface) and `dmarfadd` (a CIAO tool)[2]. This method is transparent to summing orders or observations.

[2] `http://space.mit.edu/cxc/analysis/add_pha/index.html`

`Add_pha` with `dmarfadd` supercedes two scripts, `add_grating_orders` and `add_grating_spectra`, though these are still available.

Higher HETGS orders: For most observations, you can ignore them. Exceptions: multiple observations (12 Capella spectra), bright X-ray binaries: you might have enough signal in HEG 2^{nd} or MEG 3^{nd} orders.

Combining RMFs: We don't. There is practically little difference between positive and negative orders, nor between observations. There are differences for non-standard extraction region widths, so if the spectrum's extraction aperture was narrowed to avoid confusing sources, then the RMF's line profile (and enclosed energy fraction) will change. *IF* you added data as files, then you can use a set from one observation (and from one side if positive and negative were combined).

Background: is usually ignorable for HETGS, or LETG/ACIS-S. For LETG/HRC-S it is important and must be included in modeling. (See 3.2 & 6.1.)

Multiple orders of LETGS are handled by assigning multiple responses to a single spectral counts histogram. For example:

```
isis> load_data("letgs_pha", 2 ) ;
isis> load_arf("leg_1.arf") ;
...
isis> load_arf("leg_8.arf") ;
isis> load_rmf("leg_1.rmf") ;
...
isis> load_rmf("leg_8.rmf") ;
isis> assign_rsp( [1:8], [1:8], 1 ) ;
```

When the model counts are evaluated, each ARF-RMF pair are applied and summed. (See additional examples on the ISIS web pages.)

Black = 'fakeit' powerlaw (alpha=−1.5) with log Nh = 20
including sum of LETGS orders m=1−11

Red = 1st order
Green = 2nd order
Blue = 3rd order
Lt−blue = sum m=4−11

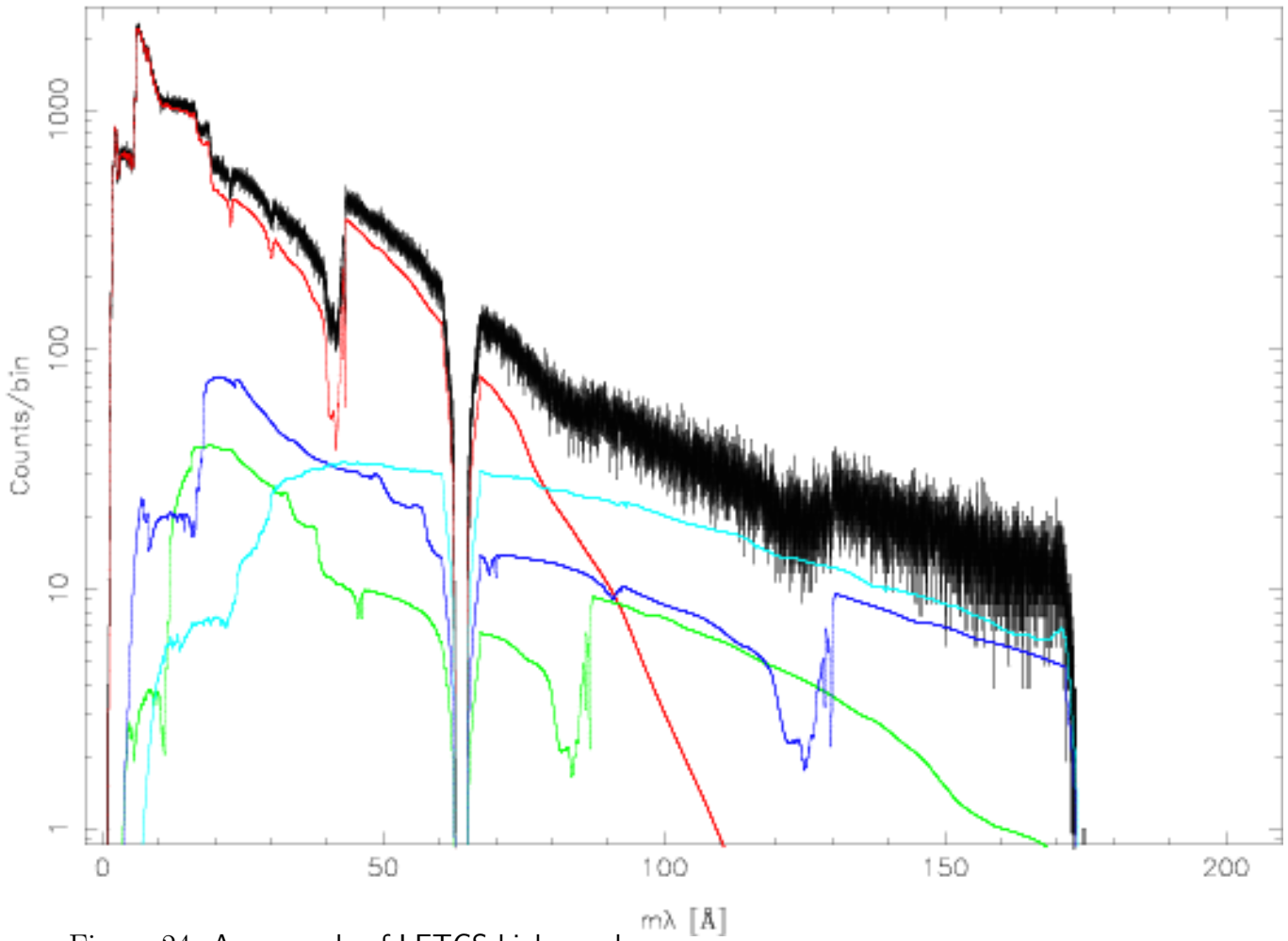
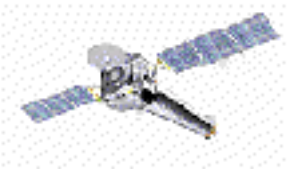


Figure 24: An example of LETGS higher orders.



6 Various Other Details

6.1 Backgrounds

Don't *NEVER EVER* subtract background! Your statistics will be tricky. There is no necessity for subtracting background for analysis.

If background is important, use a system which *adds background to the model counts.*

(It is perfectly fine, however, to *inspect and display* background subtracted data.)

6.2 ACIS CC-mode: risky business?

It's not so bad. CC-mode spectral extraction works basically the same way as for TE. Input data might look funny, but we still do the same basic steps and produce the same products. Some of the calibration products may not be as good, and CTI correction is not done. So some care is needed in interpretation.

6.3 Extended Sources, Multiple Sources

Extra care is needed with source and background regions. See the options on `tg_create_mask` and `tgextract`.

For extended sources, you typically want to increase the widths.

For crowded sources you probably want to decrease the widths.

For LETG/HRC-S, you may also need to adjust the background regions.

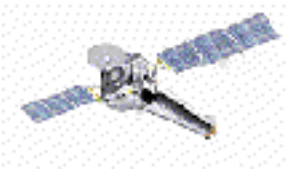
6.4 Flux Correction?

Flux correction can be done by dividing the counts by the ARF and exposure time to get units of [photons $\mathrm{cm}^{-2}\,\mathrm{s}^{-1}$]. It is more accurate to use both the ARF and RMF in analysis. So, always, *ALWAYS* use the RMF.

Flux correction in ISIS, for example, doesn't just divide the counts by the ARF, but divides the counts by the $\int \mathrm{ARF} \times \mathrm{RMF}\, dE$.

The Chandra grating RMF also contains a portion of the effective area, related to the cross-dispersion selection region which clips the wings of the spatial distribution.

We don't normally model flux corrected data, but it is very useful for *visualization* of data and models.



6.5 Time Slicing

Many sources are variable and we may want spectra vs time or state. An easy way to produce spectra for different times is to `dmcopy` your event file using your externally derived `GTI` tables. Then you run those individual event files through the same grating processing threads.

7 Links to Additional Resources

APED: A spectroscopy database for X-ray emission

`http://cxc.harvard.edu/atomdb/`

CIAO dictionary: `http://cxc.harvard.edu/ciao/dictionary/`

CIAO grating threads: Detailed recipes for performing some common tasks;

`http://cxc.harvard.edu/ciao/threads/gspec.html`

ISIS: The the Interactive Spectral Interpretation System, developed especially for working with Chandra grating spectra; includes an interface to an atomic database (APED)

`http://space.mit.edu/cxc/isis/`;

POG: The Proposers' Observatory Guide - detailed descriptions of all components of Chandra.

`http://cxc.harvard.edu/proposer/POG/`

summing spectra: `http://space.mit.edu/cxc/analysis/add_pha/index.html`

TGCat: The recently released catalog and archive of Chandra grating data;

`http://spacebase-alpha.mit.edu/tgcat`.

Tool help "ahelp" for CIAO tools:

`http://cxc.harvard.edu/ciao/ahelp/`

WebGuide: interactive atomic data;

`http://cxc.harvard.edu/atomdb/WebGUIDE/`

Appendices

A LETG/ACIS-S Images

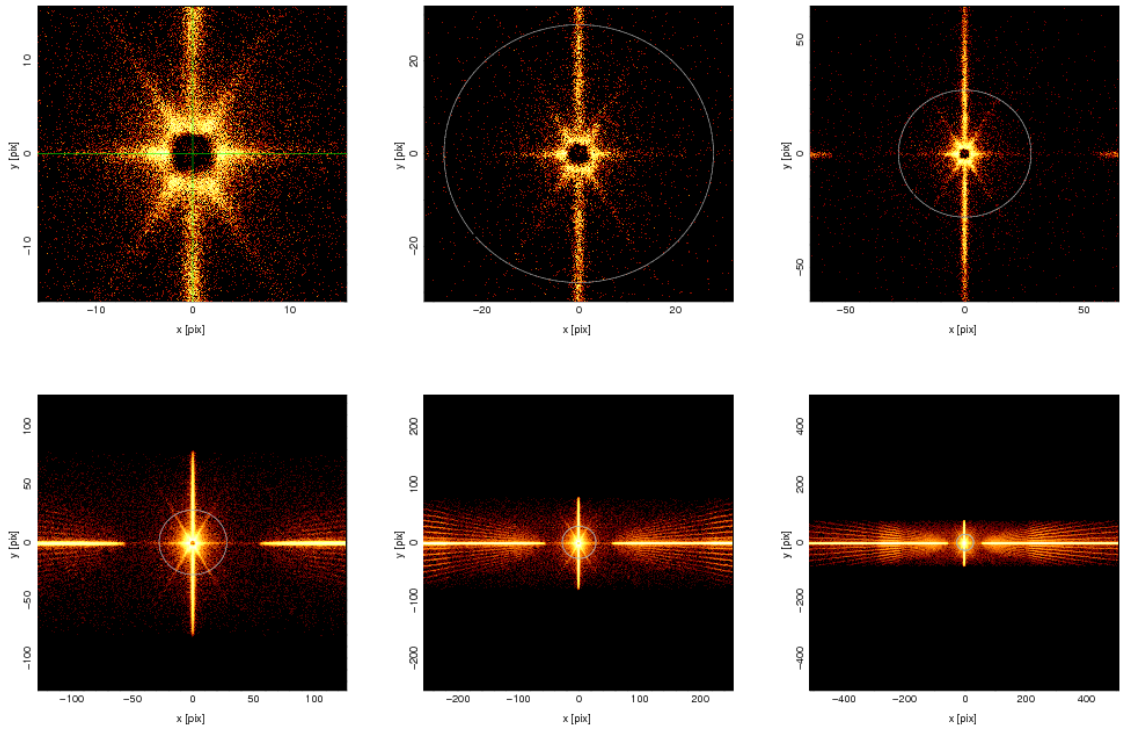
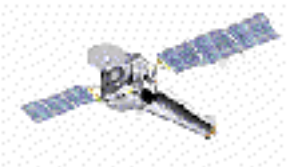


Figure 25: The zero order region of an LETG/ACIS-S spectrum. We step out by factors of two from upper-left to lower-right. As we step out, you begin to see the detector boundary, the "frame shift streak" (vertical feature) and the diffracted spectra. We can also see that the zeroth order is heavily distorted, so much that it has a "crater" (hole in the center) — this is due to severe photon pile-up and rejection of events before telemetry. The LETG cross-dispersion "star" and radial lines are also apparent. (The green cross and circle were added as markers for the zero order position and region.)



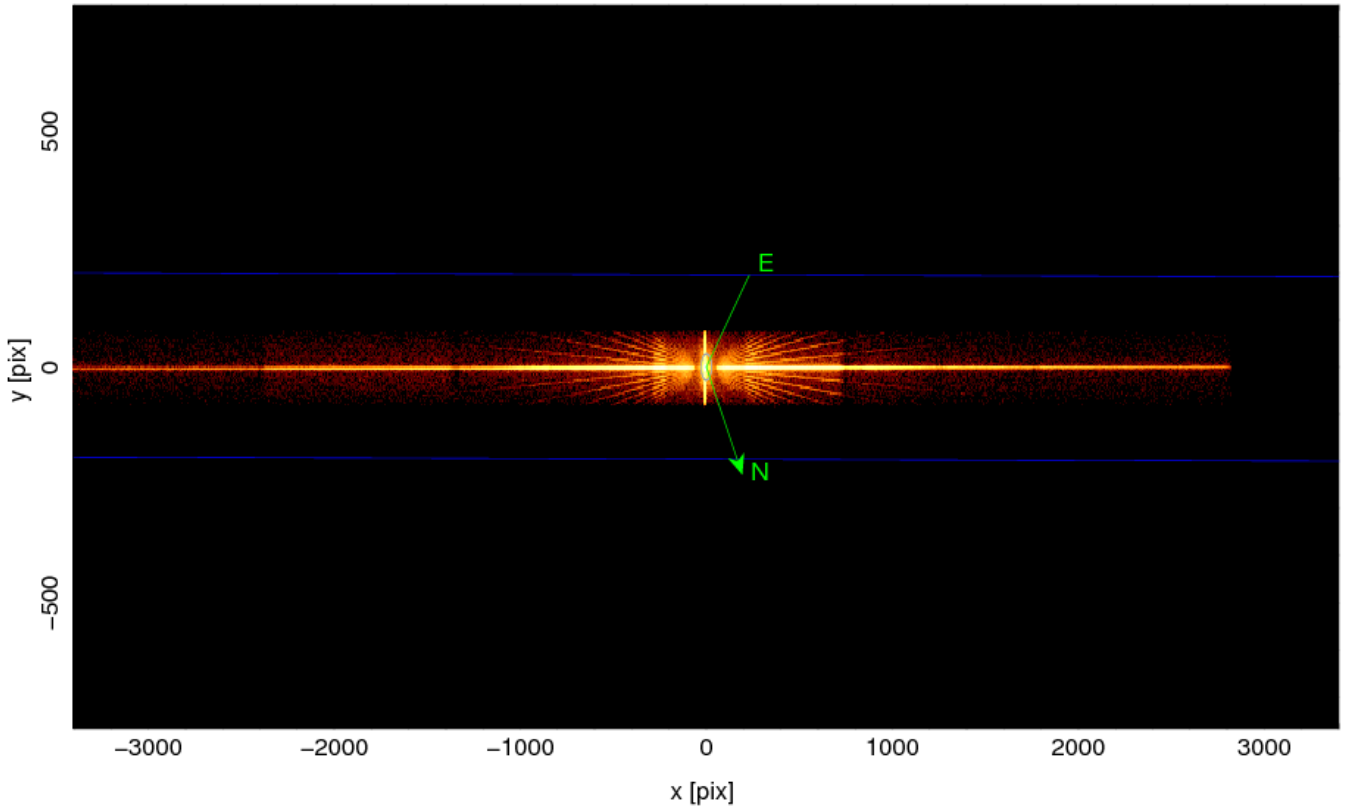
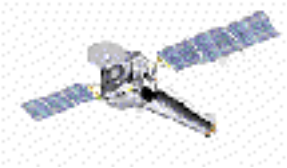


Figure 26: This is an image in sky coordinates, rotated to horizontal for better display. It shows the full ACIS-S detector area with an LETG/ACIS-S spectrum. The source spectrum is the bright horizontal streak. The gaps between the 6 CCDs show as darkest vertical lines. The chips with brighter background (2^{nd} and 4^{th} from the left) are back-illuminated (BI) devices. The LETG cross-dispersion features are clear. North is marked by the green arrow, and east by a green line (they are not orthogonal in this view because of the non-square aspect ratio).



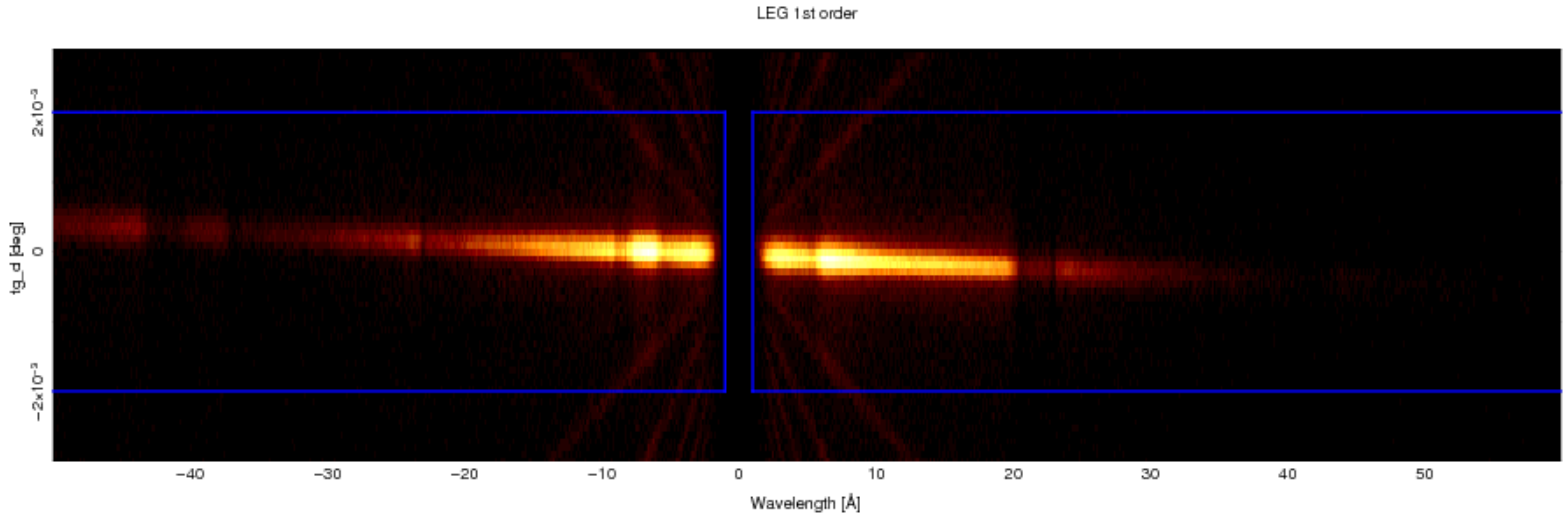
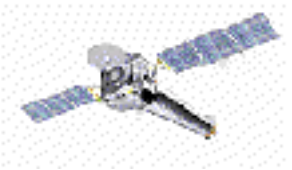


Figure 27: This is an LETG/ACIS-S spectrum in grating diffraction coordinates. The slight tilt is an unsolved calibration or software issue. The colored outlines mark our default spectral extraction regions.



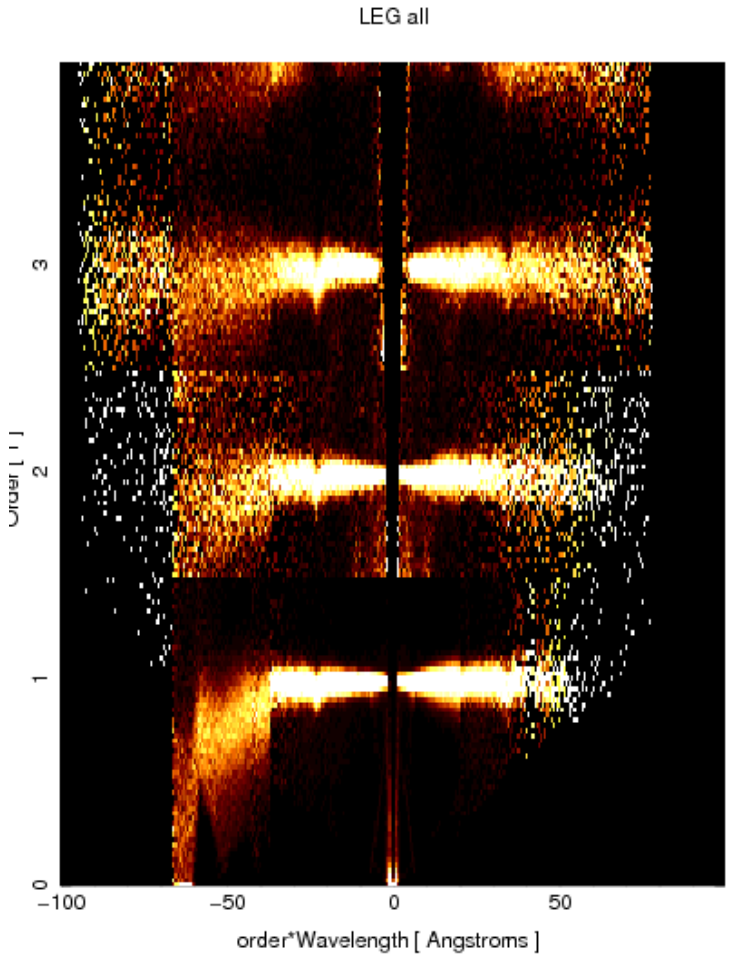
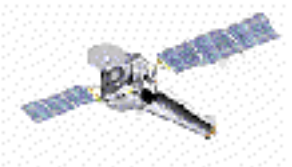


Figure 28: This is an LETG/ACIS-S "order sorting" image. The horizontal axis is $m\lambda$, and the diffraction order, m, is on the vertical axis. The distribution in the y-axis is essentially from the intrinsic CCD energy resolution. Order-sorting selects the bright horizontal regions and excludes the background in between. With LETG on ACIS-S, we get to wavelengths longer than the CCDs can detect and resolve well.



B Spectral Image Visualization with Ds9

Some of the images shown in Section 2.2 can be made in ds9 using the "`Bin` → `Binning Parameters...`" and "`Zoom` → `Pan Zoom Rotate Parameters...`" menus. For example, choosing a Capella HETGS observation (ObsID 1103) (use a log-intensity scale and delete regions for a good view):

```
> ds9 evt2 &
```

To set binning parameters for the full field image:

1. Choose "Bin columns" `x` and `y`;
2. Block each by 8
3. Choose "Bin center" `or center of data` checkbox.

The rotation depends on the observation. You can get it from menu "`File` → `Display Fits Header..., evt2[EVENTS]`", and look for `ROLL_NOM`. (98.2° for this observation).

For diffraction coordinates, we can use something like

1. Choose "Bin columns" `tg_mlam` and `tg_d`;
2. Block `tg_mlam` by 0.08, and `tg_d` by $5.0e-05$.
3. Choose "Bin center" checkbox "`or center of data`";
4. Set a `Bin Filter` to `tg_part==2, abs(tg_m)==1`.

Set the rotation to 0.0.

C Thanks

Thanks to Nancy Brickhouse and Randall Smith for previous versions of this Workshop topic, from which I borrowed heavily.