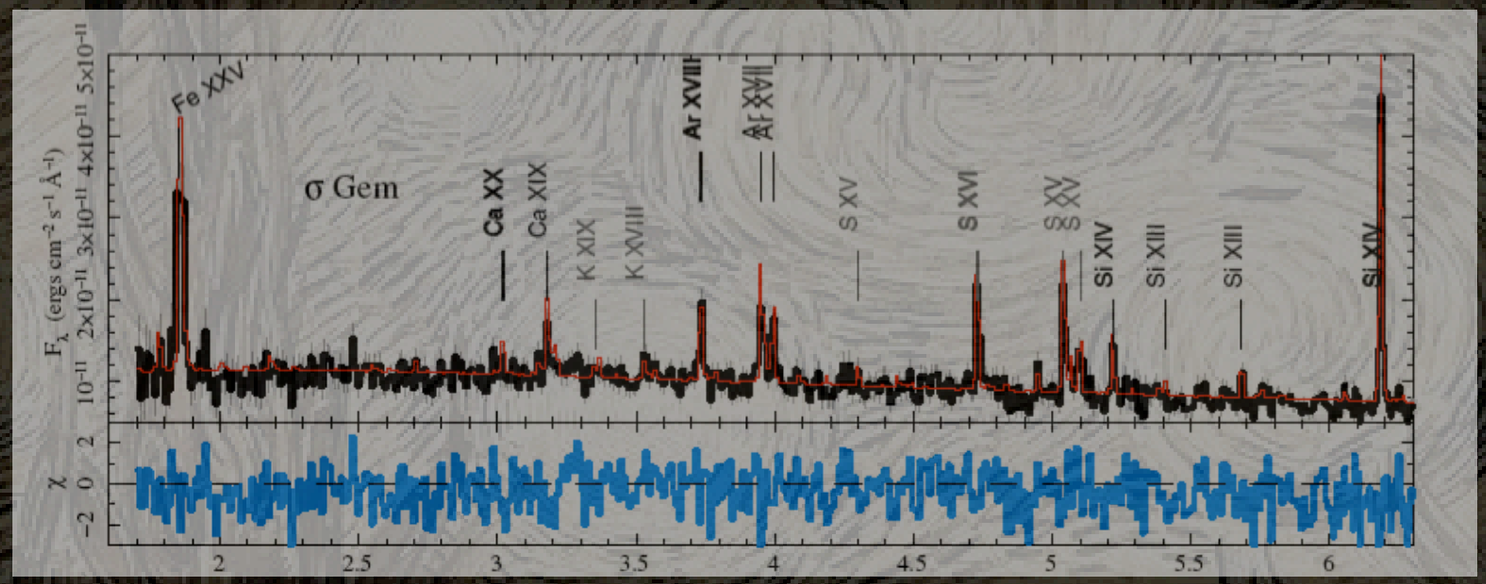
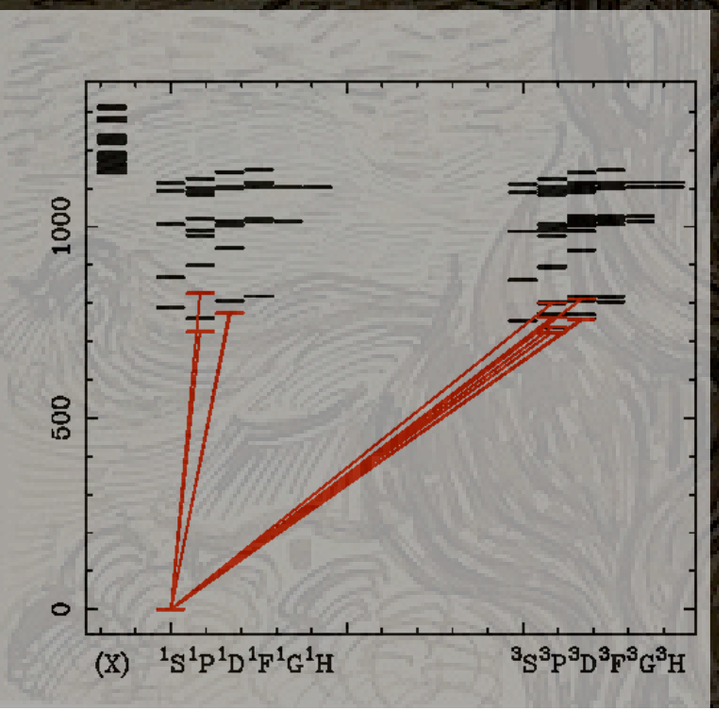
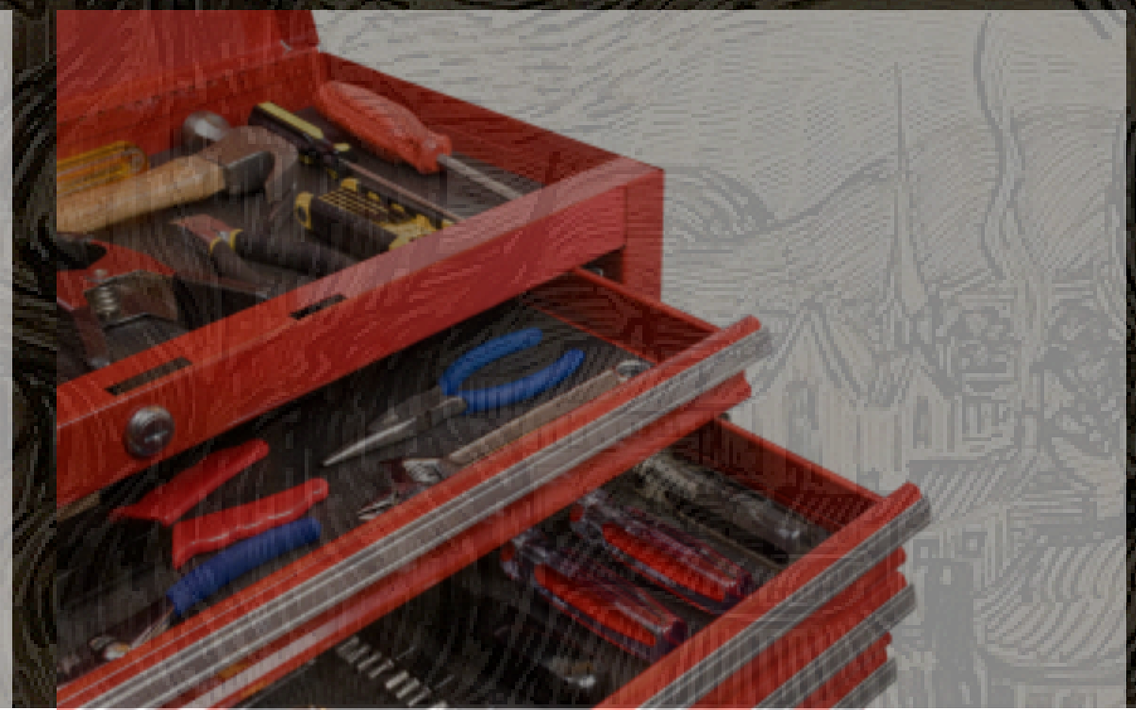
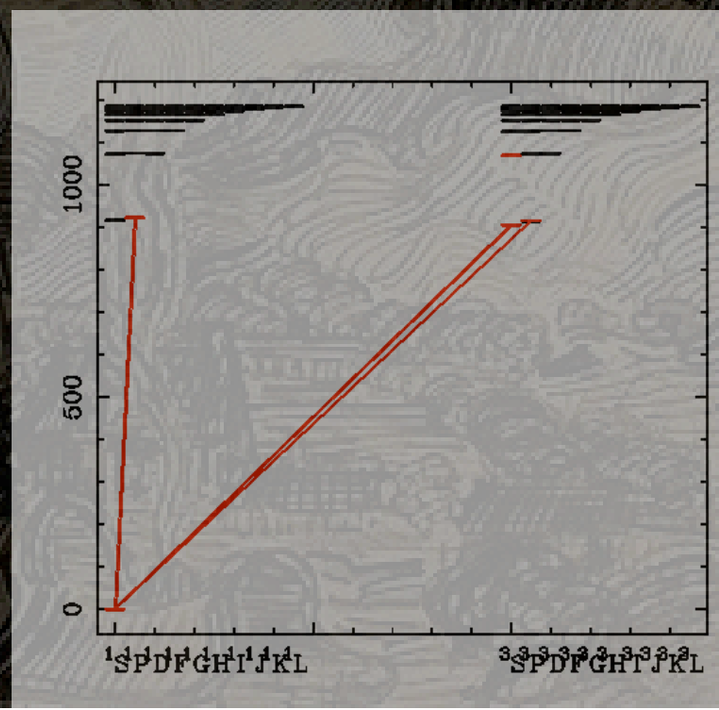
Database browsing, scripting, and spectral modeling

David Huenemoerder / MIT
(with help from John Houck, Norbert Schulz, Mike Nowak, John Davis)







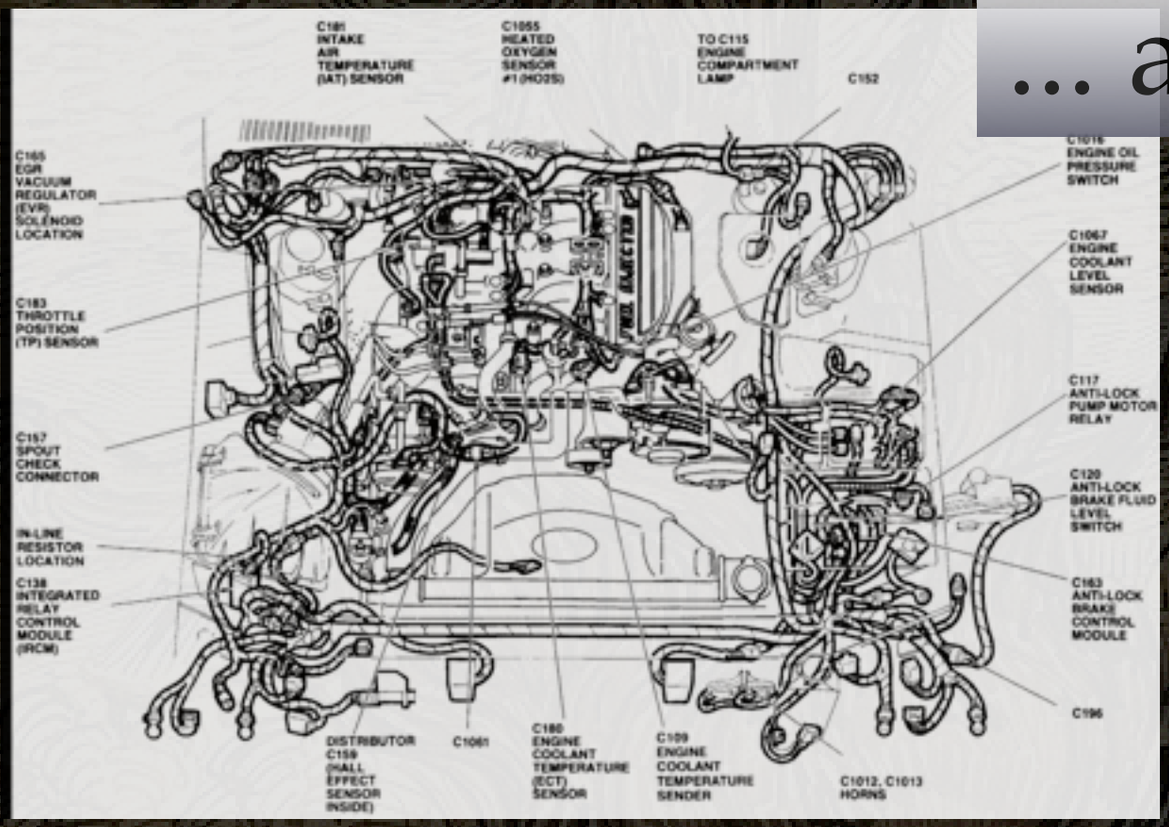


Traditional “global” spectral modeling (the hammer):

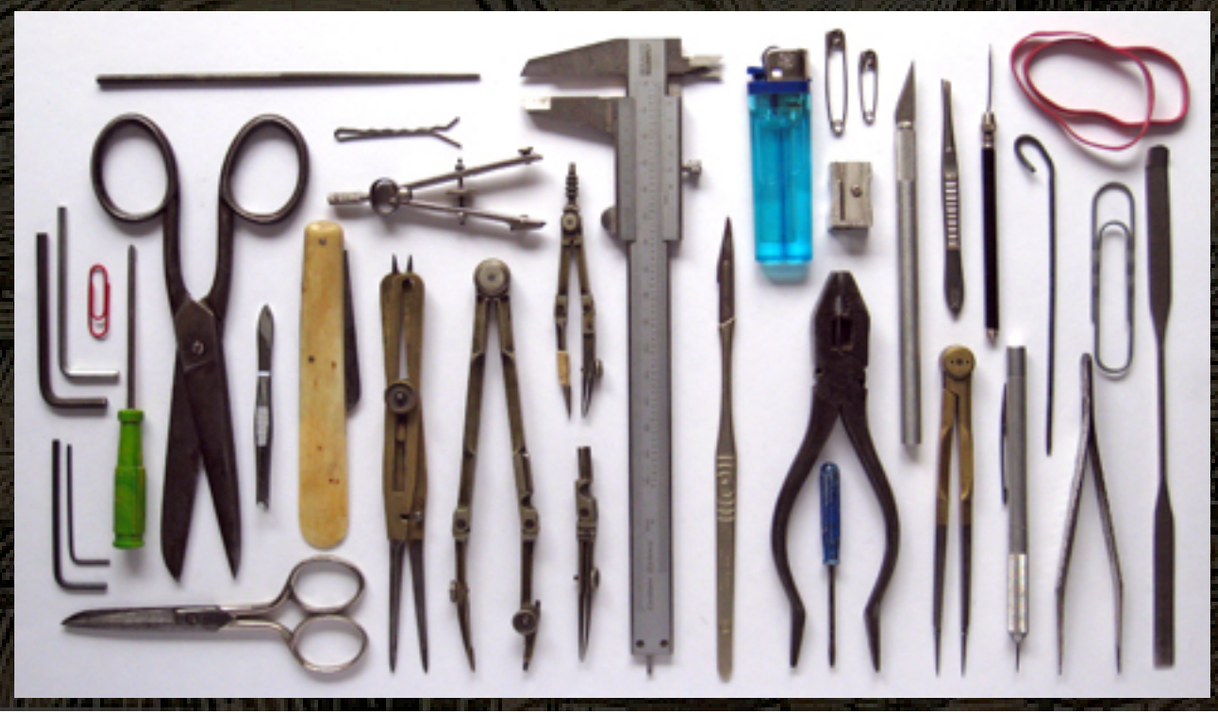
- define a model
- set the parameter guesses
- fit (minimize a statistic) to obtain a model spectrum (best-fit parameters)
- compute parameter uncertainties (which might take a very long time)

Necessary, but not sufficient!

Sometimes, you need to get under the hood,



... and you need more tools



What's in a (simple thermal, CIE: Collisional Ionization Equilibrium) spectral model?

flux at earth* [phot cm^{-2} s^{-1}]

elemental abundance

emissivity [phot cm^{3} s^{-1}]

volume [cm^{3}]

$$f_\lambda = e^{-N_H \sigma_\lambda} \frac{A_Z}{4\pi d^2} \int \Lambda_\lambda(T) n_e^2 dV(T)$$

Atomic Data/Code

Emission Measure (plasma model)

foreground column density and bound-free cross-section

geometric dilution

electron number density [cm^{-3}]

* Note: we have omitted the transformation from counts to flux through the instrumental response.

flux at earth*
[phot cm^{-2} s^{-1}]

elemental
abundance

$$f_\lambda = e^{-N_H \sigma_\lambda} f_c(\lambda)$$

Atomic Data/Code

foreground
column density
and bound-free
cross-section

* Note: we have omitted the transformation from counts to flux through the instrumental response.

A photoionized absorption spectrum can be expressed similarly:

THE ASTROPHYSICAL JOURNAL, 708:981–994, 2010 January 10 doi: 10.1088/0004-637X/708/2/981

X-RAY ABSORPTION ANALYSIS OF MCG –6-30-15: DISCERNING THREE KINEMATIC SYSTEMS

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AMD analysis in order to obtain the total hydrogen column density N_H along the line of sight. The AMD can be expressed as

$$\mathrm{AMD} \equiv \partial N_H / \partial(\log \xi) \quad (3)$$

and

$$N_H = \int \mathrm{AMD} d(\log \xi). \quad (4)$$

The relation between the ionic column densities $N_{\rm ion}$ and the AMD is then expressed as

$$N_{\rm ion} = A_z \int \frac{\partial N_H}{\partial(\log \xi)} f_{\rm ion}(\log \xi) d(\log \xi), \quad (5)$$

where $N_{\rm ion}$ is the measured ion column density, A_z is the element abundance with respect to hydrogen taken from Asplund et al. (2009) and assumed to be constant throughout the absorber, and $f_{\rm ion}(\log \xi)$ is the fractional ion abundance with respect to the total abundance of its element. Here, we aim at recovering the AMD for MCG –6-30-15

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we identify
-15, and one
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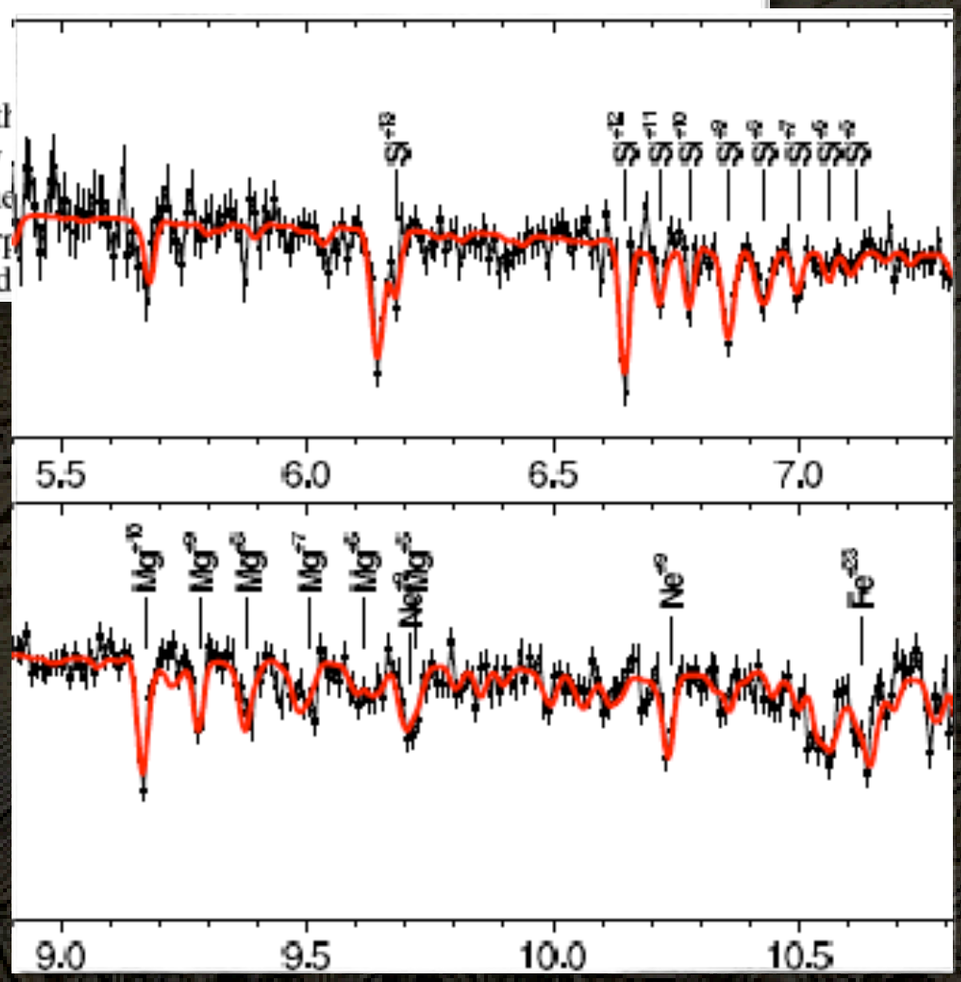
n measure d



measurement

plasma model

atomic data (or ion fractions derived therefrom)

Using ISIS as an interactive, scriptable AtomDB browser, calculator, & spectral modeler.

"ISIS, the Interactive Spectral Interpretation System, is designed to facilitate the interpretation and analysis of high resolution X-ray spectra. It is being developed as a programmable, interactive tool for studying the physics of X-ray spectrum formation, supporting measurement and *identification of spectral features*, and *interaction with a database of atomic structure parameters and plasma emission models*."

Main web page: **<http://space.mit.edu/cxc/isis>**

Reference: Houck & deNicola (2000)

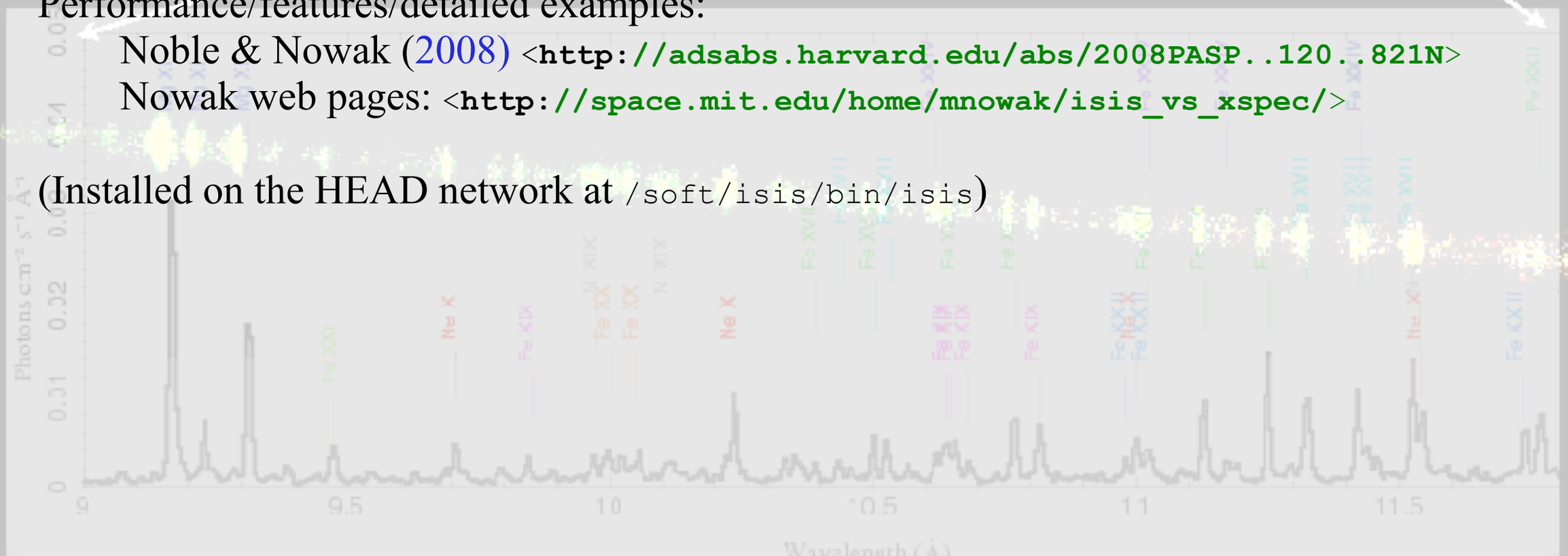
<**http://adsabs.harvard.edu/abs/2000ASPC..216..591H**>

Performance/features/detailed examples:

Noble & Nowak (2008) <**http://adsabs.harvard.edu/abs/2008PASP..120..821N**>

Nowak web pages: <**http://space.mit.edu/home/mnowak/isis_vs_xspec/**>

(Installed on the HEAD network at `/soft/isis/bin/isis`)



Two general features are useful for spectral modeling:

1. After spectral model evaluation, *KEEP* pointers to the atomic data used;

2. Provide (model independent) low-level interfaces to the atomic data

Simple example: after a 4-T global fit, query AtomDB for the actual lines in the model contributing to the spectrum:

Accepted for publication in the Astrophysical Journal.

Multiwavelength Observations of the SS 433 Jets

Herman L. Marshall[1], Claude R. Canizares[1], Todd Hillwig[2], Amy Mioduszewski[3], Michael Rupen[3], Norbert S. Schulz[1], Michael Nowak[1], Sebastian Heinz[4]

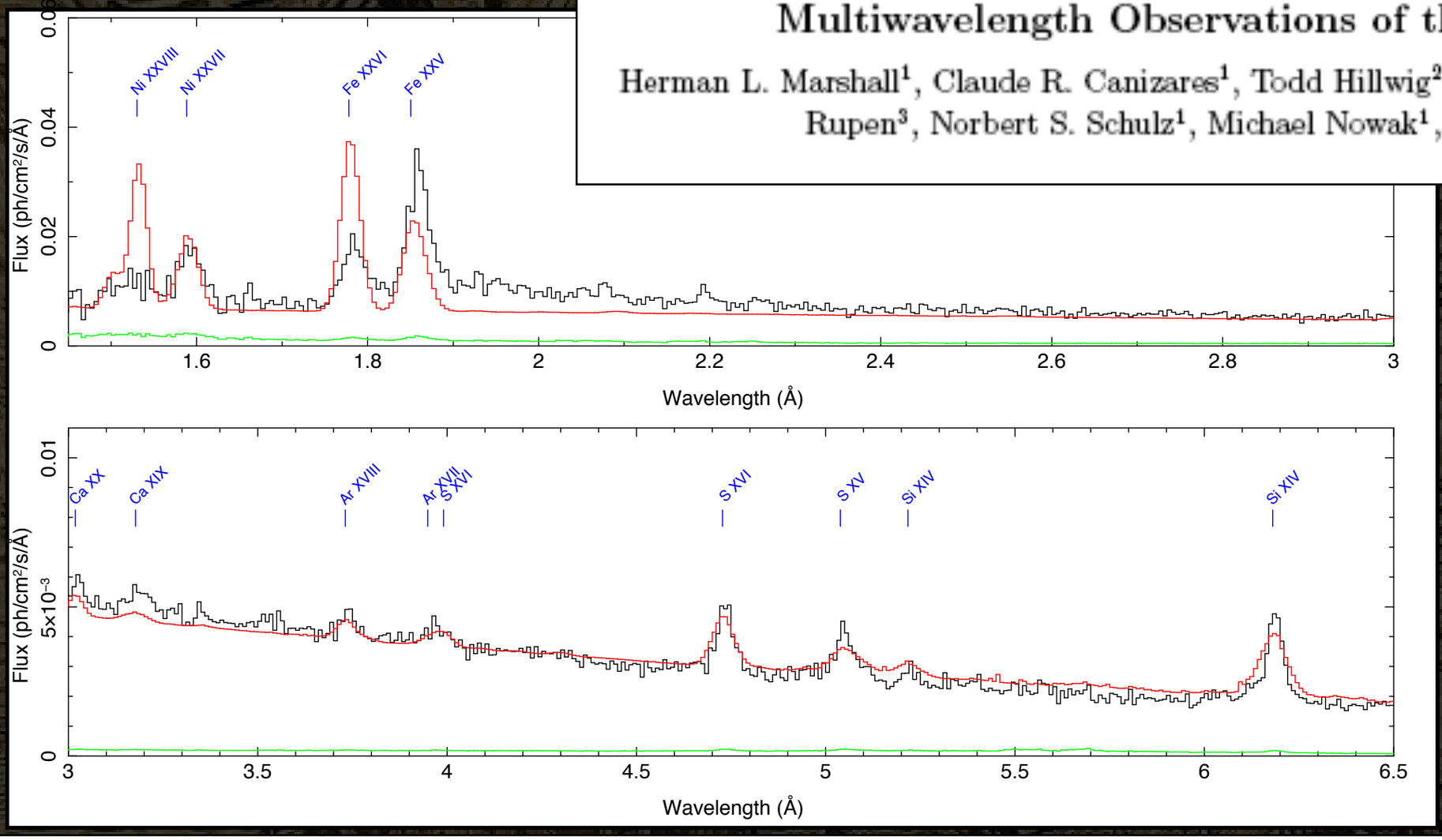
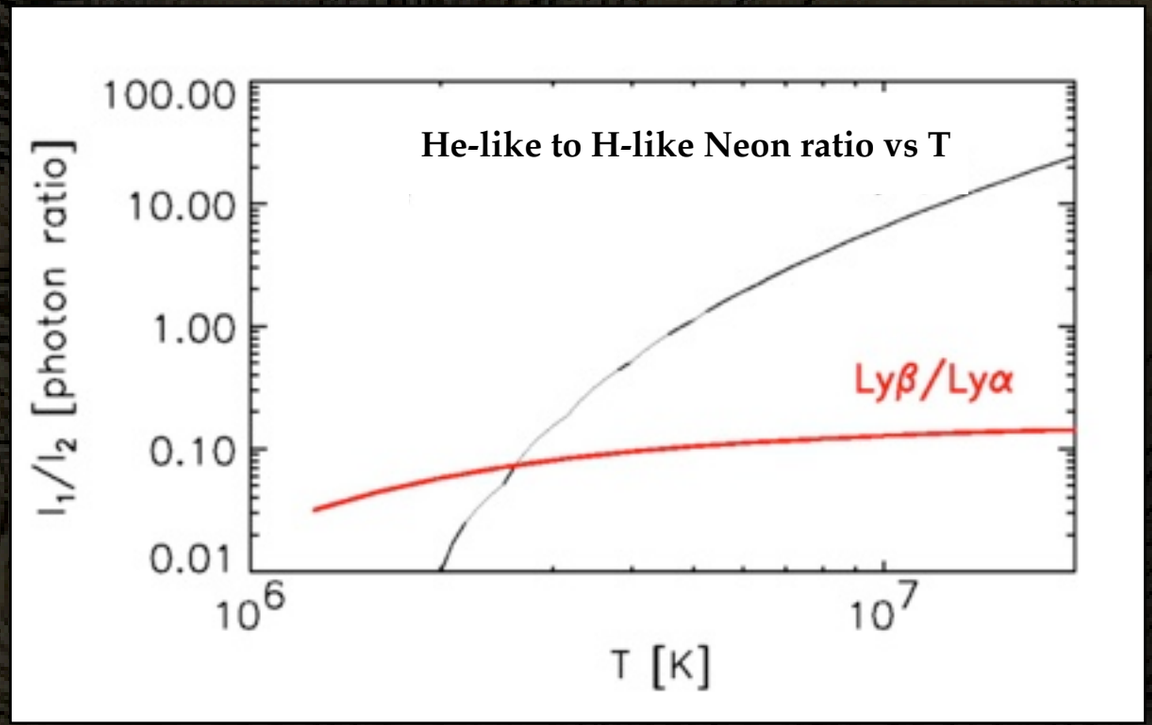


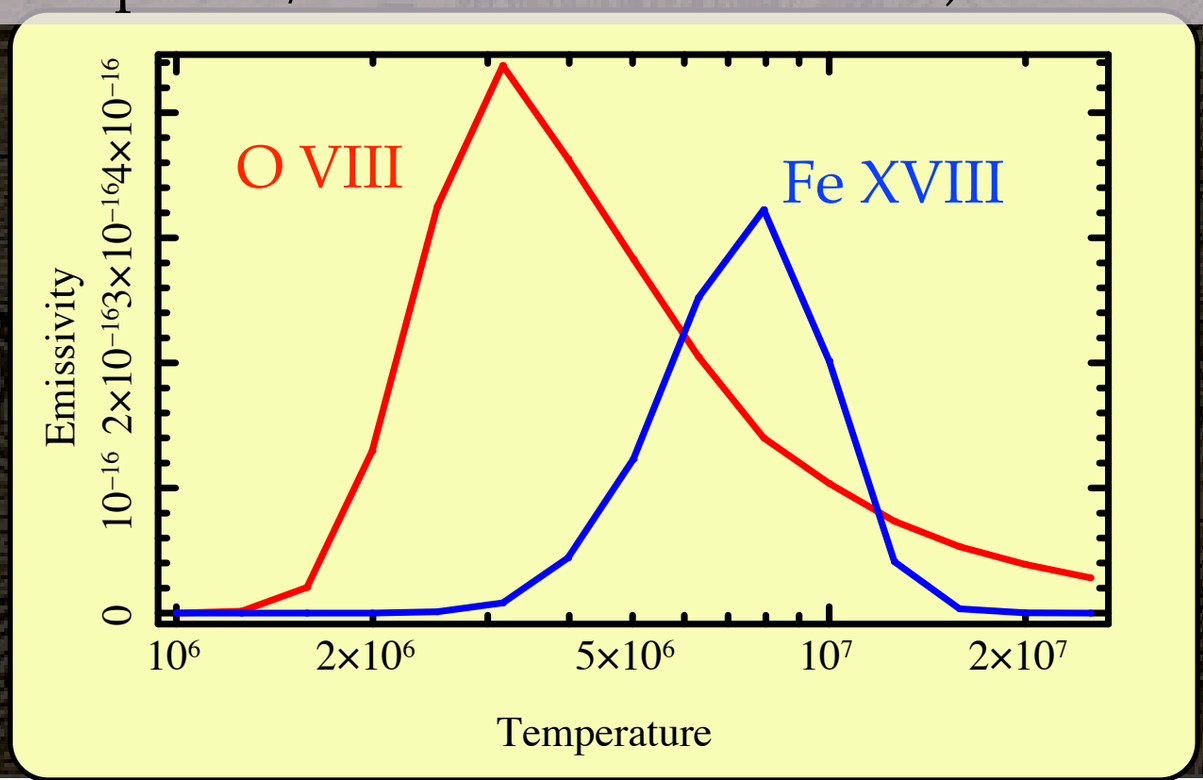
Fig. 13.— X-ray spectrum formed from the HEG data (top panel only) or combining the HEG and MEG data after correcting for the Doppler shift of the blueshifted jet. *Green line:* Statistical uncertainties in the flux measurements. *Red line:* Four temperature plasma model providing a generally adequate fit to the spectrum. Residuals near 2 Å are primarily due to the redshifted jet's continuum, which is somewhat weaker than those of the blueshifted jet. Line identifications are labeled where there are features in the spectrum and confirmed by the model.

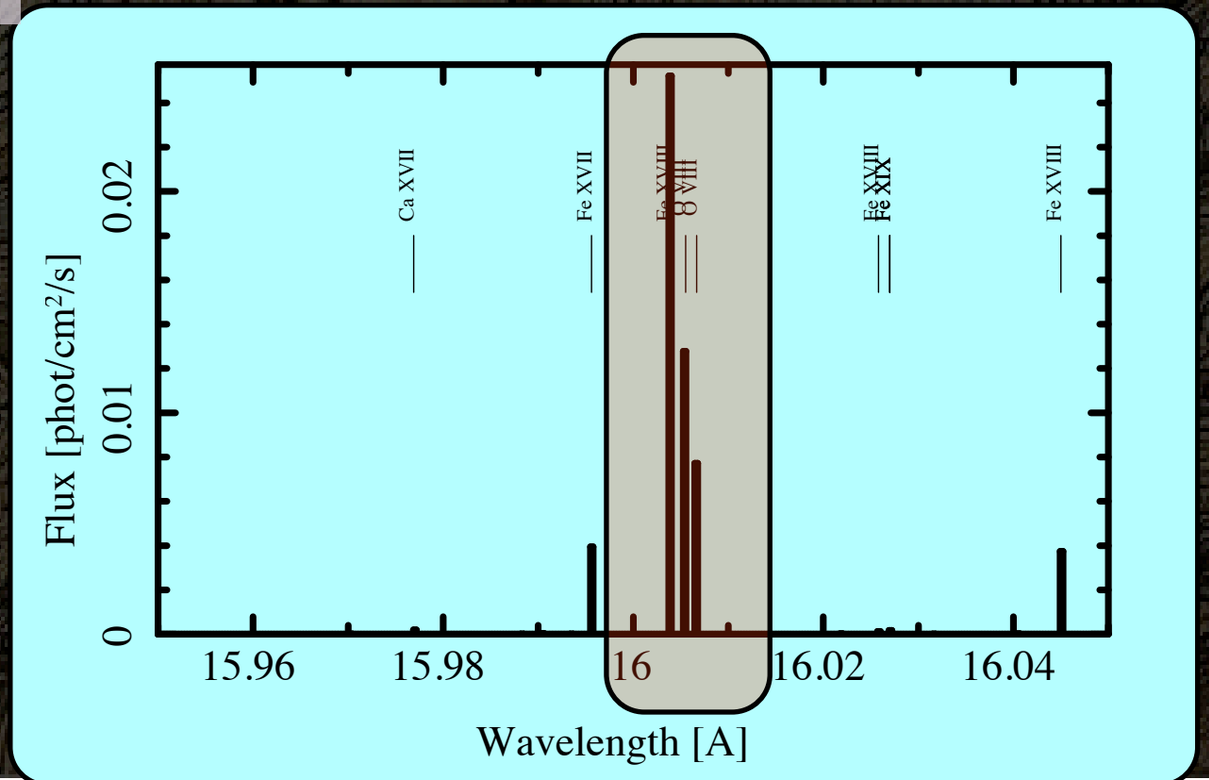
Low-level interfaces, Direct data access:

Why provide low-level interfaces?
To support very general types of analysis:

- Direct line-ratio diagnostics (for temperature, opacity, and density sensitivity);
- Sleuthing features by attributes (e.g., same upper level), or by ion state;
- Assessing unresolved blends;
- Emission measure analysis, using line strengths, database emissivity (and modeling/fitting infrastructure from your scriptable/extensible environment)







Line-Based Analysis

$$L_{ul}(Z,J) = \int \Lambda_{ul}(T;Z,J)\,(A(Z)[n_e n_H dV/dT])\;dT$$

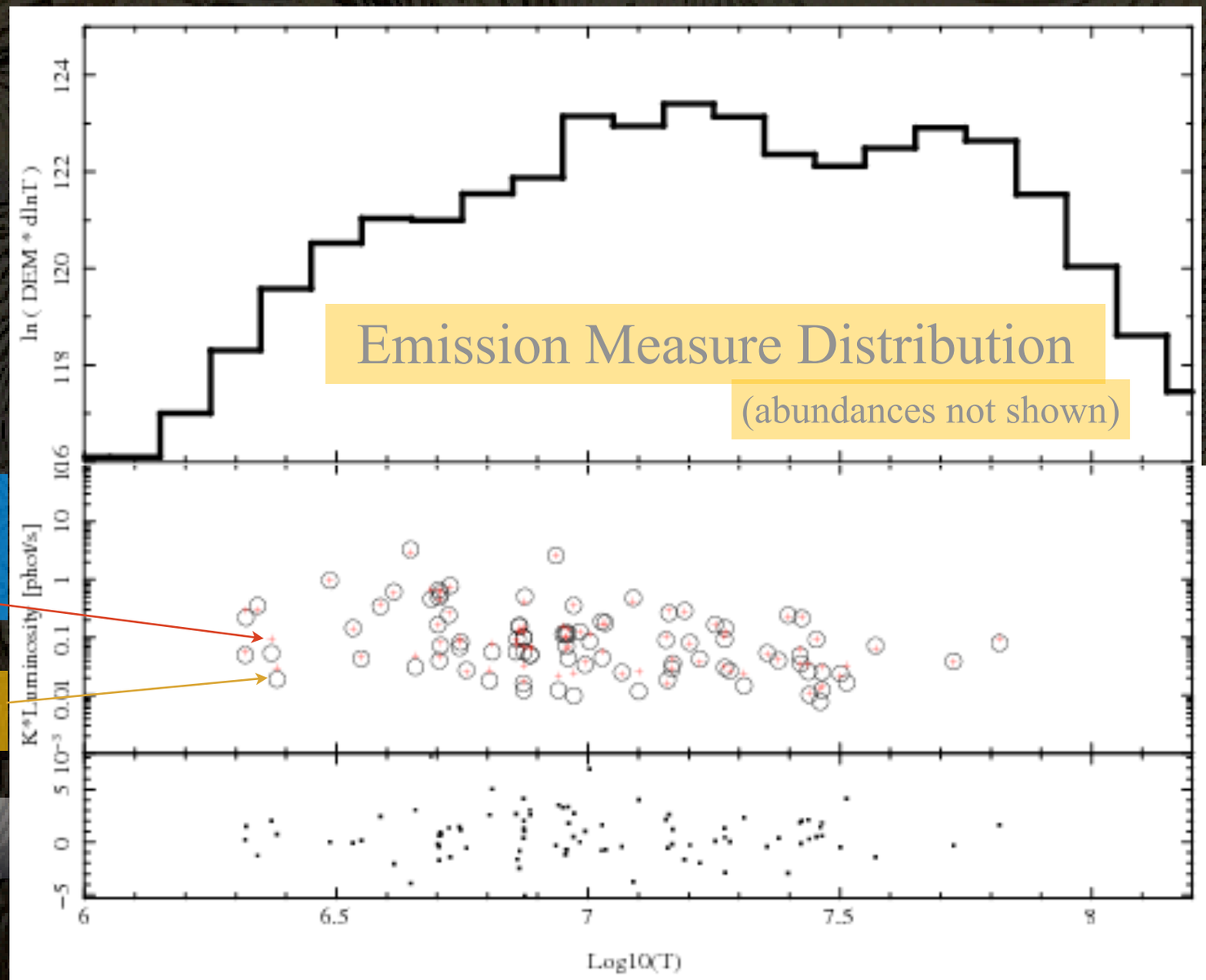
Line Luminosity | Emissivity | Model

AtomDB provides emissivities for each line.

Each small dot is a line flux measurement (parametric fit)

Each circle is a model line flux

(residuals)



Mis-IDs (large wavelength residuals) and blends (large flux residuals) iteratively removed.

e.g., σ Gem spectral models:

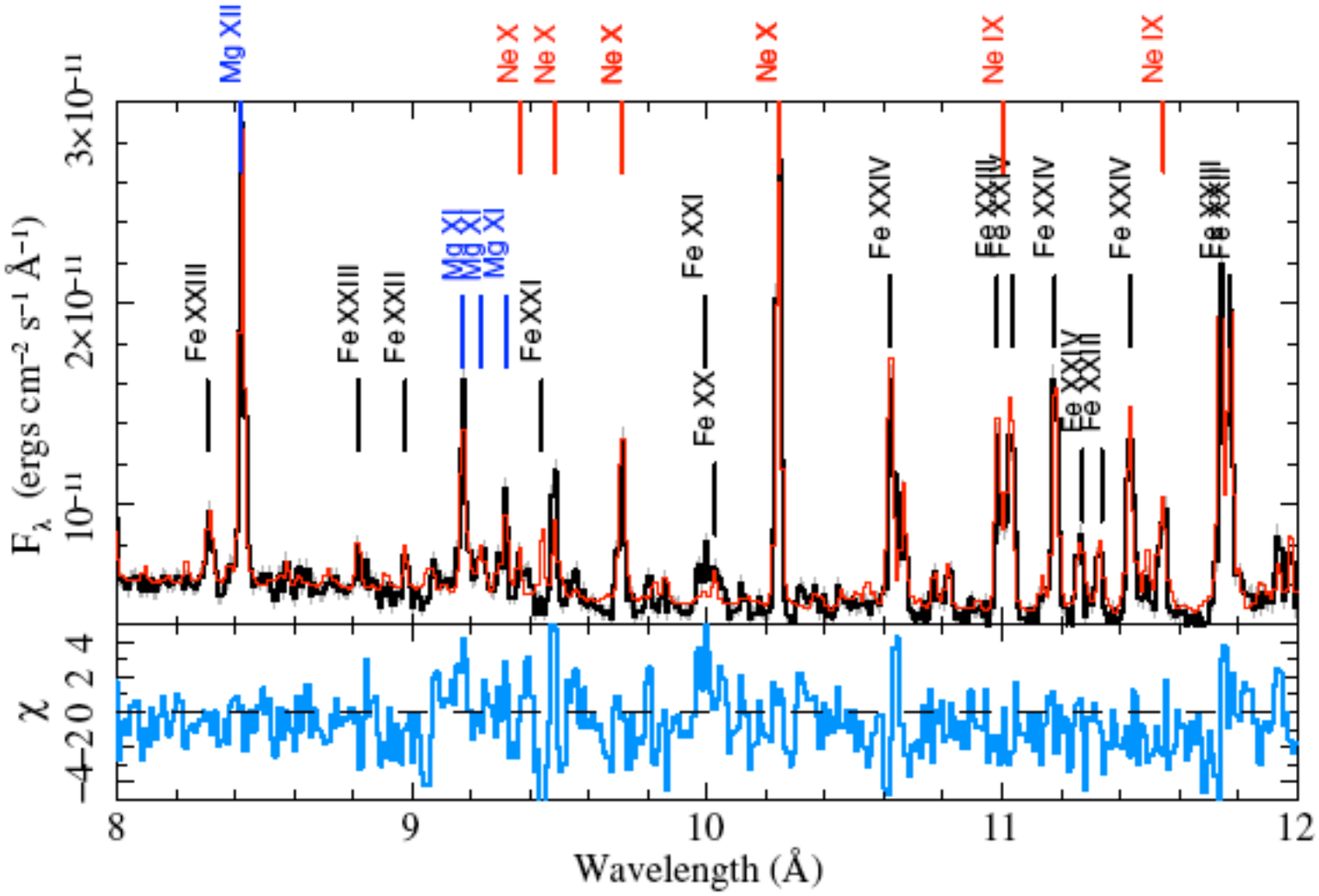
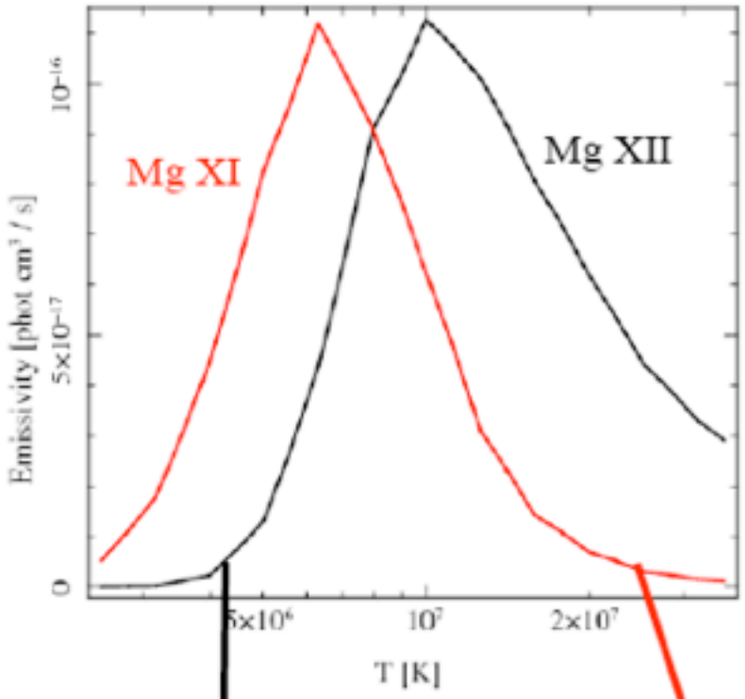


Figure 7

Example: Simple Line-Ratio Temperature Diagnostic




```
% Get AtomDB indices for Mg XI r and Mg XII H-Ly-alpha lines:

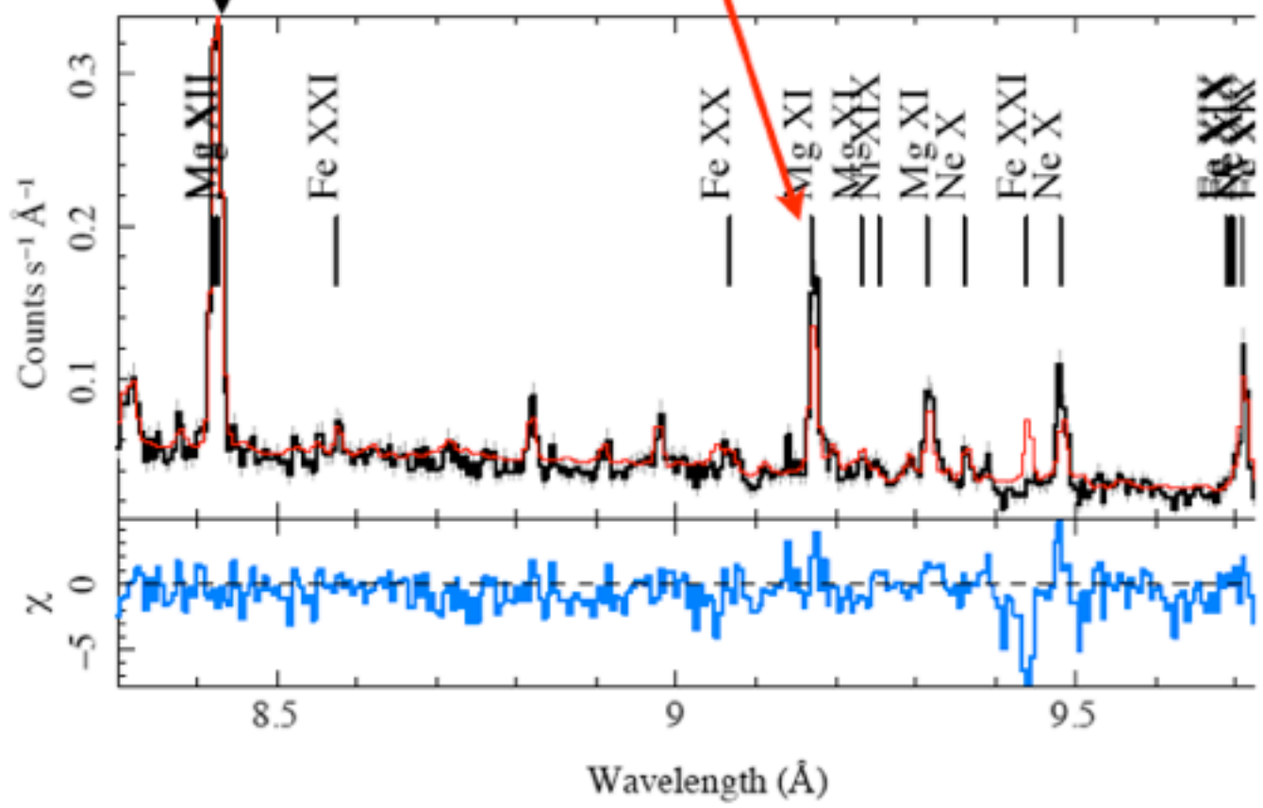
k1 = where( trans( Mg, 11, 7, 1 ) ) ;
k2 = where( trans( Mg, 12, [3,4], 1 ) ) ;

t = 10^[ 6.4 : 7.6 : 0.05 ] ;   % Define a temperature grid

% evaluate the emissivities, and the ratio, vs T:

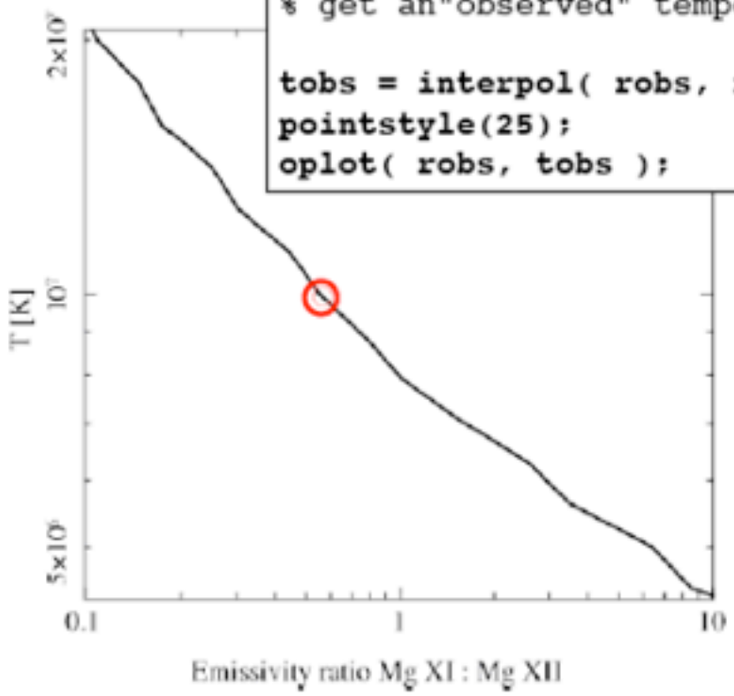
e1 = line_em( k1, t );
e2 = line_em( k2, t );
r12 = ratio_em( k1, k2, t );

% What is model's ratio?
f1 = line_info( k1[0] ).flux;
f2 = line_info( k2[0] ).flux + line_info(k2[1]).flux ;
f1/f2;
0.36    % a little less ("hotter") than isothermal value
```

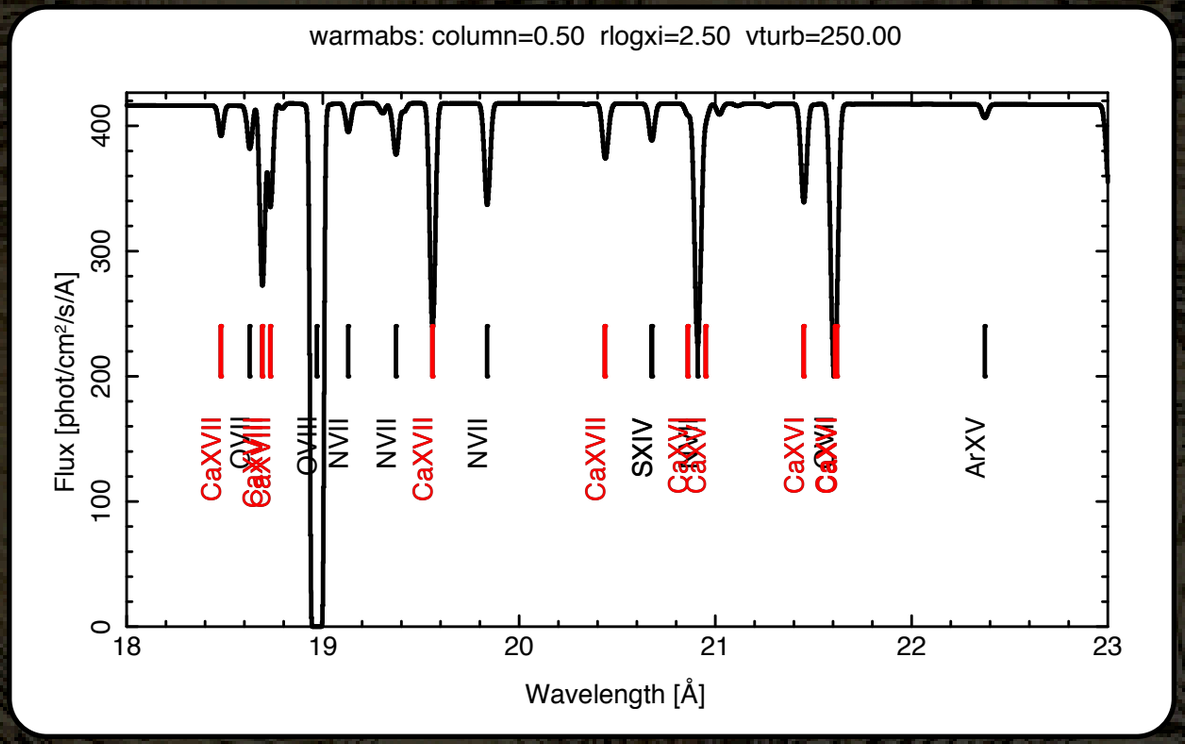


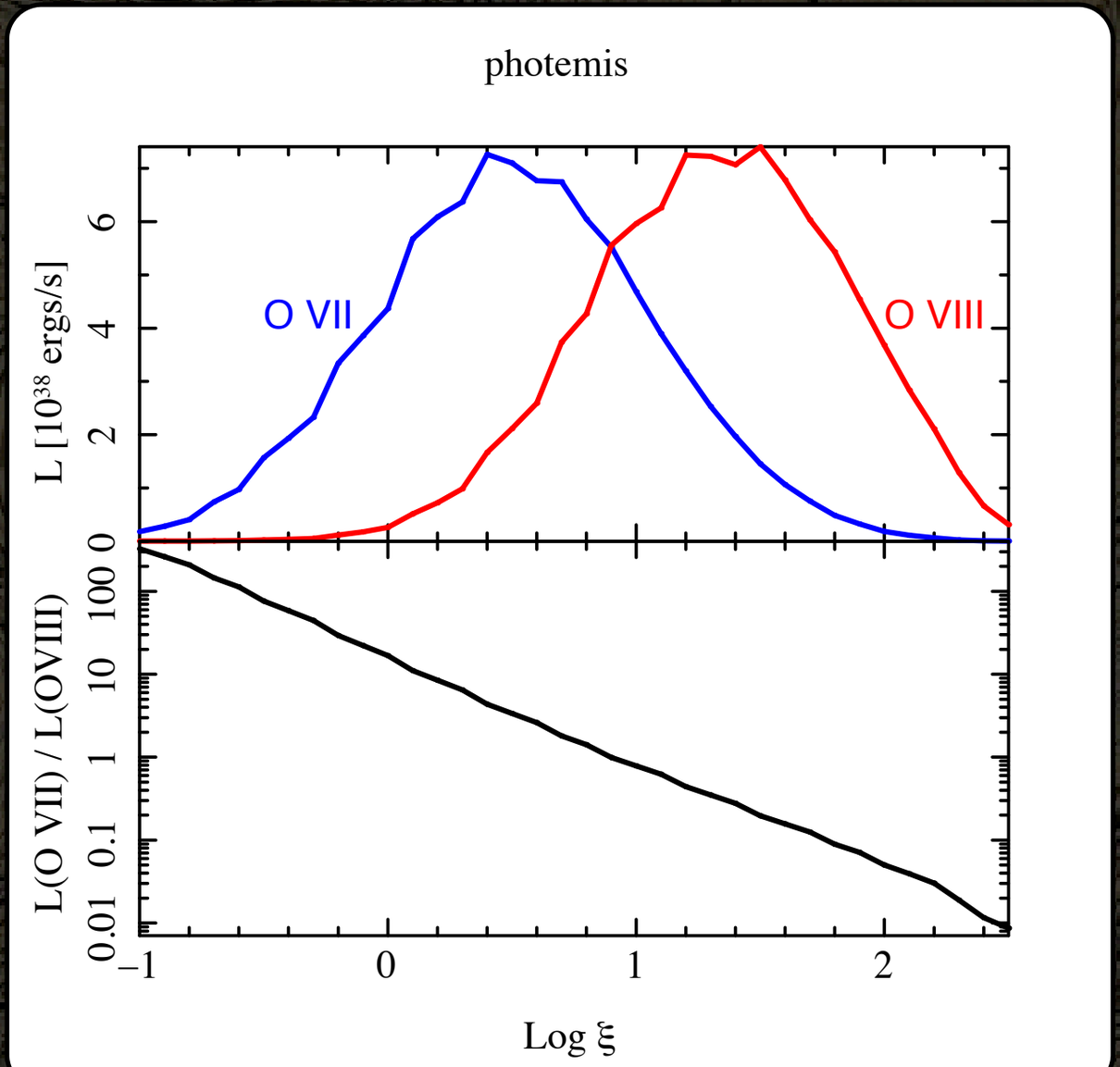

```
% interpolate the measurement to
% get an"observed" temperature:

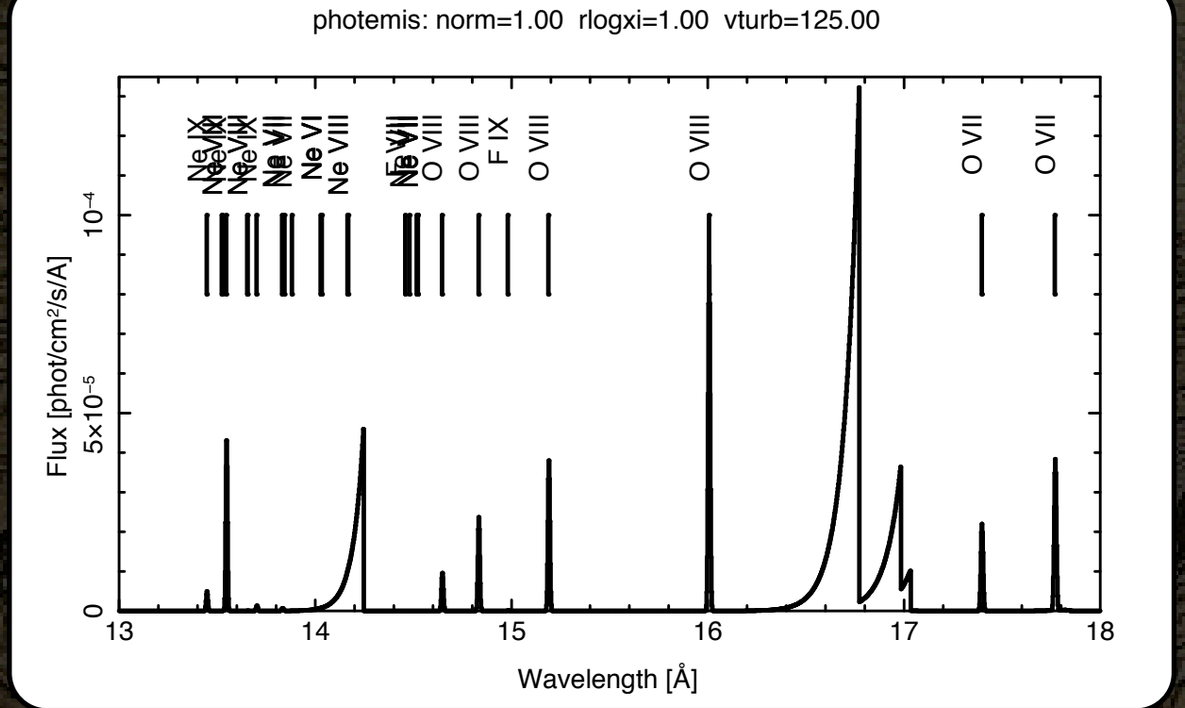
tobs = interpol( robs, r12, t );
pointstyle(25);
oplot( robs, tobs );
```



warmabs/photemis prototype examples



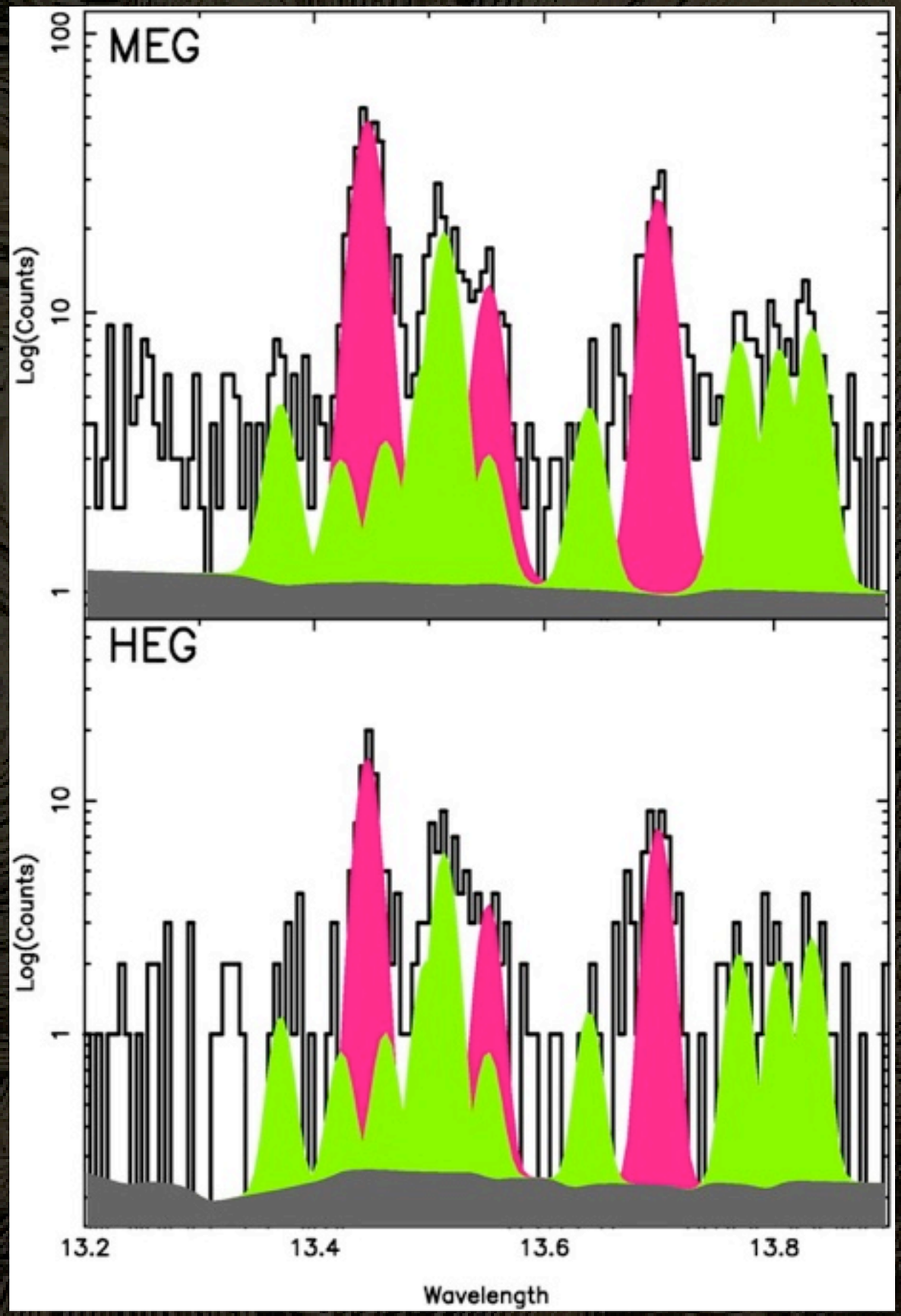




# id	ion	lambda	A[s^-1]	f	gl	gu	tau_0	W(A)	L[10^38 ergs/s]	label
64839	Ca XVII	18.480	2.674e+11	4.106e-02	1	3	5.990e-02	6.369e-02	0.000e+00	2s2 - 2s02p.3s
5687	O VII	18.627	9.333e+11	1.456e-01	1	3	9.128e-02	1.001e-01	0.000e+00	1s2.1S - 1s.3p.1P*
64914	Ca XVIII	18.691	2.311e+12	2.420e-01	2	4	4.290e-01	3.983e-01	0.000e+00	1s2.2s - 1s2.3p
64927	Ca XVIII	18.732	2.358e+12	1.240e-01	2	2	2.203e-01	2.187e-01	0.000e+00	1s2.2s - 1s2.3p

Example of model evaluation by components:

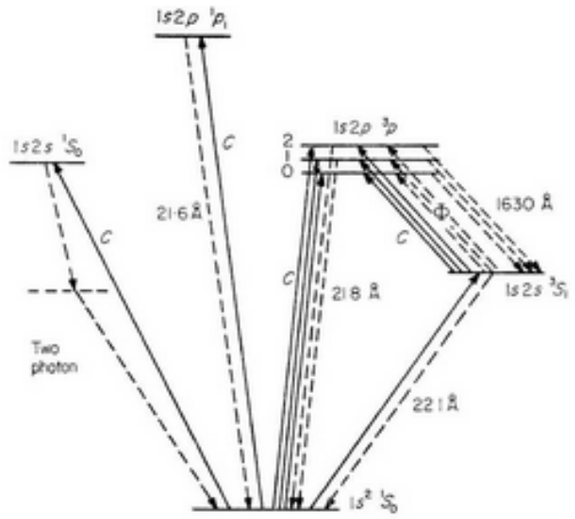
- Ne lines (pink),
- Fe lines (green),
- continuum (gray);

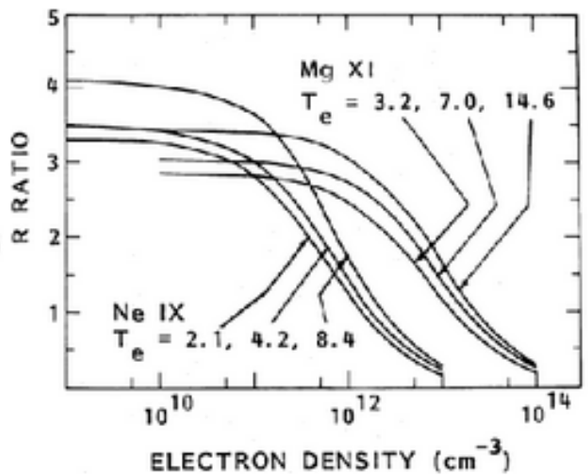


Flexibility, extensibility example

space.mit.edu/cxc/analysis/he_modifier/index.html

He-like Ion Line Emissivities for X-Ray Spectral Modeling





(From Gabriel and Jordan 1969 MNRAS 145, 241; Wolfson et al 1983 ApJ 269, 319)

Emissivity Modifier for He-like triplets

The He-like triplet lines which occur in the X-ray band from 4-42 A are powerful diagnostics of density or photoexcitation. The APED (Astrophysical Plasma Emission Database), however, only contains emissivities for low density.

To provide better support for more *direct fitting and modeling within a data-analysis enviroment*, we have

- constructed tables of coefficients which parameterize the electron density dependence of the triplet lines' collisionally excited emissivities for a grid of temperatures, for several astrophysically important elements;
- written an ISIS plasma model interface to define and apply "emissivity modifiers" for the atomic database (APED), which can be used directly in X-ray spectral modeling and fitting;
- constructed similar coefficients tables using Chianti (Dere et al., 1997 A&AS, 125, 149; Dere et al., 2009, A&A 498, 915) emissivities;
- constructed a coefficients table for photoexcitation-dominated triplet emission (also using Chianti) in which the independent parameter is photon energy density (further controlled by a dilution factor).

ISIS' "emissivity modifier" allows one to change the emissivity for any line, here to implement He-triplet density dependence *without* having the entire AtomDB density-dependent database.

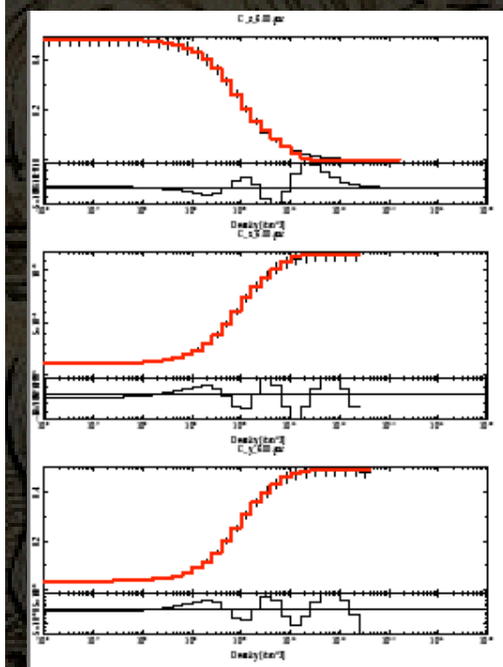
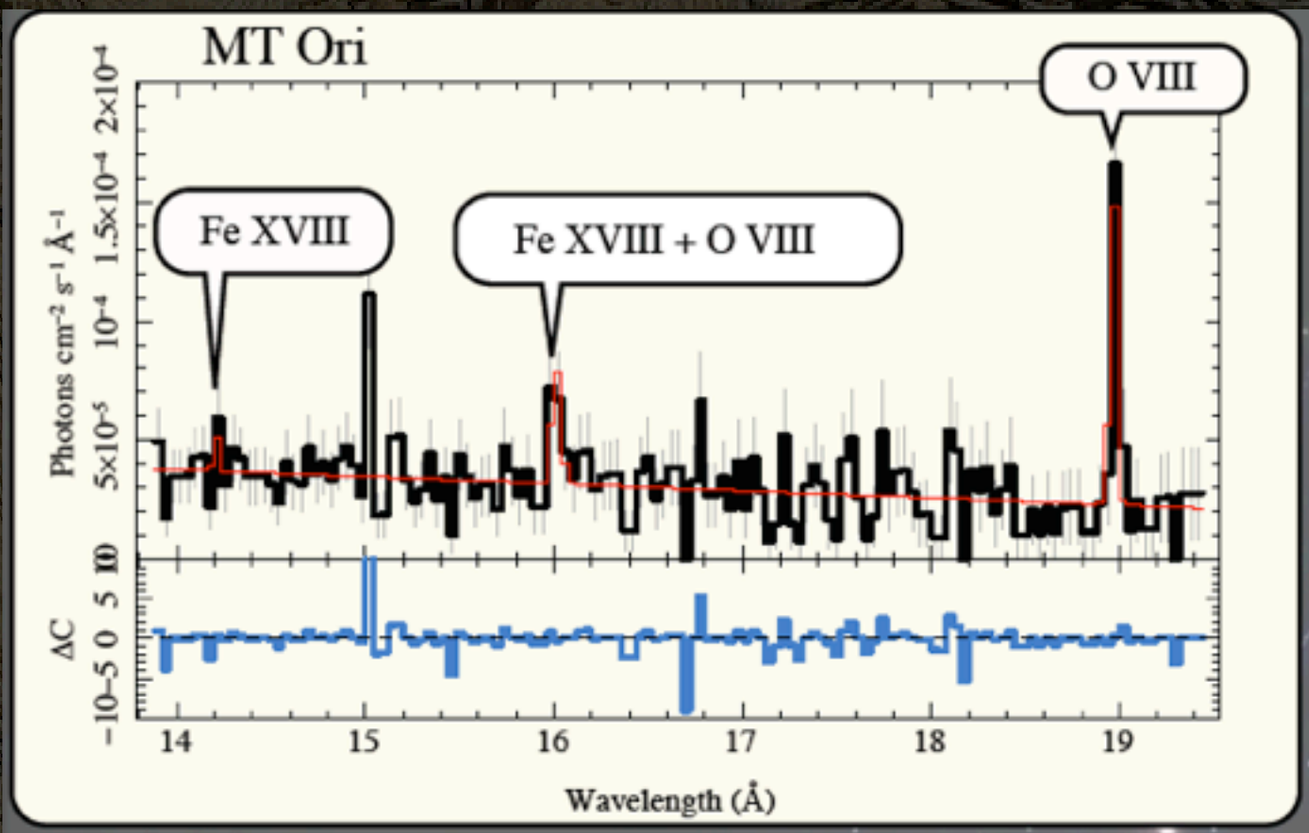


Figure 3: Example fit of the emissivities of z (top), x dle), and y (bottom) for log 6.00. The red curve is the the underlying black histo and below are the resi

Table 1: FITS file Block Structure

No.	Name	Type	Dimensions
1	PRIMARY	Null	
2	he_coefs_C	Table	5 cols x 56 rows
3	he_coefs_N	Table	5 cols x 56 rows

Solving for N_H (degenerate in low-res spectra)



Know:

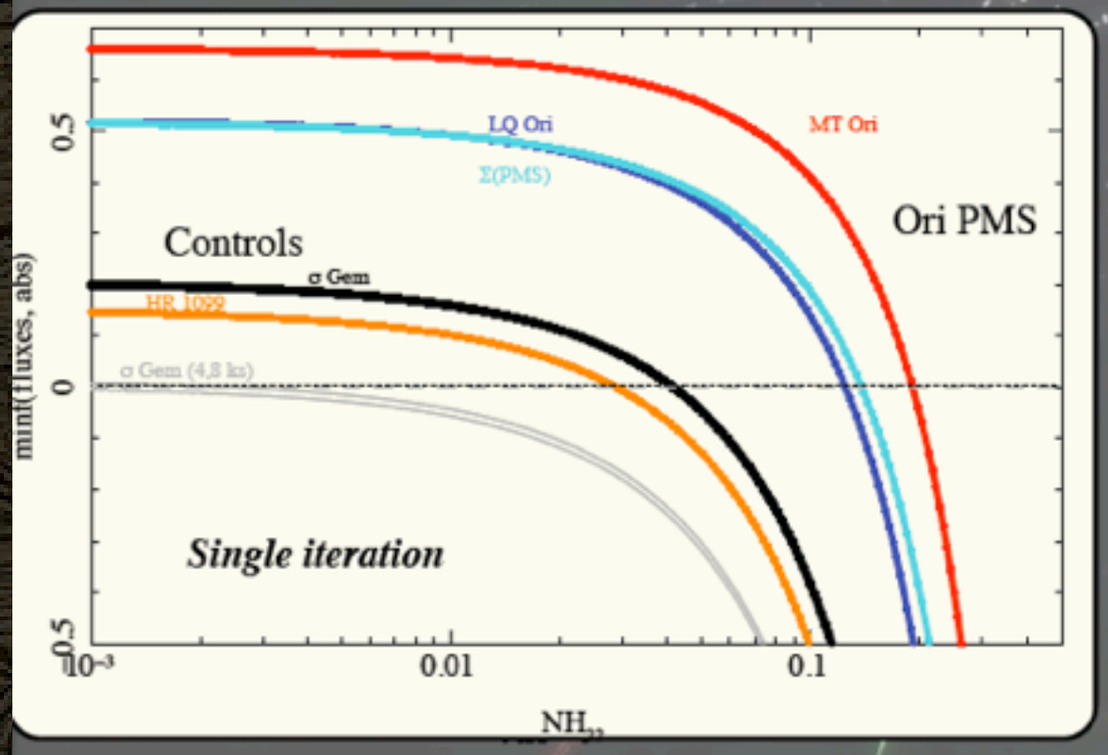
- ★ 3 measured fluxes (with unknown absorption)
- ★ Fe XVIII ratio (from atomic data)
- ★ O VIII ratio (from atomic data)
- ★ absorption function vs N_H

Can write 5 equations with 5 unknowns (the unabsorbed flux for 4 lines, and N_H) => solve for N_H

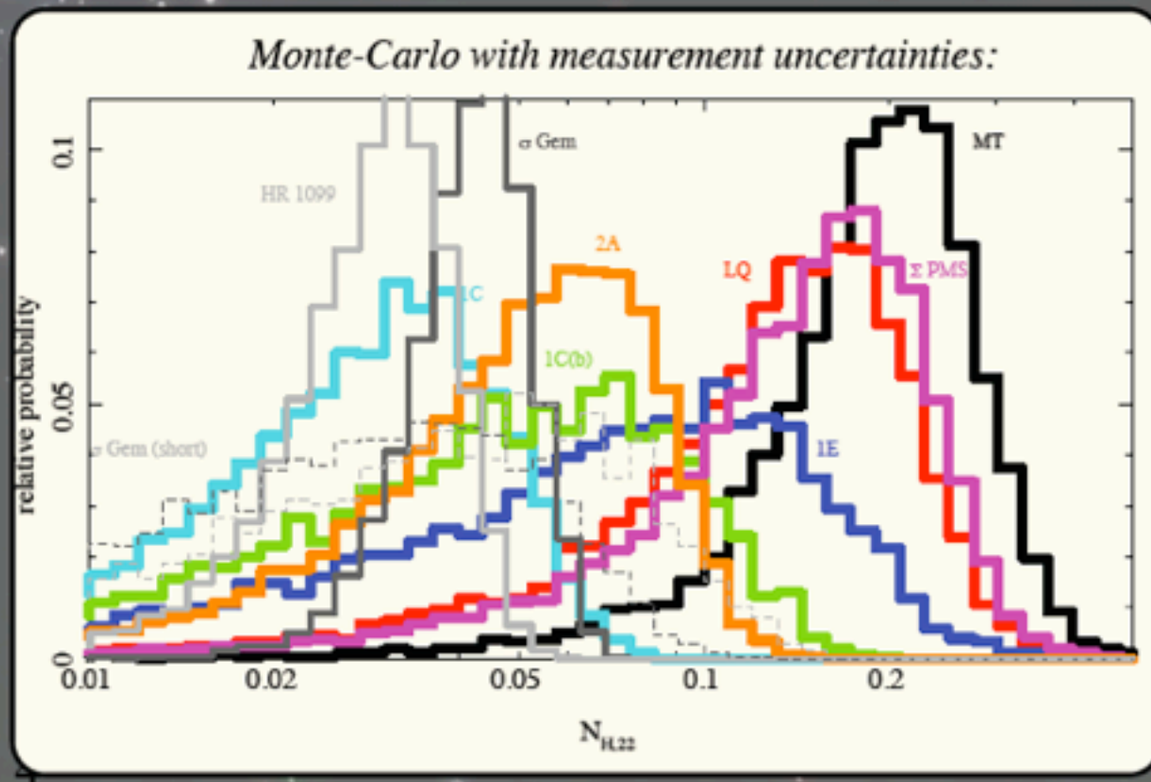
Non-linear, but simple; find the zero of a function; fast to evaluate:

$$0 = 1 - a_1 / t(N_H, \lambda_1) - a_2 / t(N_H; \lambda_2)$$

(COUP for MT Ori found: $N_{H22} = 0.15$)



Monte-Carlo with measurement uncertainties:



Interfacing With Atomic Codes (& Data)

Essential infrastructure:

- Modern mathematical scripting language (S-Lang, Python)
- Automatic binding generator (e.g., SLIRP for S-Lang; see `<http://space.mit.edu/cxc/software/slang/modules/slirp>`)
- Parallel/distributed computing (ISIS `plm` method or S-Lang `pvm` module; see `<http://space.mit.edu/cxc/isis/parallel.html>`; see Noble & Nowak (2008) "*Beyond XSPEC: Toward Highly Configurable Astrophysical Analysis*" for discussion of issues and methods `<http://adsabs.harvard.edu/abs/2008PASP..120..821N>`; also see SLIRP features.

Desired characteristics of codes:

- C is easiest (robust, portable); Fortran, C++ possible (Fortran compilers make life difficult)
- Codes developed as libraries make for easier interfaces; (don't write library-class code in Python or IDL - no one else will be able to use it)
- Code versioning is critical (meaningful major.minor.patch or equivalent)
- Code regression tests are useful (for validation/verification against new versions)

Data-Source References (and a *conundrum*...)

```
b = aped_bib(aped, where(trans(Ne,9,[2:20],1)));
s = aped_bib_query_string( b );

s;
http://adsabs.harvard.edu/cgi-bin/nph-bib_query/?bibcode=2006ApJS.. ICFT&bibcode=...

system( "lynx -dump '$s' > /tmp/s.bib"$);     % (I learned this from the on-line help...)

! cat /tmp/s.bib

Query Results from the ADS Database
Retrieved 6 abstracts, starting with number 1.  Total number selected: 6.

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  adsnote = {Provided by the SAO/NASA Astrophysics Data System}
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Higher Energy
n = 3
n = 2
n = 1
+Ze