Interfacing With Atomic Codes (& Data)

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

"Traditional" spectroscopic analysis:

- pick a model
- set the parameters
- obtain a binned spectrum and a statistic.

Necessary, but not sufficient!

Interfacing With Atomic Codes (& Data)

"Modern" methods (to take advantage of multiple fast CPUs, ample memory, large disk volume):

- (as above for "traditional", plus:)
- save all input information
- provide evaluation/retrieval of underlying functions and data (emissivities, ionization balance, energy levels, wavelengths, ...)

Interfacing With Atomic Codes (& Data)

Example: ATOMDB interfaces in ISIS*:

Database interface: relatively easy - DB is ***static***. Requires data specification, optionally interface library (and very important: a machine-readable ***VERSION*** number).

ISIS initializes the database: `plasma(atomdb);` (<15s to read data for 1 million lines; also supports load of multiple DB versions and can toggle between them).

After defining a model (via temperature(s), norm(s), abundances, redshifts, broadening) and evaluating a model, one can make *source-model-dependent* queries like:

```
ne10 = brightest( 8, where( el_ion( Ne, 10 ) and wl( 9.0, 12.5 ) ) );
fe17 = brightest( 20, where( el_ion( Fe, 17 ) ) );
page_group( fe17 );
fe17_model_flux = line_info( where( trans( Fe, 17, 27, 1 ) )[0] ).flux ;
```

Or we can make *source-model-independent* (in CIE) queries about the atomic data, such as:

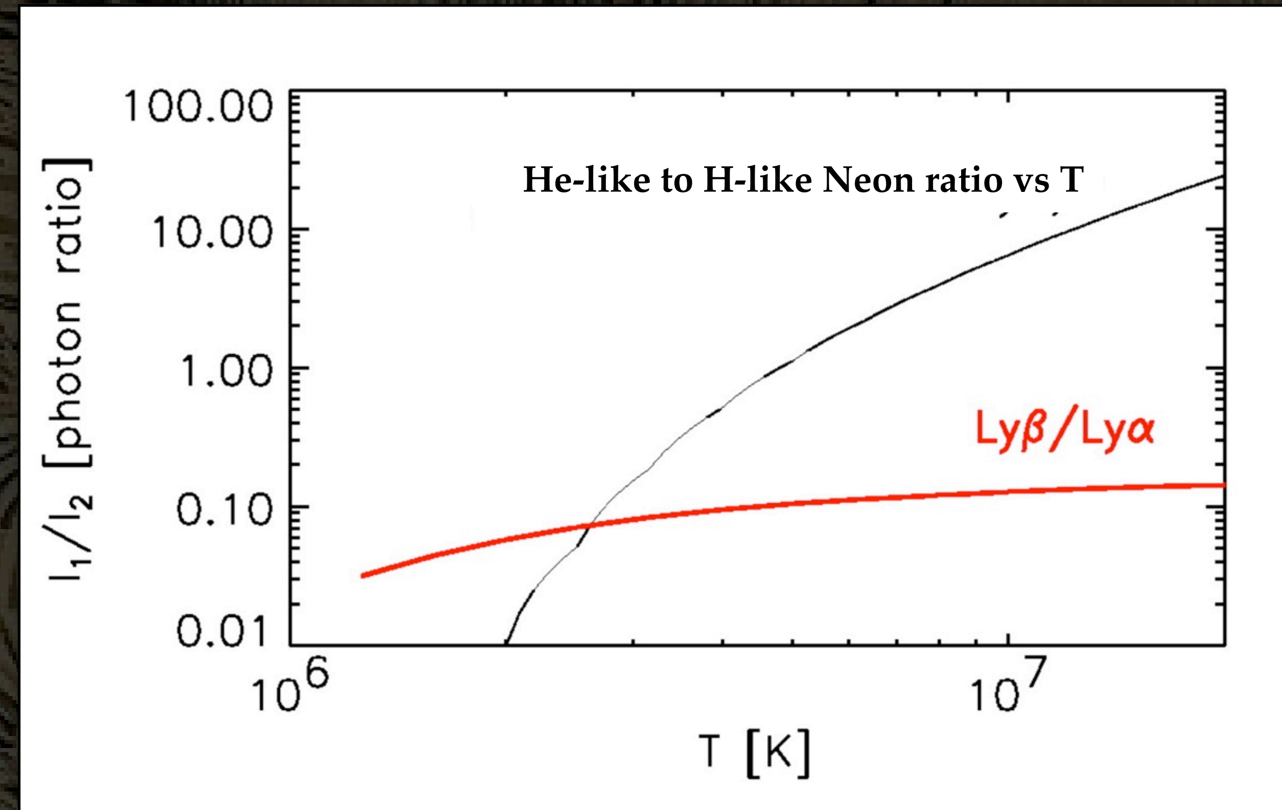
```
tgrid = 10^[6.0 : 8.0 : 0.1 ] ;
emis_fe17 = line_em( where(trans(Fe,17,27,1) ), tgrid);
plot(tgrid, emis_fe17);
```

*ISIS: Interactive Spectral Interpretation System <`http://space.mit.edu/cxc/isis`>, or on the HEAD network, `/soft/isis/bin/isis`

Interfacing With Atomic Codes (& Data)

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.
- Emission measure analysis, using line fluxes, database emissivity (and modeling/fitting infrastructure from your scriptable/extensible environment):



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

- flux at earth [phot cm^{-2} s^{-1}] → f_λ
- foreground absorption → $e^{-N_H \sigma_\lambda}$
- elemental abundance → A_Z
- geometric dilution → $4\pi d^2$
- loss function [phot cm^3 s^{-1}] → $\Lambda_\lambda(T)$ (Atomic Data/Code)
- electron number density [cm^{-3}] → n_e
- volume [cm^3] → $dV(T)$ (Emission Measure)

Interfacing With Atomic Codes (& Data)

Interfaces to Codes: ***Trickier!***

- Mix of data and computation.
- Depends critically on interfaces (and documentation) provided by the code's authors.

Example: `warmabs/photemis` models:

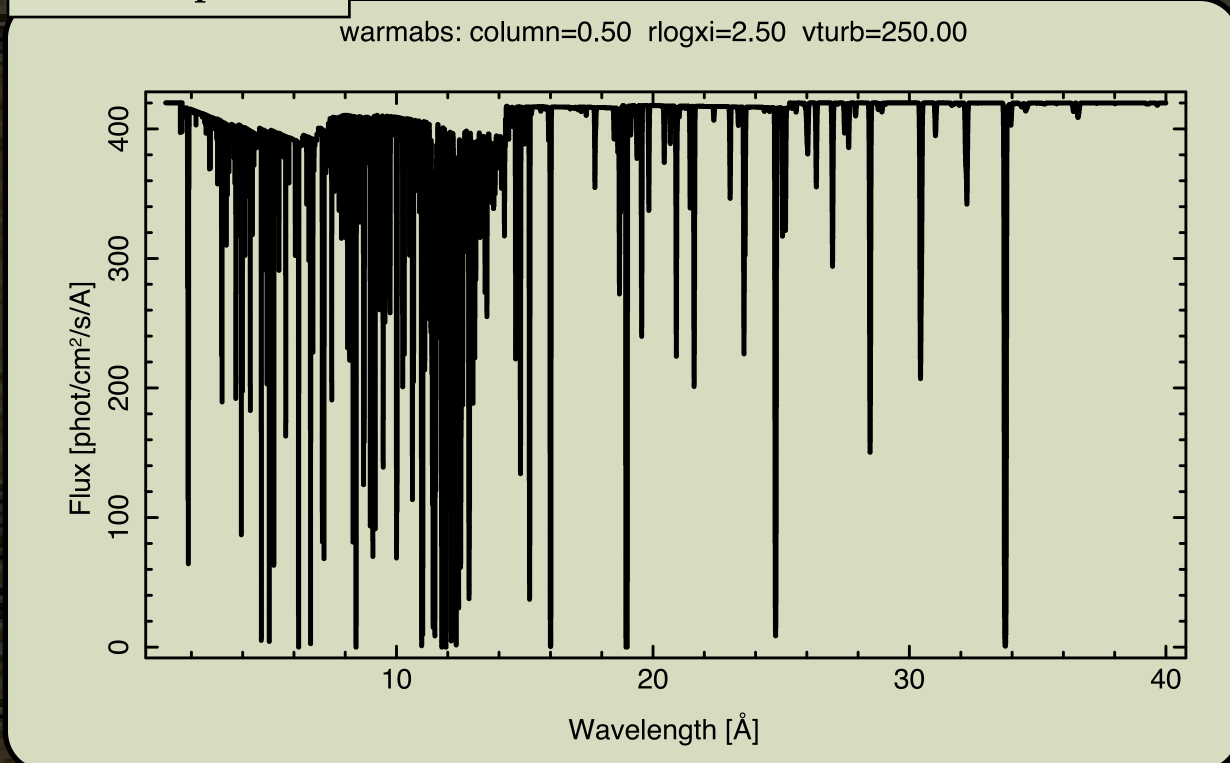
- The external code (an Xspec local model) defines a Fortran common block ("`ewout`") containing atomic data and model results.
- An ISIS module provides bindings (C to Fortran, S-Lang to C) which expose the common block variables to an interactive ISIS session. (C code: about 300 lines, mostly boilerplate. S-Lang code, about 80 lines.)

All Xspec models, as well as local models, are available in ISIS as "black-box" functions. One can always use the `warmabs` model in a fit. With the `ewout` module, one can "get under the hood"...

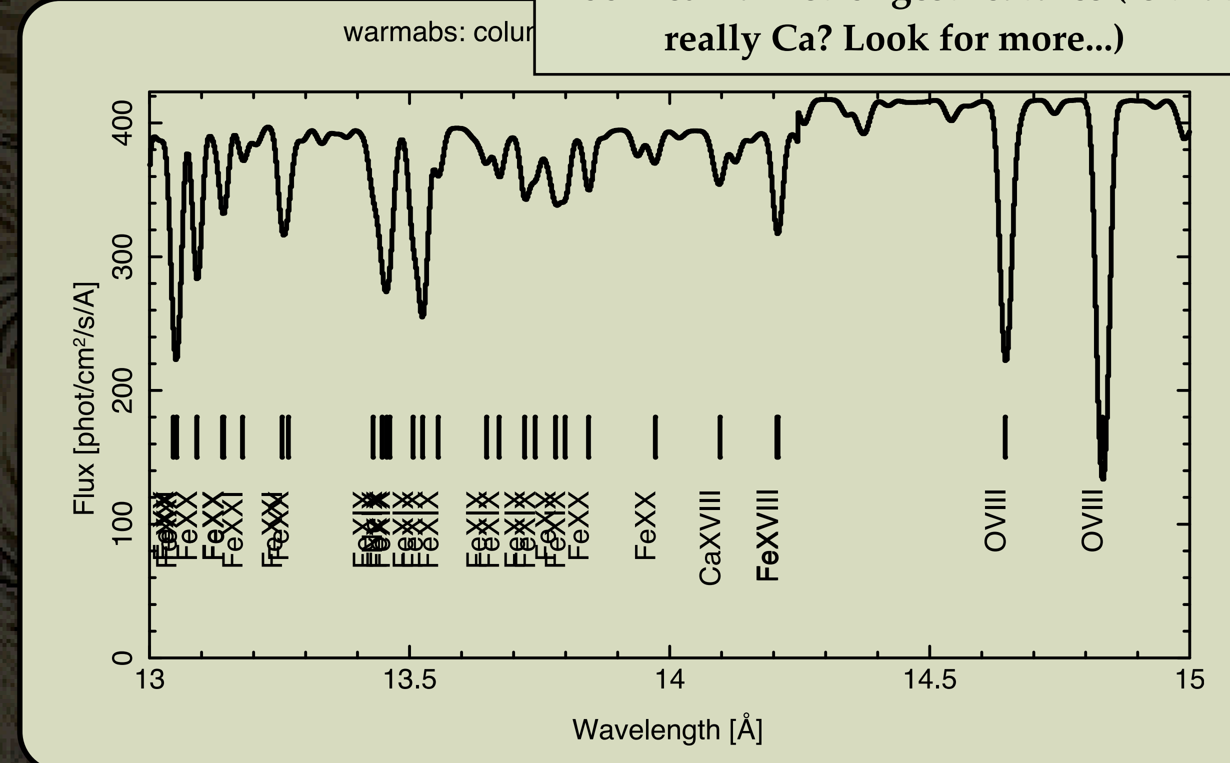
Interfacing With Atomic Codes (& Data)

warmabs/ewout examples

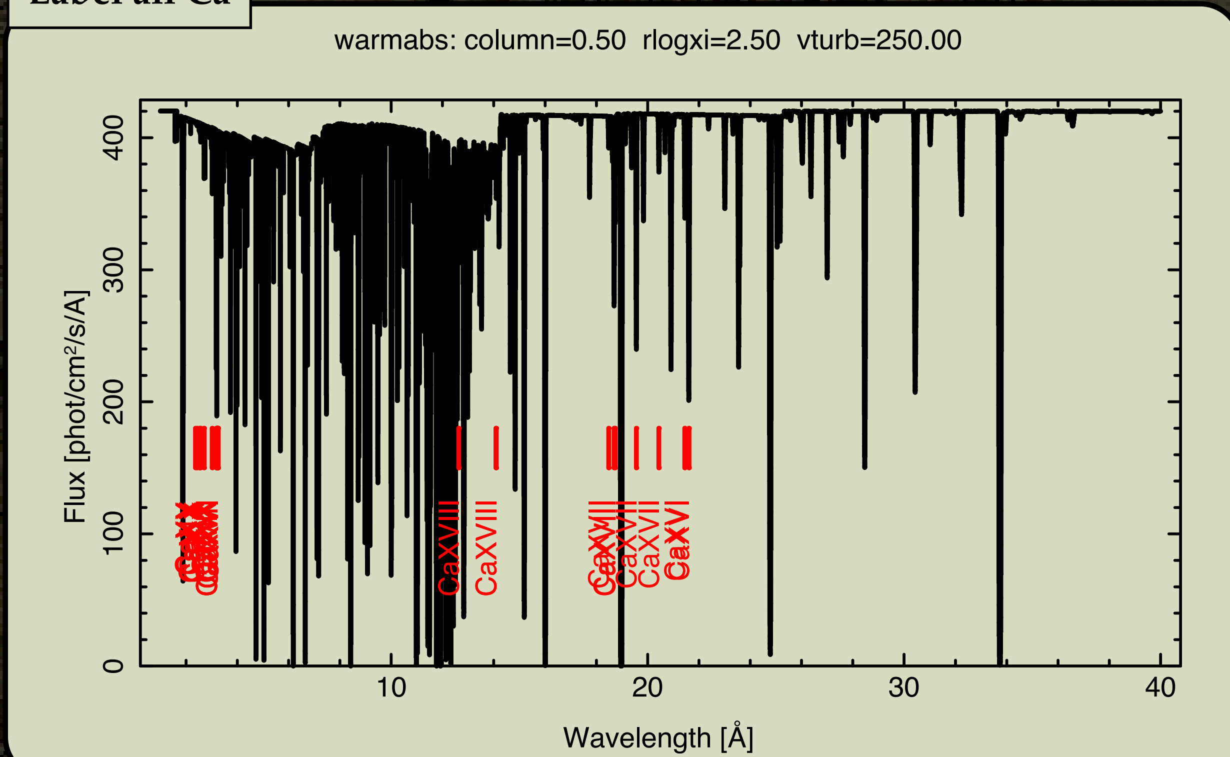
A model spectrum



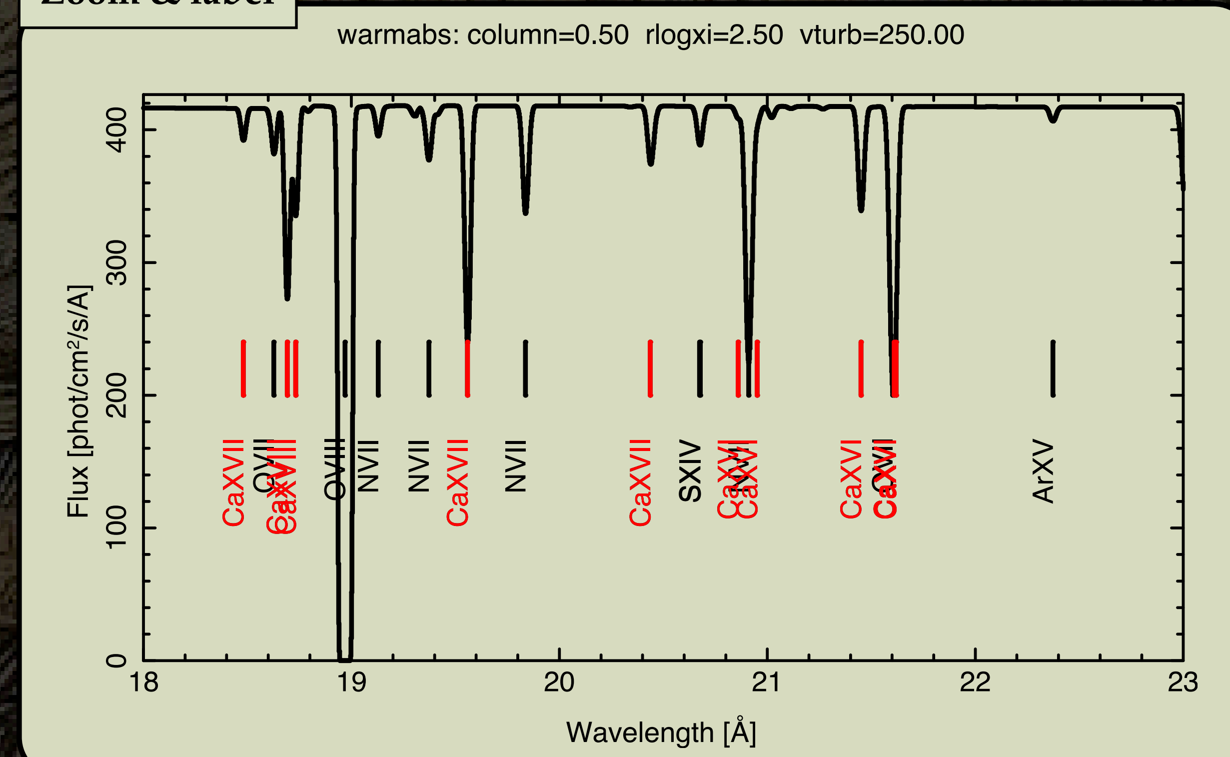
Zoom & mark strongest features (Is that really Ca? Look for more...)



Label all Ca



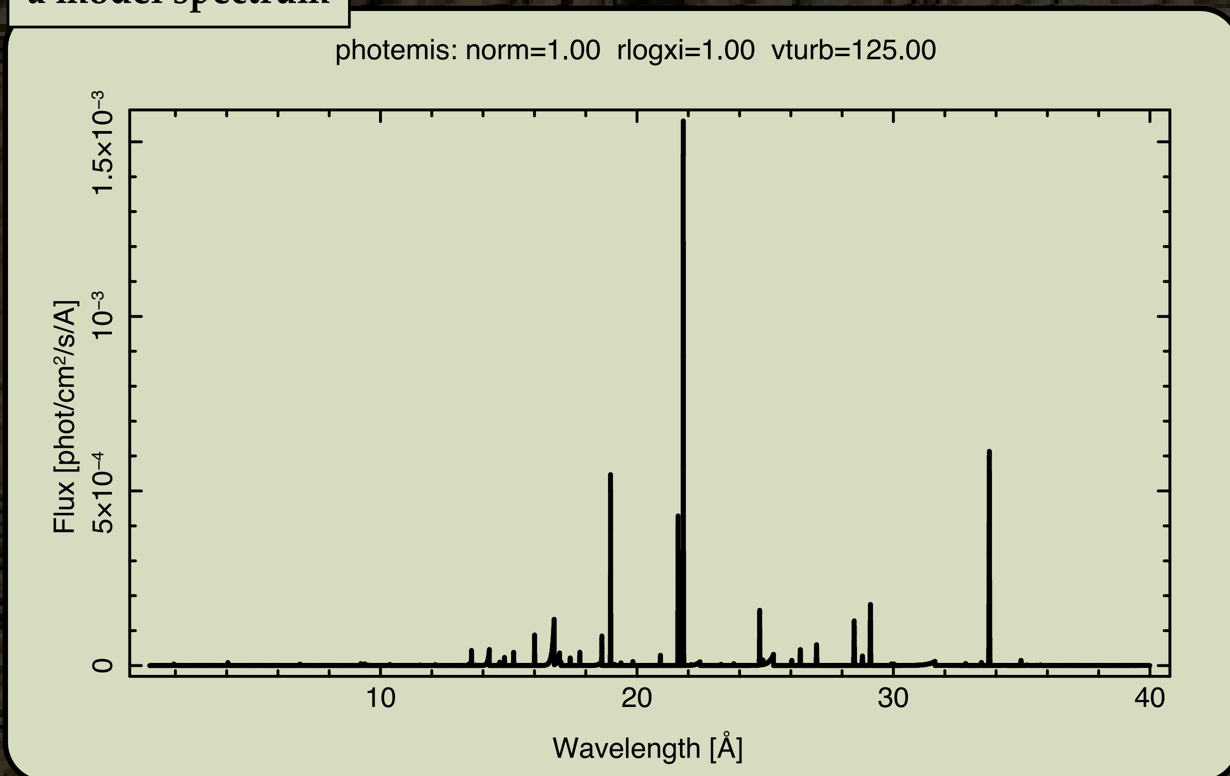
Zoom & label



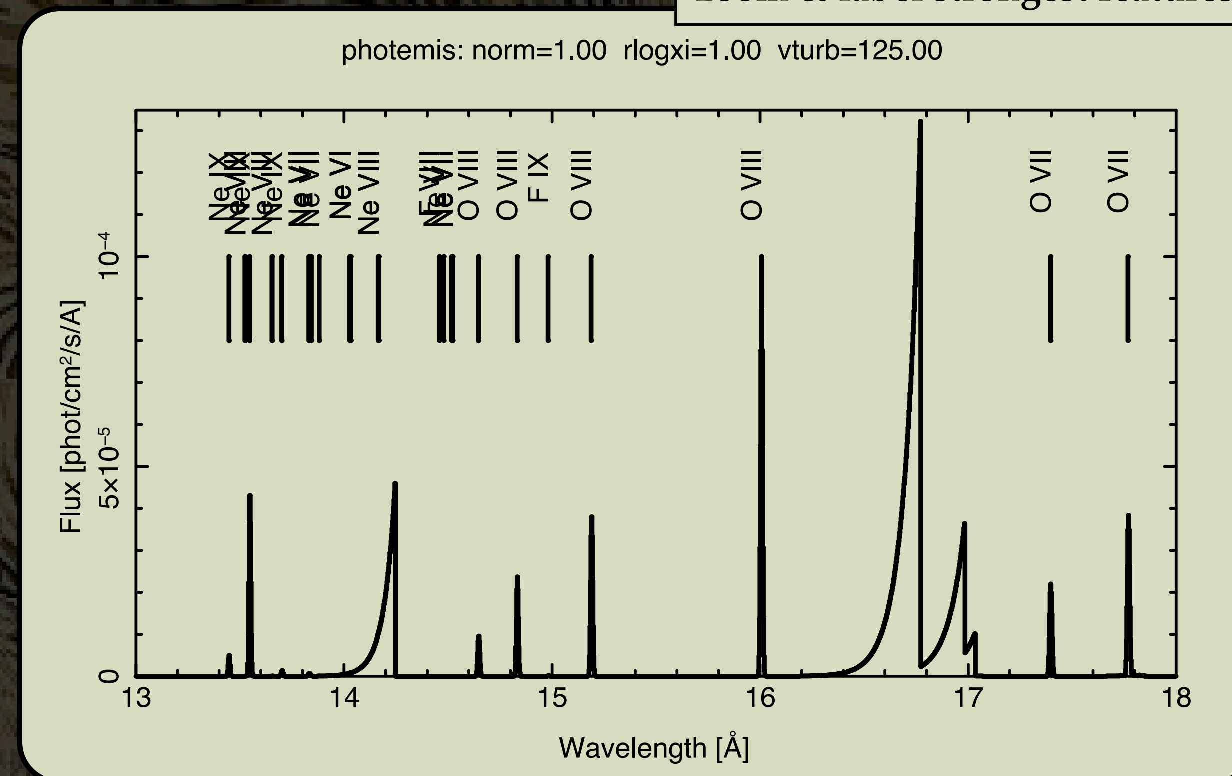
Interfacing With Atomic Codes (& Data)

photemis/ewout examples

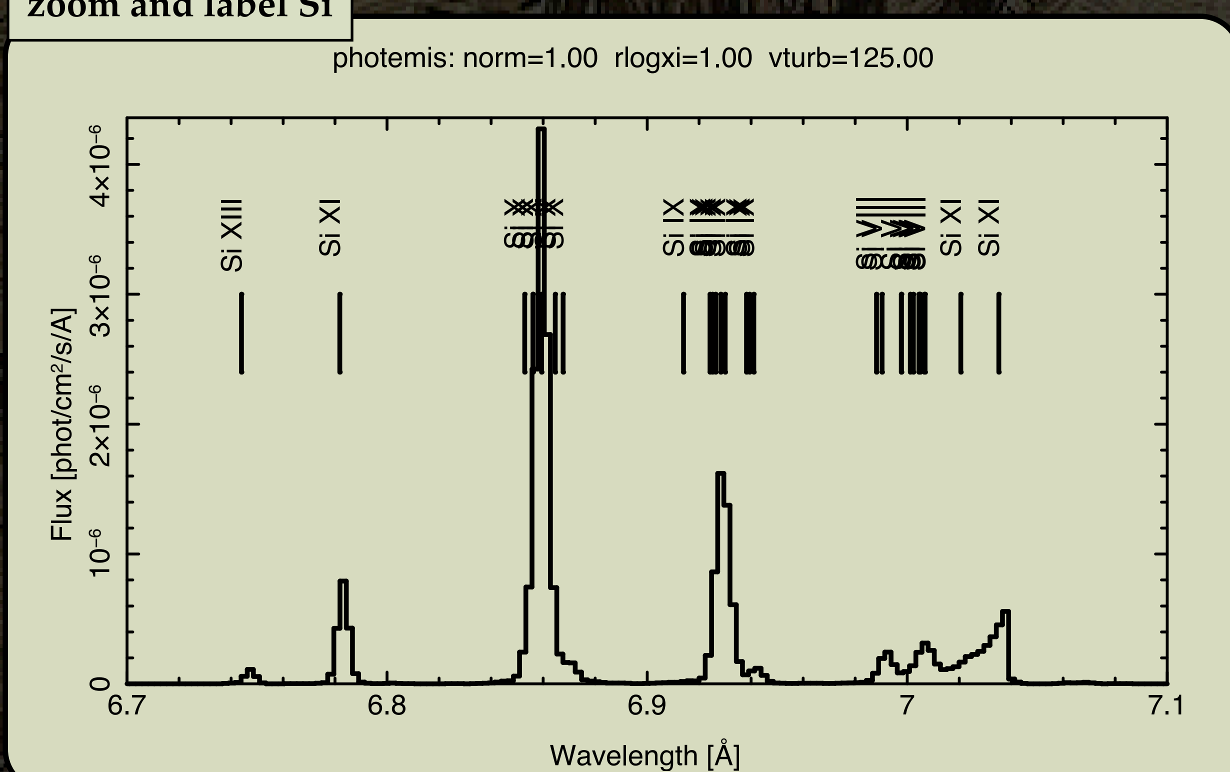
a model spectrum



zoom & label strongest features



zoom and label Si



Interfacing With Atomic Codes (& Data)

We can list the `warmabs` features (or access the values directly):

# 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
5806	O	VIII	18.969	2.566e+12	4.1						
2991	N	VII	19.129	4.737e+10	7.7						
2997	N	VII	19.372	8.254e+10	1.3						
64736	Ca	XVII	19.558	2.102e+12	3.6						
2998	N	VII	19.837	1.637e+11	2.8						
64688	Ca	XVII	20.437	7.141e+12	6.2						
21075	S	XIV	20.674	1.967e+11	2.5						
21024	S	XIV	20.678	1.982e+11	1.2						
63874	Ca	XVI	20.859	5.056e+11	6.5						
2994	N	VII	20.910	4.016e+11	7.8						
63957	Ca	XVI	20.951	1.268e+12	8.3						
64058	Ca	XVI	21.450	4.481e+12	6.1						
5697	O	VII	21.602	3.303e+12	6.9						
64332	Ca	XVI	21.610	5.260e+12	5.5						
64420	Ca	XVI	21.619	8.850e+11	6.1						
42233	Ar	XV	22.373	1.486e+11	3.3						

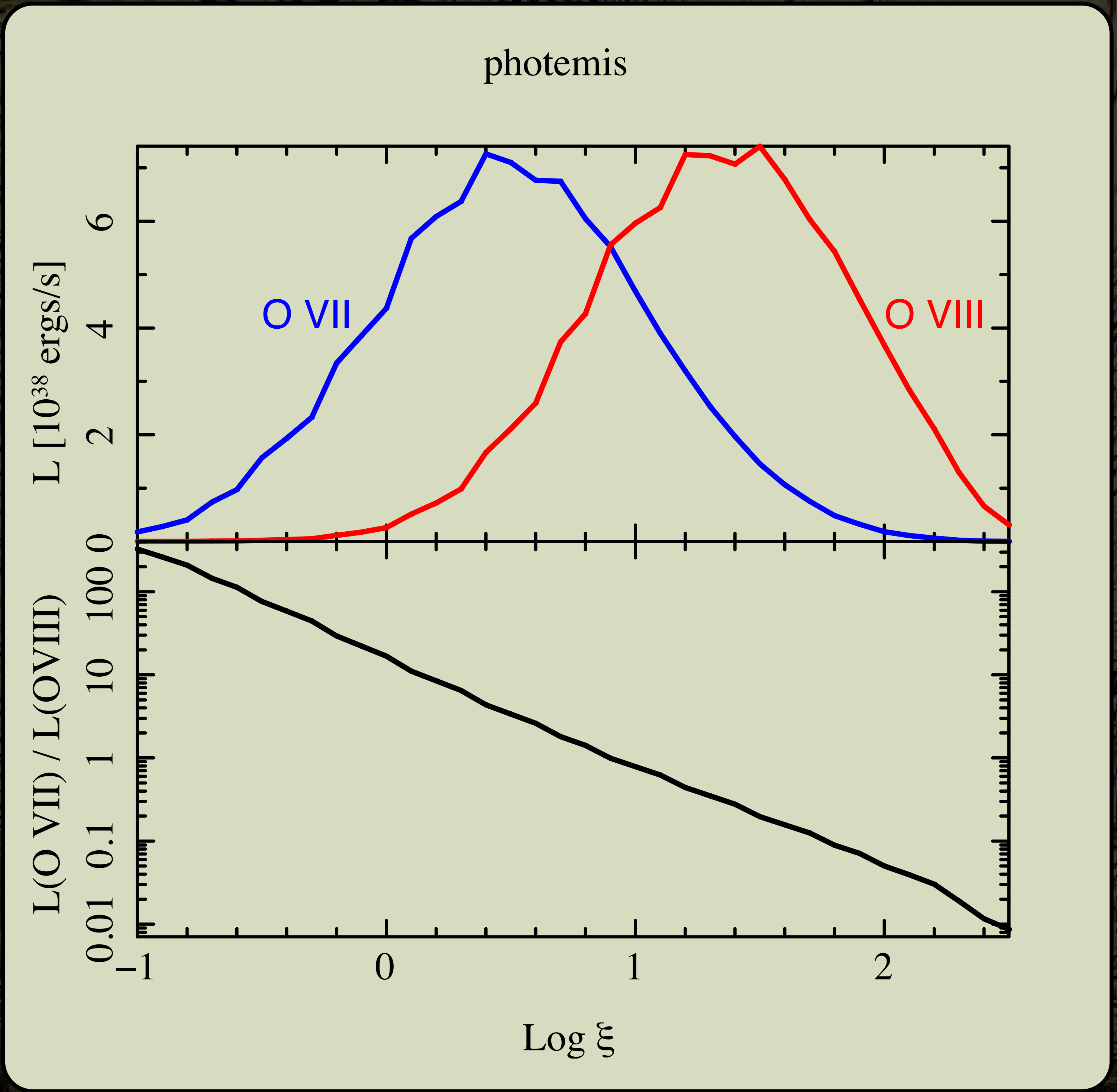
(using filters as appropriate: element, ion, wavelength, strength).

Features list for `photemis` (now *W(A)<0* and *L > 0*):

# id	ion		lambda	A[s^-1]	f	gl	gu	tau_0	W(A)	L[10^38 ergs/s]
9143	Ne	IX	13.447	8.867e+12	7.208e-01	1	3	0.000e+00	-5.537e-16	5.431e-02
8984	Ne	VIII	13.524	1.210e+12	3.316e-02	2	2	0.000e+00	-1.522e-18	1.502e-04
9005	Ne	VIII	13.527	2.730e+12	3.743e-02	4	2	0.000e+00	-3.433e-18	3.387e-04
9123	Ne	IX	13.546	5.612e+07	1.389e-05	1	9	0.000e+00	-4.718e-15	4.662e-01
9025	Ne	VIII	13.653	8.130e+12	4.542e-01	2	4	0.000e+00	-4.635e-18	4.616e-04
9040	Ne	VIII	13.655	7.980e+12	2.230e-01	2	2	0.000e+00	-2.559e-18	2.549e-04
9135	Ne	IX	13.701	1.090e+04	9.199e-10	1	3	0.000e+00	-1.470e-16	1.469e-02
8779	Ne	VII	13.830	7.960e+12	6.845e-01	1	3	0.000e+00	-8.056e-17	8.128e-03
8821	Ne	VII	13.843	1.220e+13	3.503e-01	3	3	0.000e+00	-1.319e-18	1.332e-04
8771	Ne	VII	13.880	6.220e+12	1.796e-01	5	5	0.000e+00	-4.727e-19	4.786e-05
8307	Ne	VI	14.028	1.530e+12	9.024e-02	2	4	0.000e+00	-7.840e-19	8.022e-05
8512	Ne	VI	14.030	9.440e+12	2.785e-01	4	4	0.000e+00	-4.835e-18	4.949e-04
8396	Ne	VI	14.030	7.580e+12	2.236e-01	2	2	0.000e+00	-2.029e-18	2.077e-04
8426	Ne	VI	14.033	3.400e+12	5.017e-02	4	2	0.000e+00	-9.098e-19	9.314e-05
8994	Ne	VIII	14.164	1.800e+11	5.412e-03	2	2	0.000e+00	-7.988e-18	8.254e-04
9033	Ne	VIII	14.167	3.490e+11	5.249e-03	4	2	0.000e+00	-1.548e-17	1.600e-03
5878	F	VIII	14.458	1.570e+12	1.475e-01	1	3	0.000e+00	-6.405e-19	6.755e-05
8888	Ne	VII	14.479	4.700e+11	8.860e-03	5	3	0.000e+00	-4.340e-18	4.584e-04
8889	Ne	VII	14.518	6.530e+10	3.438e-03	3	5	0.000e+00	-7.115e-19	7.534e-05
8922	Ne	VII	14.519	8.630e+10	8.180e-03	1	3	0.000e+00	-5.853e-19	6.199e-05
8758	Ne	VII	14.520	1.930e+11	6.098e-03	5	5	0.000e+00	-2.102e-18	2.226e-04
8975	Ne	VII	14.522	2.550e+11	2.686e-03	3	1	0.000e+00	-5.863e-19	6.211e-05
8920	Ne	VII	14.523	1.050e+11	1.991e-03	5	3	0.000e+00	-7.119e-19	7.541e-05
5846	O	VIII	14.645	8.081e+10	7.792e-03	2	6	0.000e+00	-9.769e-16	1.044e-01
5805	O	VIII	14.832	1.408e+11	1.393e-02	2	6	0.000e+00	-2.380e-15	2.575e-01
5981	F	IX	14.981	4.121e+12	4.158e-01	2	6	0.000e+00	-1.119e-17	1.223e-03
5822	O	VIII	15.188	2.793e+11	2.896e-02	2	6	0.000e+00	-3.731e-15	4.133e-01
5823	O	VIII	16.006	6.851e+11	7.891e-02	2	6	0.000e+00	-8.141e-15	9.504e-01
5681	O	VII	17.396	1.963e+11	2.671e-02	1	3	0.000e+00	-1.882e-15	2.388e-01
5692	O	VII	17.768	3.867e+11	5.488e-02	1	3	0.000e+00	-3.207e-15	4.157e-01

Interfacing With Atomic Codes (& Data)

For `warmabs` & `photemis`, some useful quantities require multiple model evaluations (currently). E.g., if you were interested in photoionized plasma emission measure or line-ratio analysis, you have to evaluate line power vs ionization parameter (ξ) "manually":



Interfacing With Atomic Codes (& Data)

Future work:

`warmabs`/`photemis` (`ewout`) interfaces is work in progress; we would like to have better support for:

- emission measure analysis;
- curve of growth analysis;
- absorption edge data (ID, wavelength, strength)
- RRC data (ID, wavelength, strength)

APEC interfaces: in progress (Li Ji, John Houck); need top-down definition of analysis cases.

Both will require collaboration with the codes' authors.

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

appendix

extra stuff

Spectral Modeling: Collisional Plasma, detailed example of "opening the black-box"

```
isis> plasma(aped);
isis> create_aped_fun( "Aped_1T", default_plasma_state);
isis> fit_fun( "Aped_1T(1)" );
isis> set_par( "Aped_1T(1).temperature", 10^6.8);

isis> (wlo, whi) = linear_grid( 15, 20.0, 16384 );
isis> y = eval_fun( wlo, whi ) ;

isis> xrange( 15.95, 16.05 ) ;  yrange(0);
isis> hplot( wlo, whi, y ) ;
isis> plot_group( brightest( 10, where( wl( 15.95, 16.05) ) ) );
```

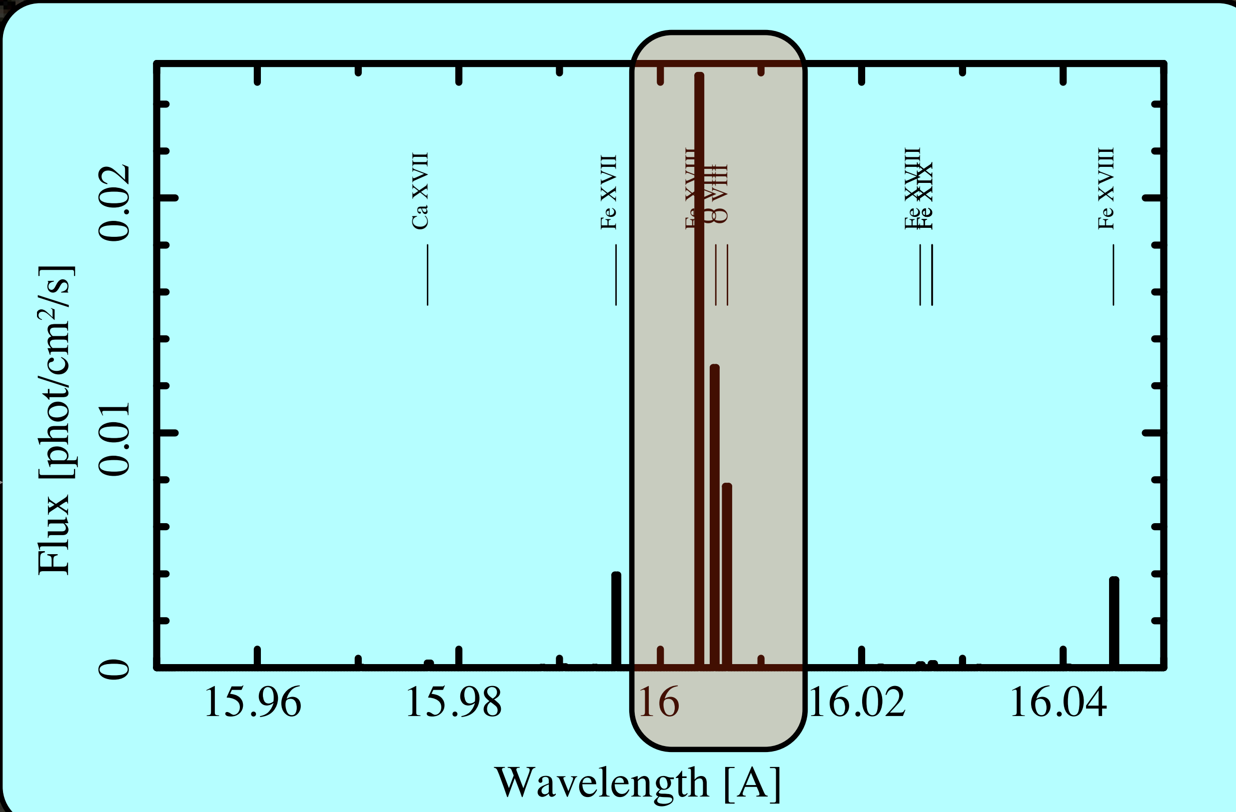
```
isis> page_group( brightest( 5, where( wl( 15.98, 16.02 ) ) ) );
```

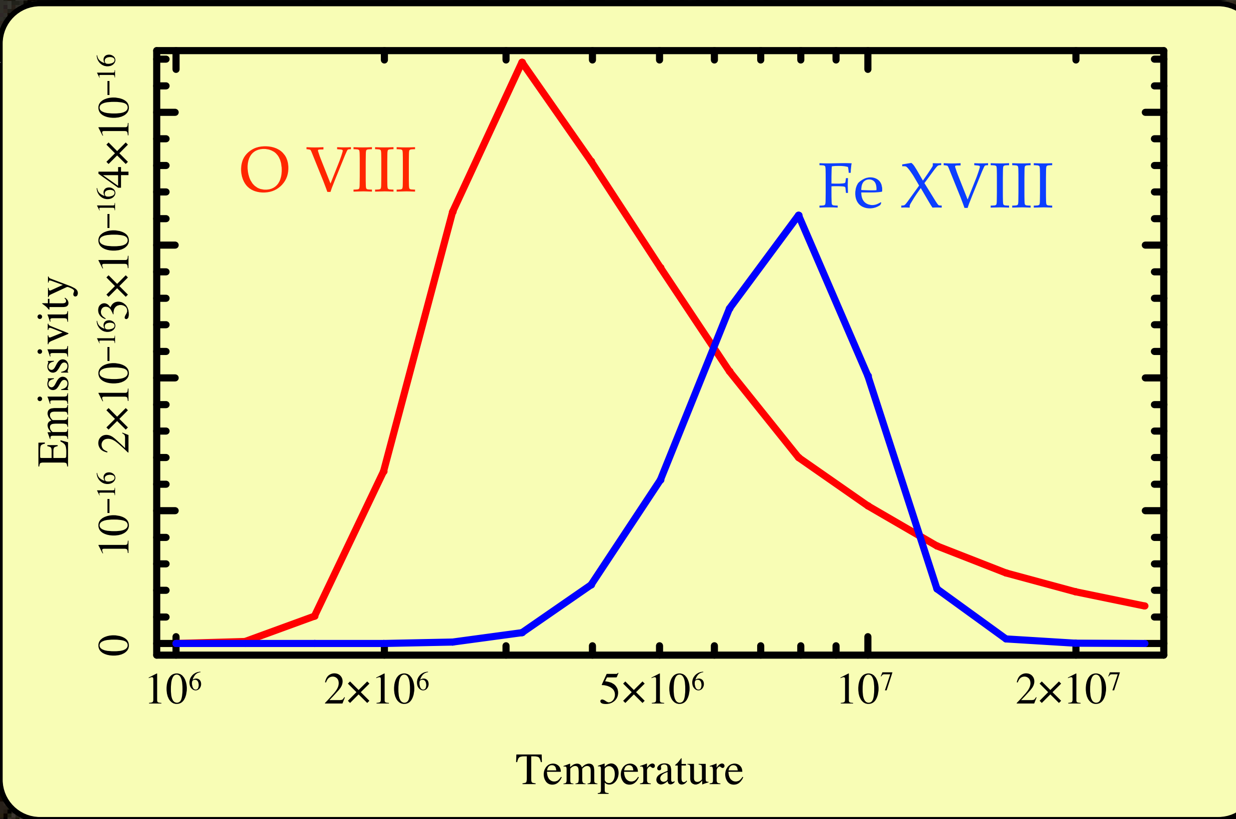
```
isis> t = 10^[ 6.0 : 7.5 : 0.1];
isis> e1 = line_em( where(trans( O, 8, [6,7], 1) ), t );
isis> e2 = line_em( where( trans( Fe, 18, 5, 1) ), t );

isis> xlog; xrange;
isis> xlabel("Temperature"); ylabel("Emissivity");
isis> plot( t, e1, 2 ) ;   oplot( t, e2, 4 );
```

```
isis> page_group( brightest(5, where( wl(15.98, 16.02))));
```

# index		ion	lambda	F (ph/cm^2/s)	A(s^-1)	upper	lower	label
421194	*	Fe XIX	15.990	2.887e-05	2.510e+10	40	6	2p3 - 2s1
390247	*	Fe XVII	15.996	3.947e-03	7.543e+08	14	1	2p5 - 2p6
404081	*	Fe XVIII	16.004	2.522e-02	1.580e+12	5	1	2p4 - 2p5
50041	*	O VIII	16.006	1.278e-02	6.829e+11	7	1	3p1 - 1s1
50034	*	O VIII	16.007	7.718e-03	1.367e+12	6	1	3p1 - 1s1

The 3 lines highlighted all fall within a single MEG bin of 0.005A. If you naively intended to measure a temperature from the ratio of O VIII Ly α to Ly β , you would be wrong.





appendix

Example of model evaluation by components:

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