High-Resolution X-ray Analysis

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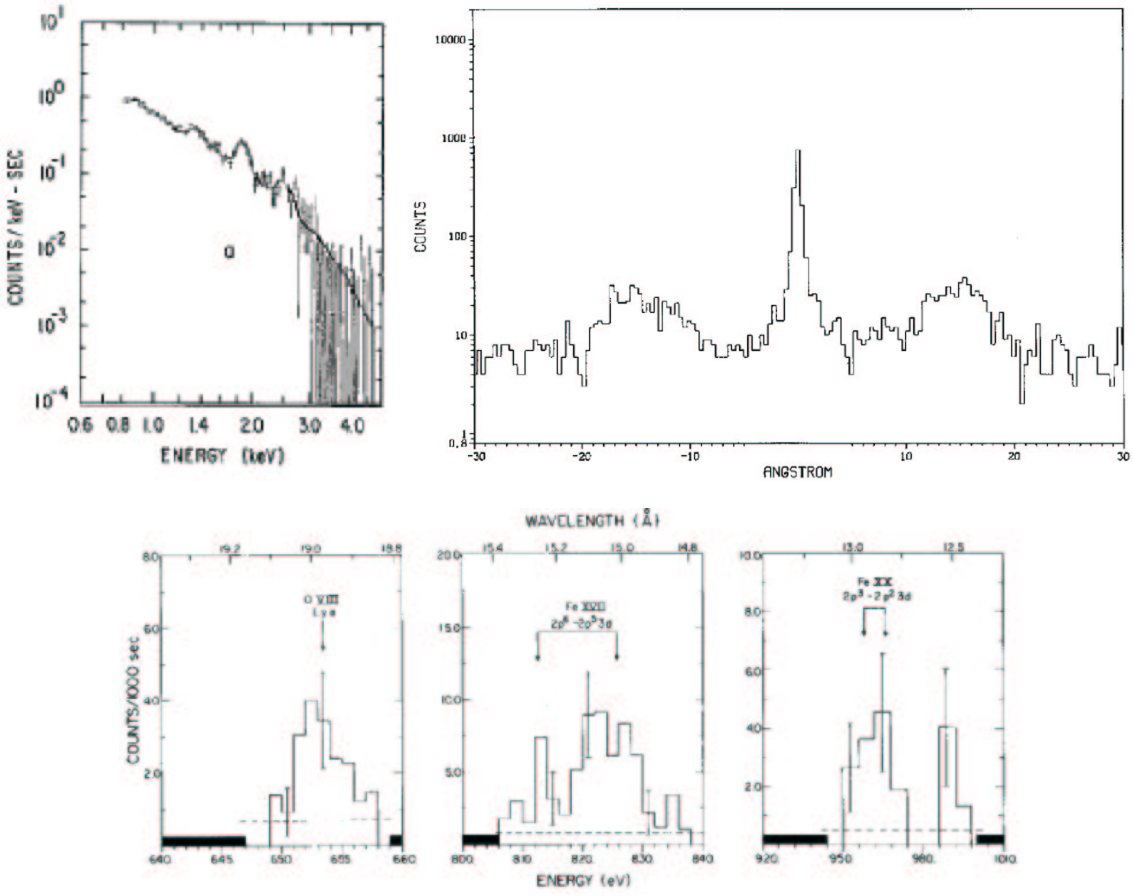
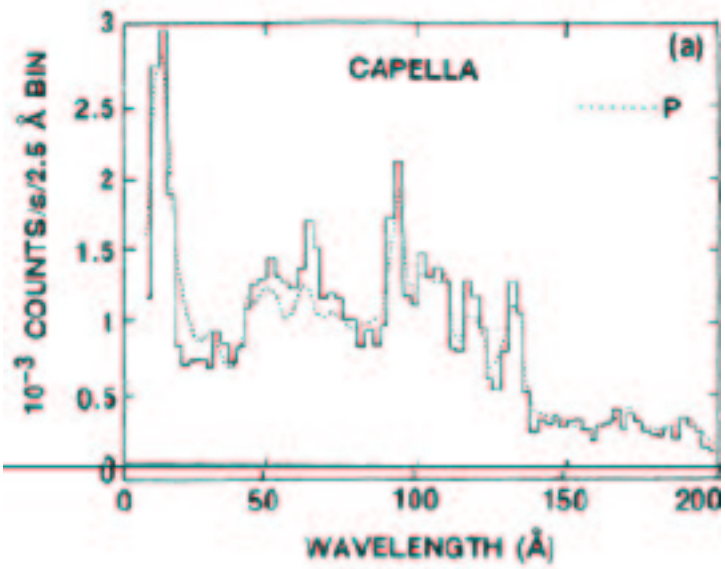
High-resolution X-ray spectroscopy did not begin with *Chandra* and *XMM/Newton*, although these two satellites have the highest resolution and throughput to date. As a sample target, I present observations of Capella, a binary star system that is bright in X-rays, and therefore a regular target for high-resolution spectrometers.

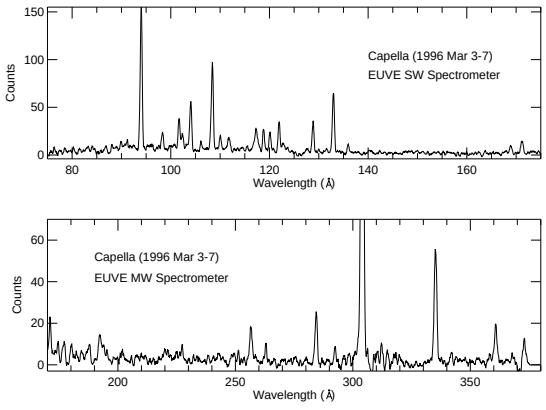
Einstein observed Capella with three separate high-resolution detectors: The Solid-State Spectrometer (SSS; 7 ksec; Holt *et al.* 1979) [Left] and the Objective Grating Spectrometer (OGS; 42 ksec; Mewe *et al.* 1982) [Right] and the Focal Plane Crystal Spectrometer (FPCS; 59 ksec; Vedder & Canizares 1983) [Bottom]:

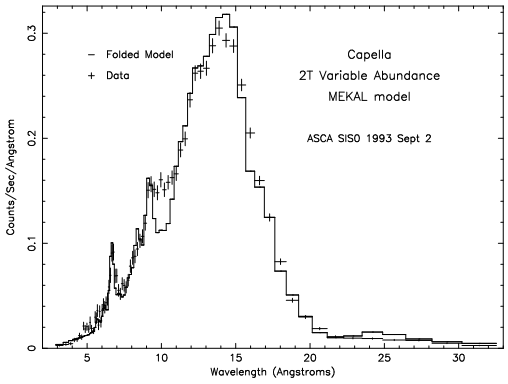


Further observations of Capella were done with the *EXOSAT* Transmission Grating Spectrometer (TGS; 85 ksec; Lemen *et al.* 1989):

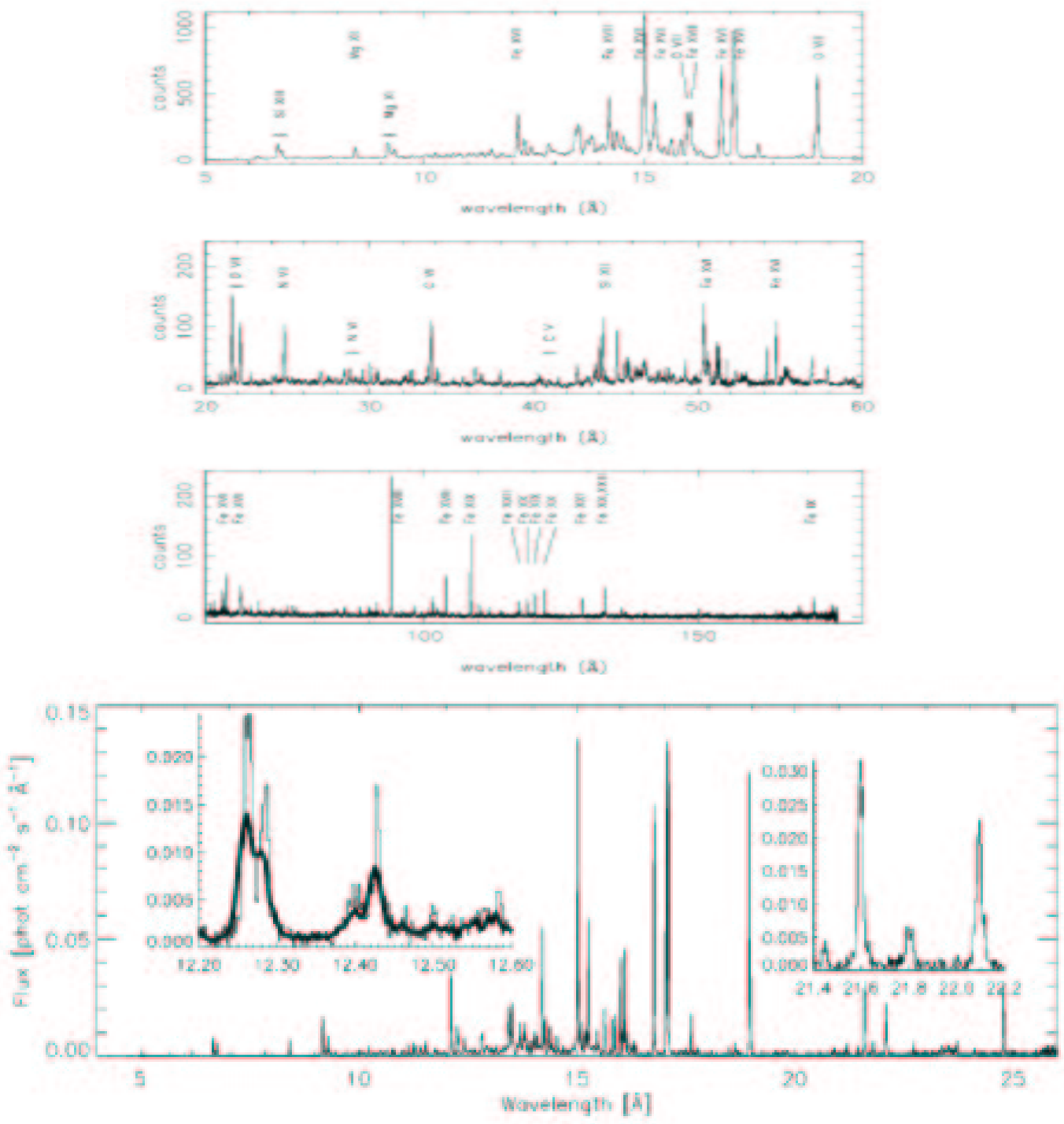


More recently, Capella was observed with the Extreme Ultraviolet Explorer (EUVE; 120 ksec) and ASCA (21 ksec) (Brickhouse *et al.* 2000)

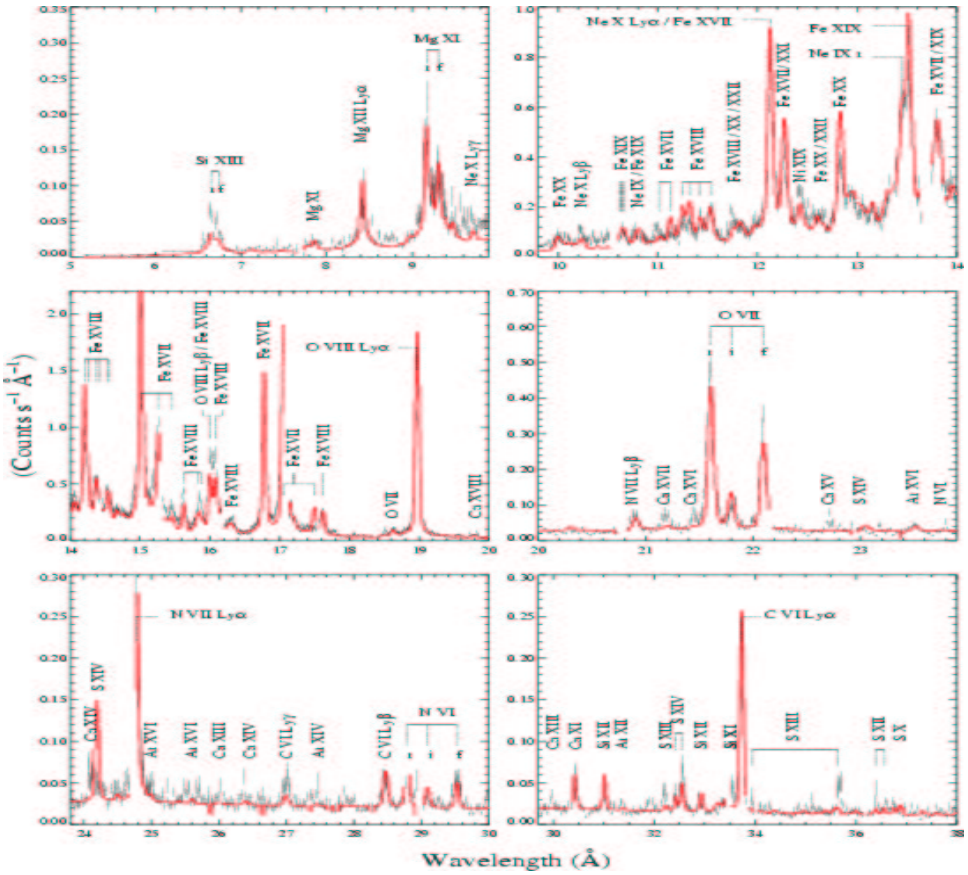




We now come to the most recent high-resolution X-ray spectrometry data on Capella from *Chandra*, using the Low-Energy Transmission Grating (LETG; 95 ksec; Brinkman *et al.* 2000) and the High-Energy Transmission Grating (HETG; 89 ksec; Canizares *et al.* 2000):

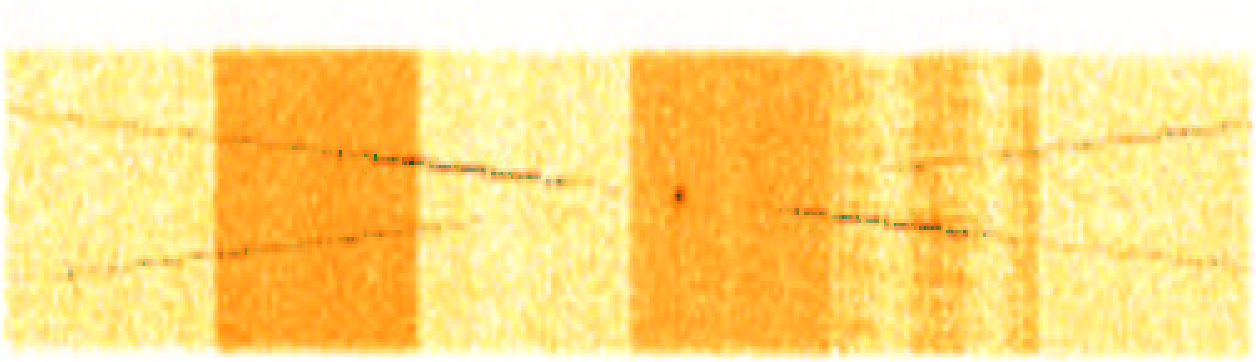


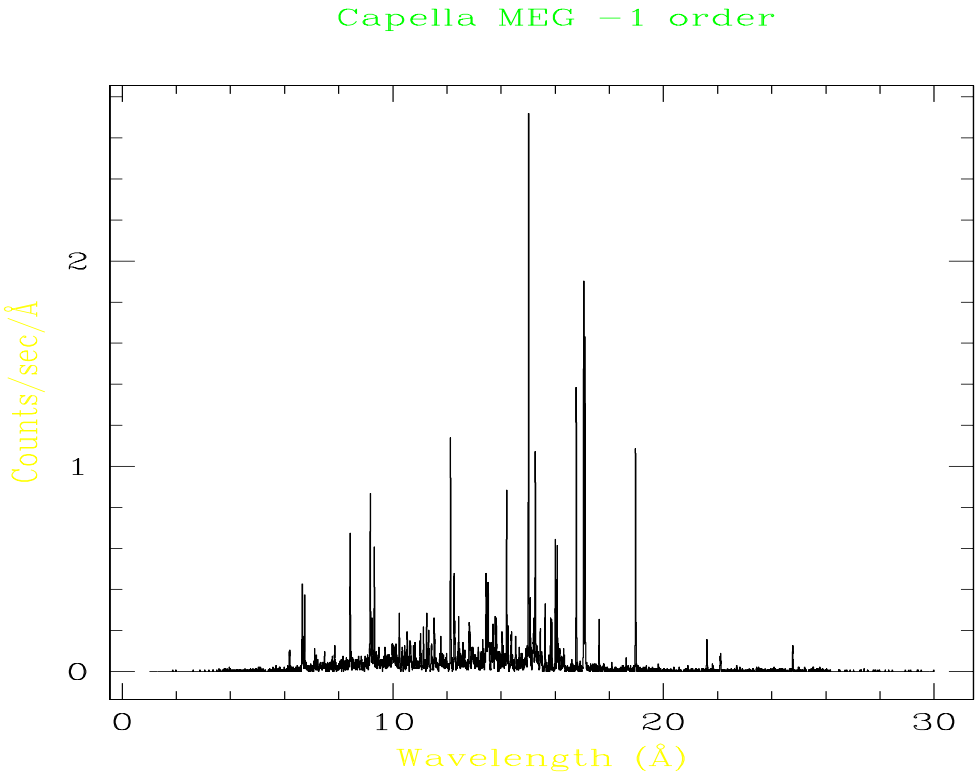
And, finally, Capella as observed by the *XMM/Newton* Reflection Grating Spectrometer (RGS; 52 ksec; Audard *et al.* 2001):



Note the increased count rates as effective areas have increased, and the general tend to higher resolution and wider bandpasses.

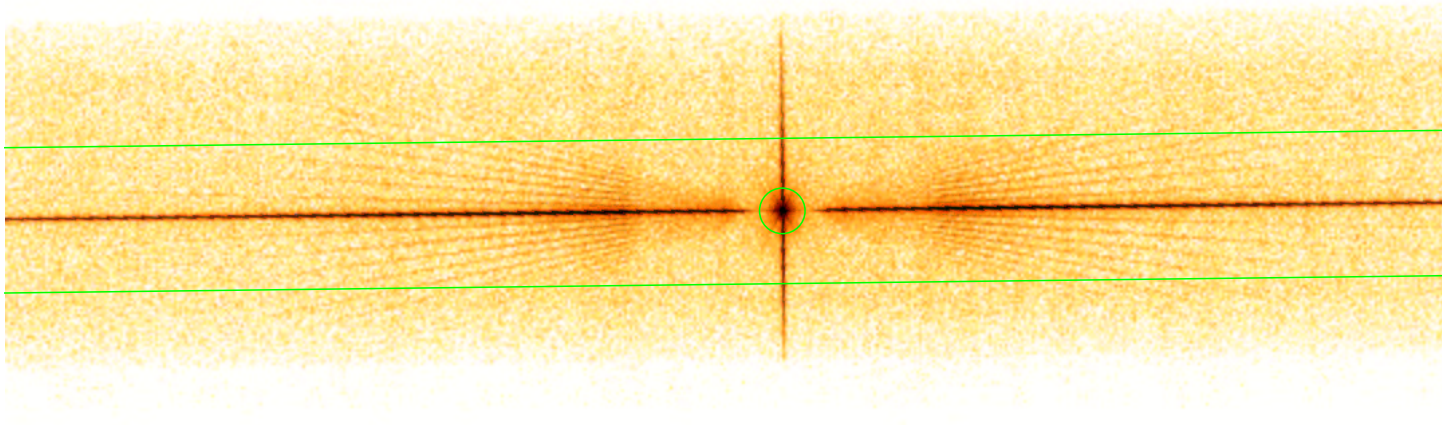
Capella with the HETG/ACIS-S detector:





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 $\pm$ order wavelengths will be offset from each other. (If this occurs, you may wish to reprocess with a new position measured by hand.)

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 data 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

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 ($\pm \Sigma_n \, i$ orders).

HRC/HETG Not a recommended configuration.

XMM/RGS By default 4 spectra are created, a 1st and 2nd order from each of two RGSs

For *Chandra* data, a single file (called a PHA Type II file) is output. This "PHA2" is a FITS format file that contains N rows of data, one for each spectral order. For the *XMM/Newton* RGS data, each spectrum is stored in a different file (a PHA Type I file). Both of these file types can be viewed with **prism** or *fv*, and has a relatively simple format. Other standard outputs are the grating arf ("garf") which stores the effective area of the detector and the grating rmf ("grmf") which tabulates the line shape as function of wavelength. These are also FITS files.

Grating spectra can be forward-fit to a model, just as lower resolution X-ray data are fit. Or, each PHA can be extracted and divided by the ARF to create a fluxed spectrum, which can be fit using any fitting program. When doing this, however, **DO NOT** ignore the line-shape; this will lead to systematic underestimation of the line flux!

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
```

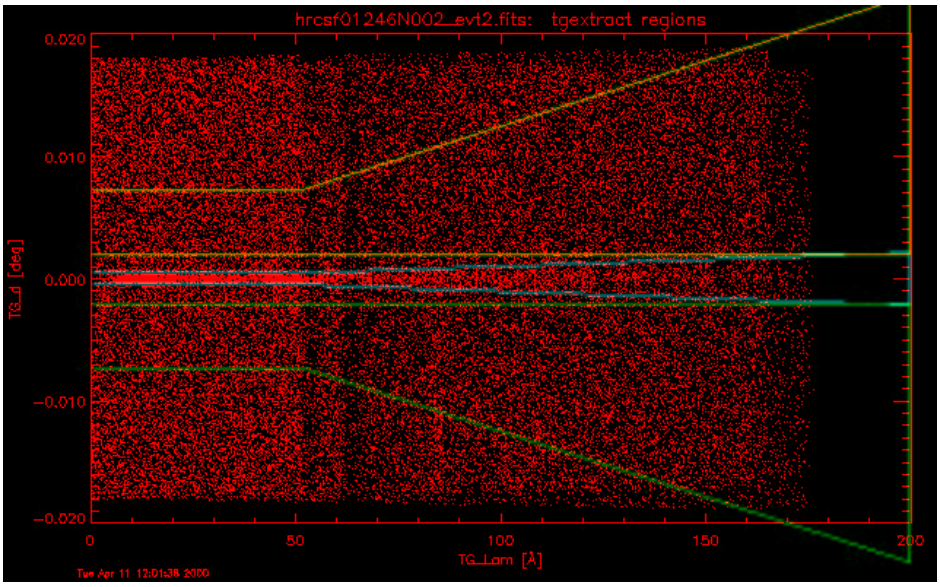
Now make the RMF

```
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
```

Again: 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 it can be large in the RGS as well.



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 different gratings, such as 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:

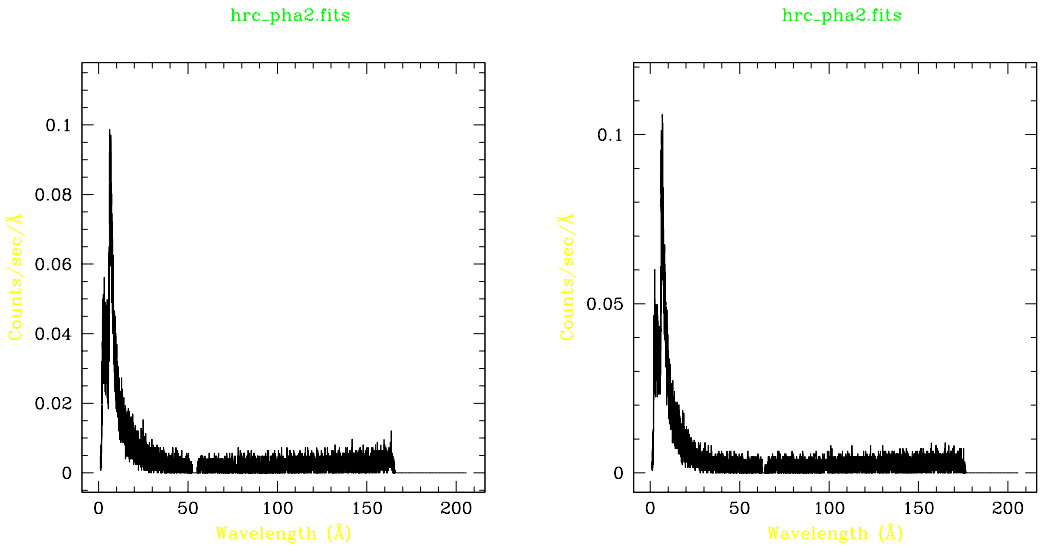
Adding together plus, minus orders

```
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

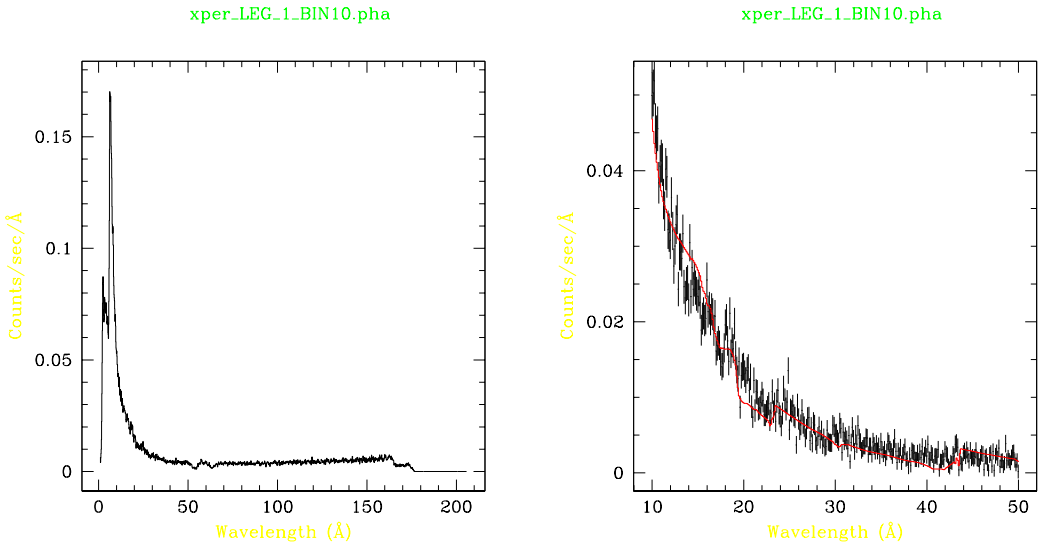
```
add_grating_spectra pha1=2463_MEG_1_BIN10.pha
  pha2=459_MEG_1_BIN10.pha garf1=2463_MEG_1.arf

  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
```



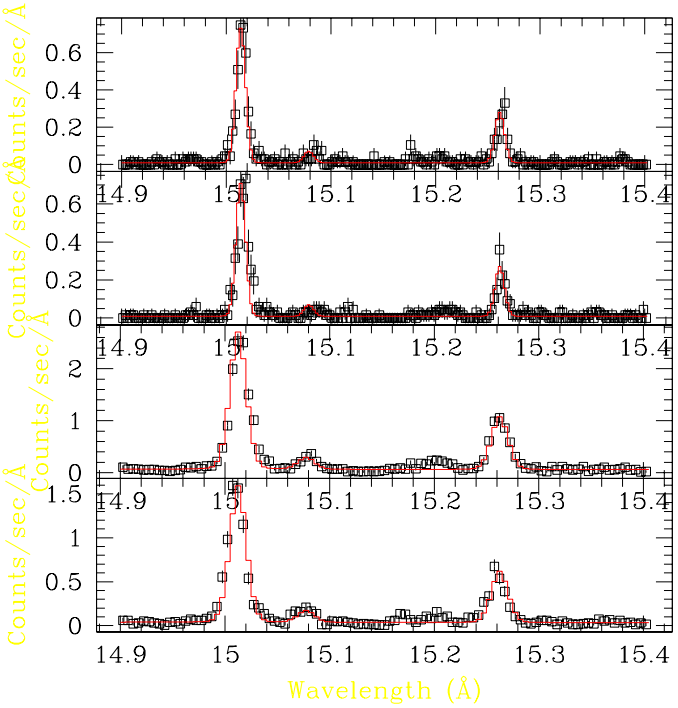
With low or moderate resolution data, forward-folding models and comparing to the data is the only analysis possible. With grating data, this becomes optional depending on the analysis needs. If the inherent resolution and line shape of the gratings is kept in mind (HEG: 0.012Å, MEG: 0.023Å, LEG: 0.05Å, RGS: $\sim$0.038Å), analysis of a fluxed spectrum using any tool may be 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 Angstrom	Flux ph/cm^2/s	Flux Error ph/cm^2/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	

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.
```

Lambda Angstrom	-- Ion	UL - LL	Approximate Emissivity@ ph cm^3/s	kT keV	RelInt	For More Info
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)

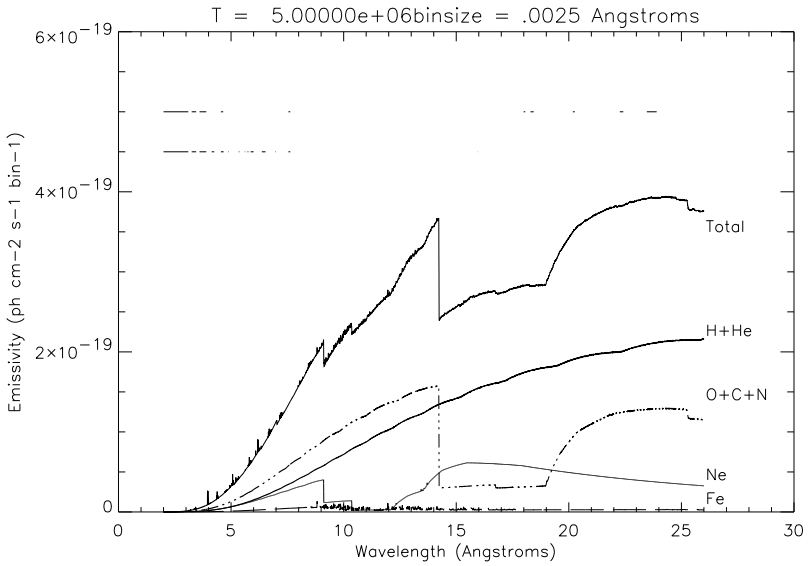
When faced with the task of understanding a high-resolution spectrum, especially a line-dominated one, it is likely that simple equilibrium models will not work adequately, despite possibly giving low reduced χ^2 values–usually because the counts/bin is low and so the errors are overestimated, not because the fits are good.

In this case, some new strategies are needed. Here are some suggestions for starting points.

First: Determine if your plasma is dominated by photoionization or collisional ionization. For example, the initial analysis of ASCA data of Cygnus X-3 used a collisional model, even though the emission is due to photoionization (see Liedahl & Paerels 1996)

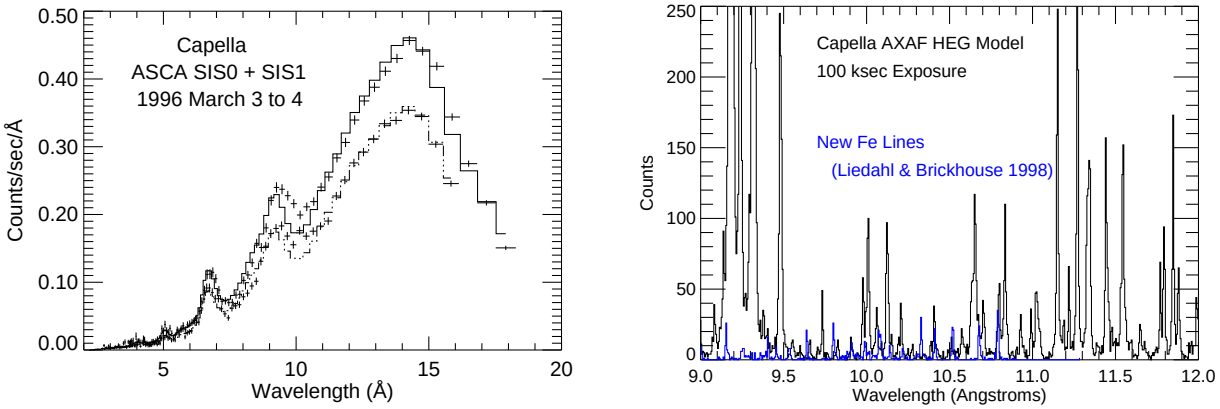
Make a list of all processes that could be affecting line emission. For example, in helium-like ions, the three dominant lines are the resonance, the forbidden, and the intercombination lines. These can be excited by direct excitation, radiative recombination, dielectronic recombination of hydrogen-like ions, innershell ionization of lithium-like ions, cascades from higher levels, or by photoexcitation or photoionization. Once created, the lines can be absorbed or scattered by like ions or by different ions. In many cases, simple physical arguments can be used to limit or exclude various processes, reducing the parameter space that must be searched. See the talk on atomic processes for more details.

Second: Attempt to determine the true continuum level with confidence. The continuum in a hot plasma is not necessarily dominated by bremsstrahlung, as shown here:



In addition, weak emission lines along with blending will make the continuum appear larger than it actually is, which will lead to a systematic underestimate of line fluxes, and therefore elemental and ionic abundances. After you have found an acceptable spectral model, search for regions in the model with no or few lines, and compare the model to the data in this region. If the model continuum overestimates the continuum here, it is likely it overestimates it everywhere due to unresolved line emission.

In some cases, the data may even show inadequacies in the atomic data. We show here Capella data from ASCA along with a best-fit model based on the ASCA plus EUVE data.



The upper figure shows the flux deficit near 10 Å in the ASCA spectrum of Capella (Brickhouse *et al.* 1998). The spectrum of Capella is shown, in simulation on the right. New iron lines are needed in order to fit the data. The new lines (in blue) betwen 9.5Å-10.5Å emit a total of 540 counts, compared to a total of 1820 counts using the best fit model. The new lines account for 23% of the emission in this small band.

In an observation with fewer counts, these weak lines may be entirely unresolvable. But they are present, and so even CCD-resolution spectra can highlight problems with atomic data. In this case, the best-fit model was tightly constrained by EUV observations. In the abscence of other checks, the entire spectrum should be used to confirm the model, paying especial attention to the continuum and to line shapes–since, for example, satellite lines may be easily confused with a red-shifted emission component.

- 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.
- A number of new facilities for atomic data analysis have been created for Sherpa and XSPEC 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
- Global fitting of generic equilibrium may be useful for guiding the analysis, but any project should begin with a physics-based approach, followed ideally by a line-based analysis and finally by checking regions which should well-understood (such as line-free areas or those dominated by a single line).