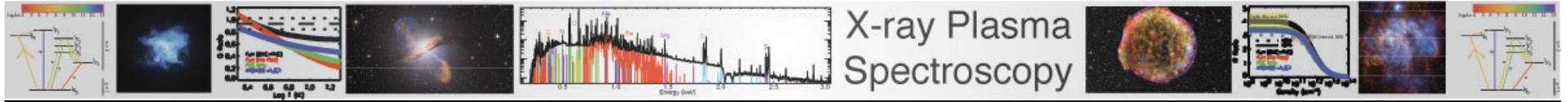


# Plasma Codes: A User's Guide

Randall K. Smith

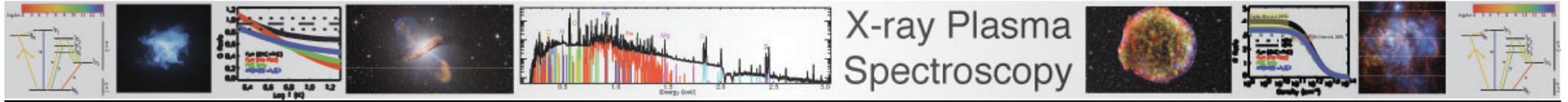
Smithsonian Astrophysical  
Observatory





## A few words to start...

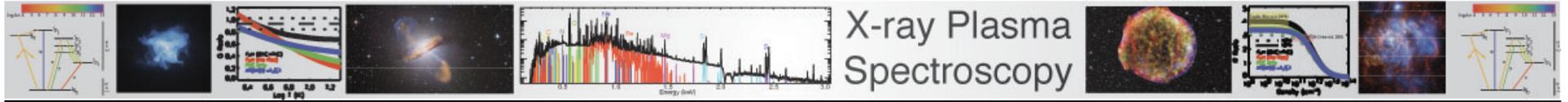
- Matching plasma codes to spectra can absorb indefinite amounts of time
- Before using a code/model/fit, think about what you hope to measure.
- Remember Ockham's Razor!



The basic atomic processes in astrophysical X-ray emitting plasmas are two-body collisional excitation & ionization, photoexcitation & ionization, spontaneous radiative decay, and two-body recombination.

A consequence of this is that the plasmas can be separated into two categories:

- Collisional:  
 $k_B T_e \sim$  Ionization energy of plasma ions
- Photoionized:  
 $k_B T_e \ll$  Ionization energy of plasma ions



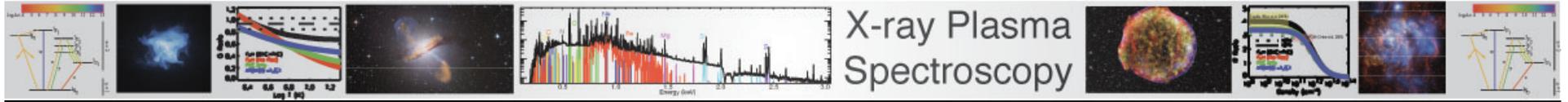
At high enough densities, collisions & photons are both important:

- **Collisional-Radiative (CR):**  $10^{14-16} \text{ cm}^{-3} < N_e < 10^{27} \text{ cm}^{-3}$
- **Coronal/Nebular:**  $N_e < 10^{14-16} \text{ cm}^{-3}$

In a **CR** plasma, collisions compete with photons in de-exciting levels; a level with a small  $A$  value may be collisionally de-excited before it can radiate.

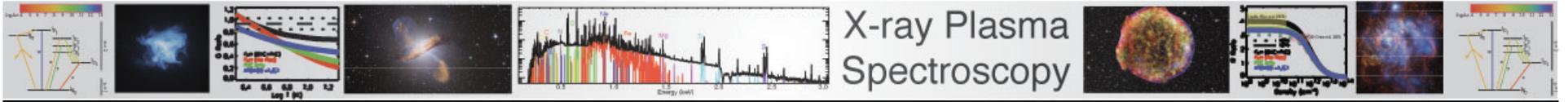
In a **Coronal** (or **Nebular**) plasma, collisions excite ions but are too rare to de-excite them; decays are purely radiative. This is also called the “ground-state” approximation, as all ions are assumed to be in the ground-state when collisions occur.



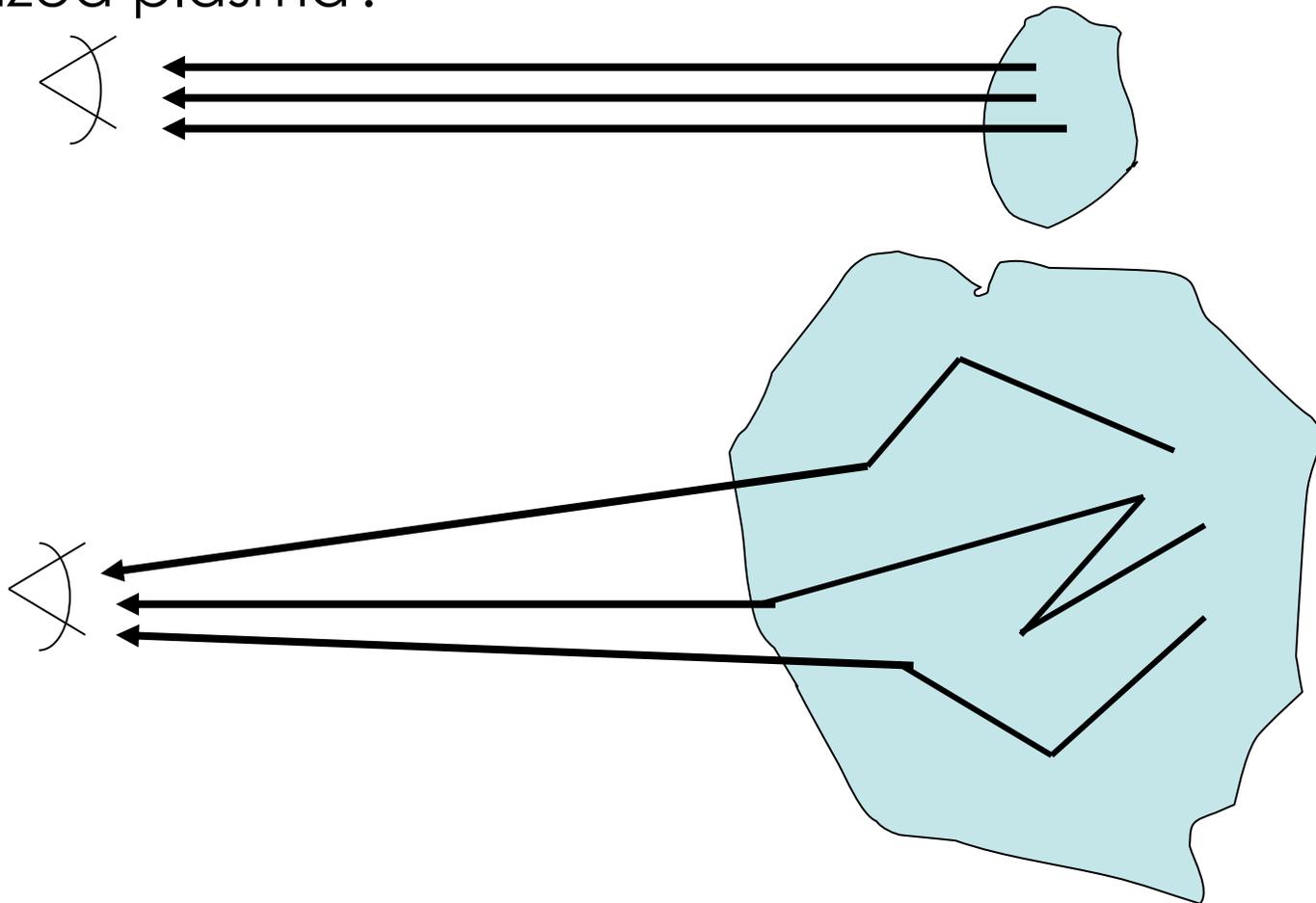


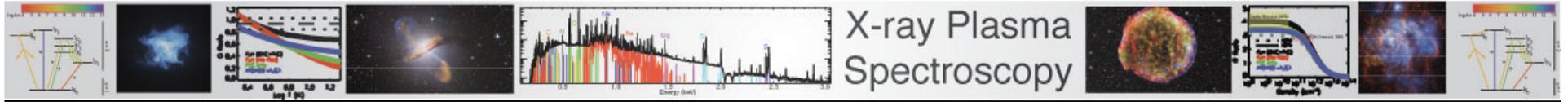
## Two common questions:

1. Can the collisional & photoionization processes both be important in a low density plasma?
  - Yes, but why would they?
2. What about plasmas in local thermodynamic equilibrium (LTE)?
  - This occurs if  $N_e > 1.8 \times 10^{14} T_e^{1/2} \Delta E_{ij}^3 \text{ cm}^{-3}$
  - For  $T_e = 10^7 \text{ K}$  for H-like Iron,  $N_e > 2 \times 10^{27} \text{ cm}^{-3}$
  - For  $T_e = 10^5 \text{ K}$  for H-like Oxygen,  $N_e > 10^{24} \text{ cm}^{-3}$ .



But what about radiative excitation? Can't photons still interact with ions, even in a collisionally ionized plasma?





So, is photon scattering an important process?

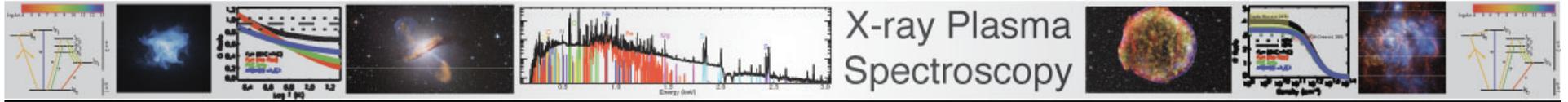
**Yes**, but only for allowed transitions; in a collisional plasma, many transitions are forbidden or semi-forbidden, and these can also occur due to cascades in a photoionized plasma.

So couldn't this show up as optical depth in allowed lines, weakening them relative to forbidden lines?

**Yes**, and this can be calculated after modeling a plasma. Using the ionization balance and the coronal approximation, along with the A value for the transition and the emitting volume, it is easy to calculate the optical depth for a line:

$$\tau = n_I \sigma l$$

This effect is often not important, but even less often checked!



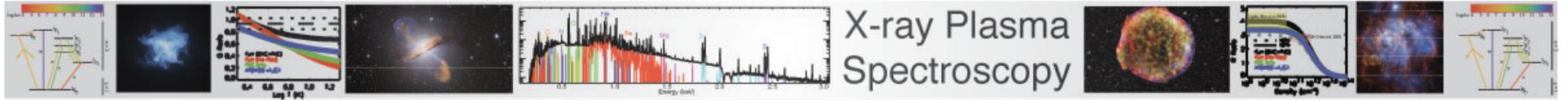
Both collisional and photoionized plasmas may be in **equilibrium** or out of it.

- A collisional or photoionized plasma in **ionization equilibrium** (usually called a **CIE** or **PIE** plasma) has the property that

$$I_{\text{rate}}(\text{Ion}) + R_{\text{rate}}(\text{Ion}) = I_{\text{rate}}(\text{Ion}^-) + R_{\text{rate}}(\text{Ion}^+)$$

- A **non-equilibrium ionization (NEI)** plasma may be:
  - **Ionizing** [ $\Sigma I_{\text{rate}}(I) > \Sigma R_{\text{rate}}(I)$ ]
  - **Recombining** [ $\Sigma I_{\text{rate}}(I) < \Sigma R_{\text{rate}}(I)$ ]
  - **Other**





# Plasma Codes for X-ray Astrophysics

## Collisional

Mekal/SPEX

Chianti

ATOMDB (APEC, APED)

## Photoionized

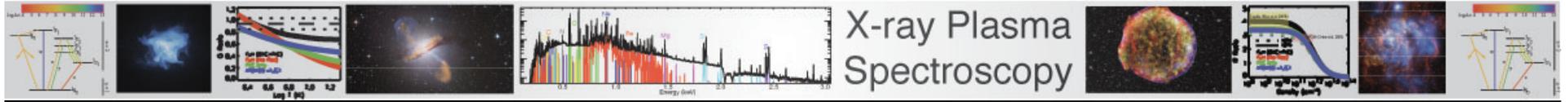
XSTAR

Cloudy

Titan

Mocassin





## Collisional Plasma Codes

Understanding a collisional plasma requires a collisional plasma model. Since even a simple model requires considering hundreds of atomic lines, and modern codes track millions, most people select one of the precalculated codes:

### Code

Raymond-Smith

Mekal/SPEX

Chianti

ATOMDB

### Source

[ftp://legacy.gsfc.nasa.gov/software/plasma\\_codes/raymond](ftp://legacy.gsfc.nasa.gov/software/plasma_codes/raymond)

<http://saturn.sron.nl/general/projects/spex>

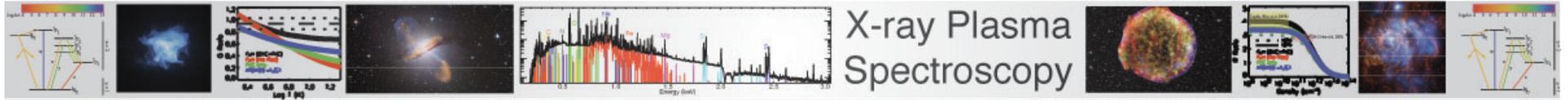
<http://www.solar.nrl.navy.mil/chianti.html>

<http://www.atomdb.org>



The calculated spectrum is also known as APEC, and the atomic database is called APED.





## Some History of Collisional Codes (from someone who wasn't there for most of it)

Raymond-Smith = John Raymond, Barham Smith (NOT ME!)

- Originally by Don Cox & Wallace Tucker
- Code still available, FORTRAN 77-ish, can do NEI.
- Led to ATOMDB, by Nancy Brickhouse & Randall Smith (ME)

MEKA = Rolf Mewe & Jelle Kaastra code...

- Based on Mewe, Gronenschild & vdOord code
- Began in 1970 at SRON to 'Develop X-ray Spectroscopy'

MEKAL = Mewe, Kaastra, & Duane Liedahl : HULLAC iron lines added

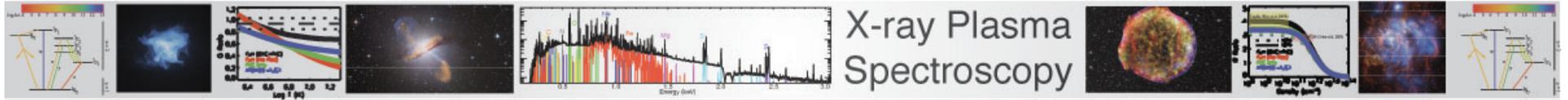
- Latest version found in SPEX

CHIANTI

- Related to ARCETRI code by Massimo Landini & Brunella

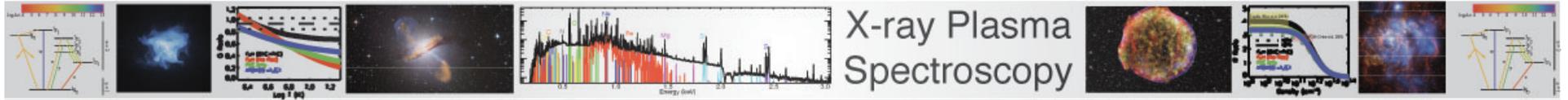
Monsignori-Fossi

- Both a database and a suite of tools; requires IDL



## When & Where are these Codes Used?

- Raymond-Smith
  - Can do NEI code output
  - Extremely fast; even suitable for hydro codes
  - Not good for high-res spectroscopy due to # of lines
- MEKAL
  - Multiple versions: older one in XSPEC, new in SPEX
  - Frequently used for both high and medium-res spectra
- CHIANTI
  - Suite of tools primarily used for solar analysis
  - Atomic Database easily used for other purposes
- ATOMDB
  - Primarily equilibrium, but some NEI versions available
  - Database has been used for other tools

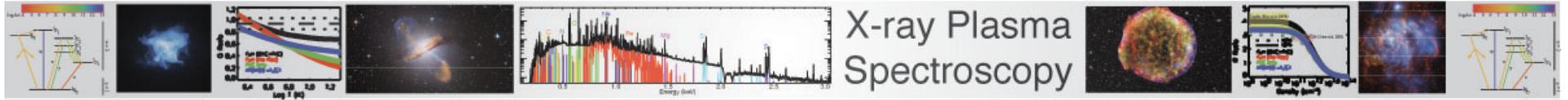


The collisional plasma models available in XSPEC or Sherpa are:

apec	ATOMDB code; good for high-resolution data
bapec	ATOMDB code; includes broadening
raymond	Updated (1993) Raymond-Smith (1977) code
meka	Original Mewe-Kaastra (Mewe <i>et al.</i> 1985) code; outdated
mekal	Mewe-Kaastra-Liedahl code (Kaastra 1992); new Fe L lines
c6mekal	mekal with an polynomial EM distribution
equil	Borkowski update of Hamilton, Sarazin & Chevalier (1983)
nei	Ionizing plasma version of equil
sedov	Sedov (SNR) version of equil
pshock	Plane parallel shock version of equil

Variable abundance versions of all these are available. Individual line intensities as functions of  $T$ ,  $n$ , etc. are not easily available (**yet**) in either XSPEC or Sherpa.





## Photoionized Plasma Codes

Understanding a photoionized plasma requires a plasma model **plus** a physical model of the system:

- Illuminated slab of gas
- Torus with central source
- Disk with 'light bulb' above it
- Central source surrounded by small absorbers
- etc...

### Code

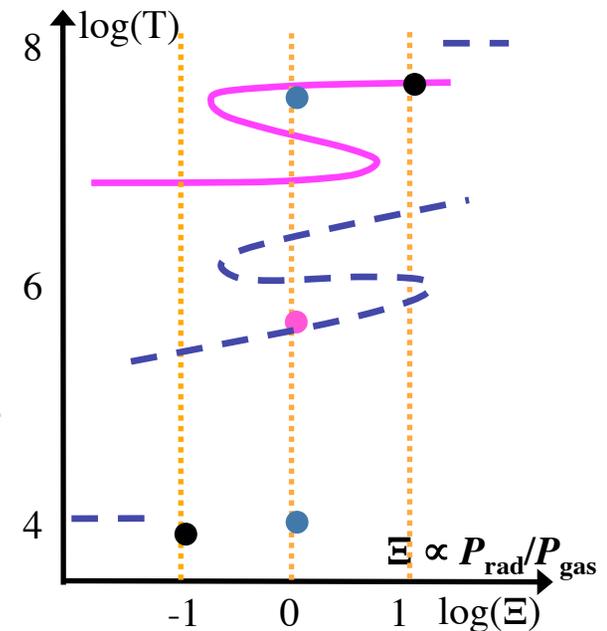
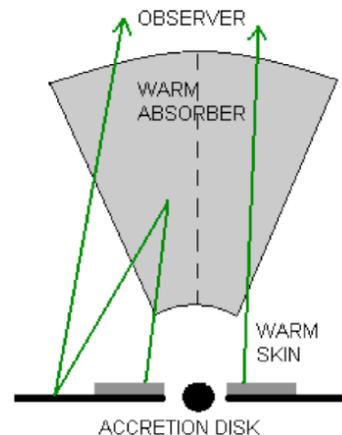
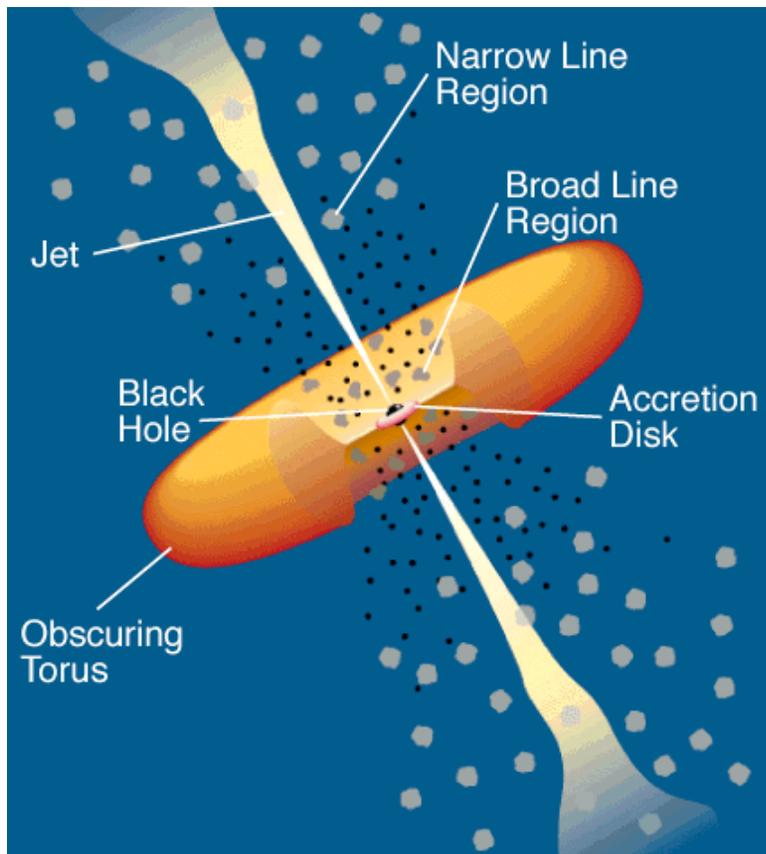
### Website

XSTAR	<a href="http://heasarc.nasa.gov/lheasoft/xstar/xstar.html">http://heasarc.nasa.gov/lheasoft/xstar/xstar.html</a>
CLOUDY	<a href="http://www.nublado.org/">http://www.nublado.org/</a>
Titan	<a href="http://Vo.obspm.fr:8888/simulation/">http://Vo.obspm.fr:8888/simulation/</a> (in progress?)
Mocassin	<a href="http://hea-www.harvard.edu/~bercolano/">http://hea-www.harvard.edu/~bercolano/</a>

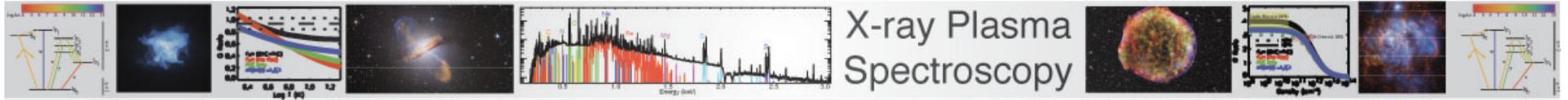


# Thermal instability in Warm Absorbers

A plasma in pressure equilibrium plasma can develop a thermal instability with 2 stable solutions (cold, hot)



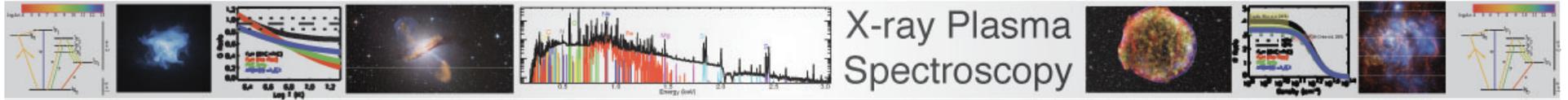
Gonçalves et al. (2007)  
Czerny et al (2003)



# XSTAR Photoionization Model

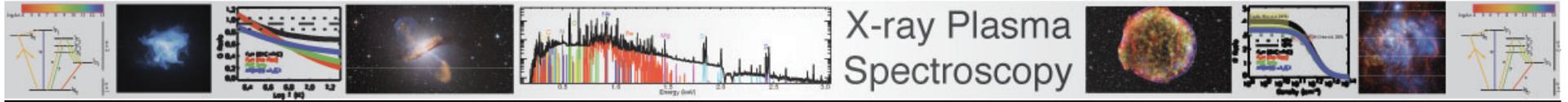
Source: <http://heasarc.nasa.gov/lheasoft/xstar/xstar.html>

- Full global model (i.e. photoionization-->synthetic spectrum --> xspec --> fit)
- Xstar version 2.1ln9
  - Inner Mshell 2-3 UTAs (FAC; Gu); >400 lines explicitly calculated
  - Chianti v5 data for iron L
  - Iron K shell data from R-matrix calculations (Bautista, Palmeri, Mendoza et al )
  - Available from XSTAR website, as are ready-made tables
- Not in current release version, 2.1kn7
- Other models have similar ingredients
- Xspec 'analytic model' warmabs
  - Not fully self consistent: assumes uniform ionization absorber, but this is small error for low columns.



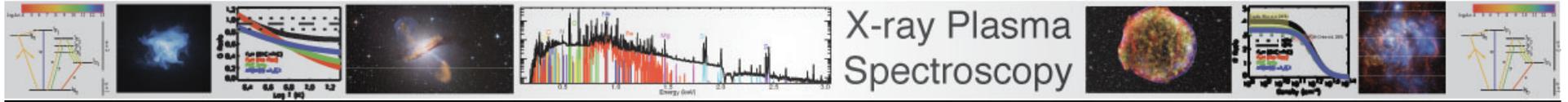
# Cloudy

- Primarily used for UV/optical/IR, but has some X-ray lines
- Massive code (now in C, was in Fortran)
- Extensive documentation (Hazy)
- Frequently used as part of larger codes
- Will be discussed more in later talks.



# The TITAN code

- A stationary, photoionization code developed at Paris Observatory (LUTH) by A.-M. Dumont & S. Collin
- Aimed at studying dense, warm ( $T \sim 10^4$ - $10^7$  K), and optically thick (Thomson thickness  $\sim$  several 10s), but also thinner ( $\sim 0.01$ - $0.1$ ) media
- Assumes a 1D plane-parallel geometry: slab of gas illuminated on one side by an irradiating X-ray source (flux and SED continuum)
- Includes all relevant processes: photoionization, radiative and di-electronic recombination, collisional ionization, ionization by high-energy photons, fluorescence, radiative and collisional excitation/de-excitation, ...
- Computes the gas structure in thermal and ionization equilibrium
- Energy balance insured locally with a precision of 0.01%, globally with 1%



# The TITAN code

- Accounts for Compton heating/cooling (coupled with the NOAR code)
- Can work in the 0.1- several  $10^5$  eV energy range (coupled with NOAR)
- Provides the gas structure in Temperature, Ionization, Density, Pressure
- Provides the outward and reflected spectra
- Atomic data: 102 ions and atoms of H, He, C, N, O, Ne, Mg, Si, S, Fe, amounting to  $\sim 1000$  lines

- Parameters' optimal range:

$$10^5 < n_{\text{H}} < 10^{14} \text{ cm}^{-3}$$

$$8000 < T < 10^8 \text{ K}$$

$$N_{\text{H}} < 10^{26} \text{ cm}^{-2}$$

$$10 < \xi = L/n_{\text{H}}R^2 < 10^5$$



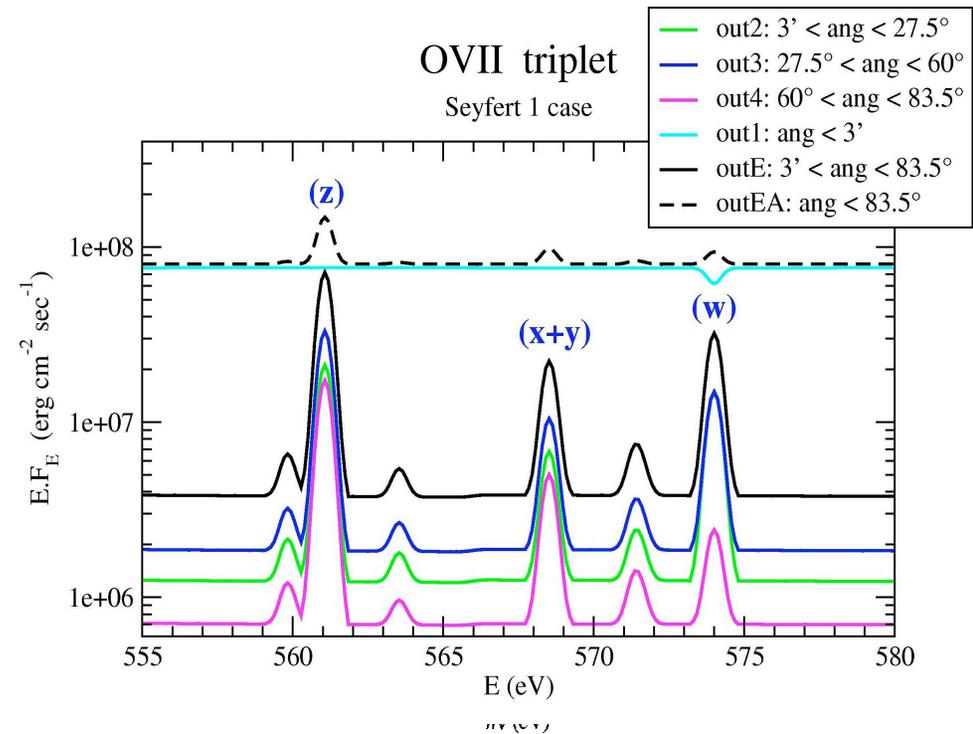
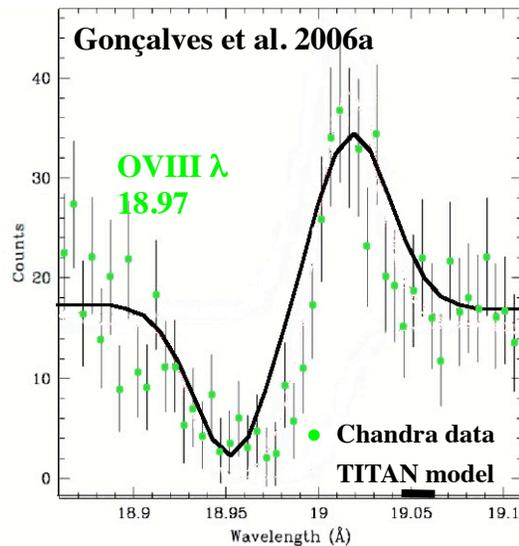
# TITAN photoionization code

## Computes the transfer of lines and continuum

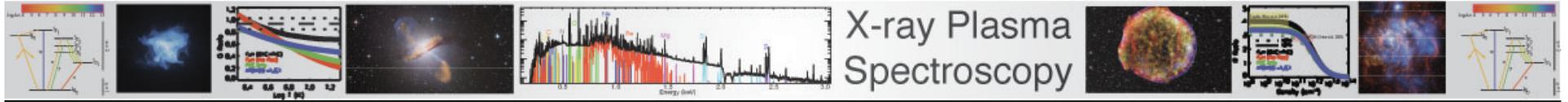
- No escape probability approximation, but throughout calculations (ALI method)

### Multi-angle spectra

- “normal direction” + 5 cones (18°, 40°, 60°, 77°, 87°)
- computes the transmitted, reflected and emitted flux



- Can account for P Cyg-like profiles
- Can simulate the expected spectrum as function of the line-of-sight



# MONteCARloSimulationSofIonisedNebulae

(Version 2.01.16)

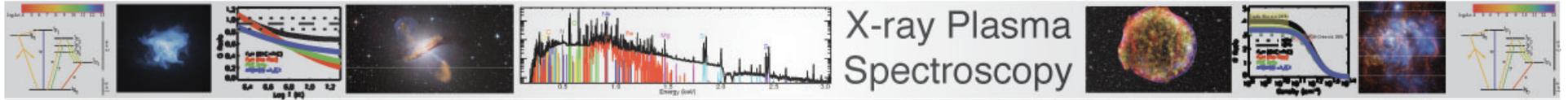
*... can treat ...*

- Bipolar, irregular geometries etc..
- Density &/or chemical inhomogeneities
- Multiple ionising sources
- **3D** gas &/or dust radiative transfer

**IN 3-D!**

*... can provide ...*

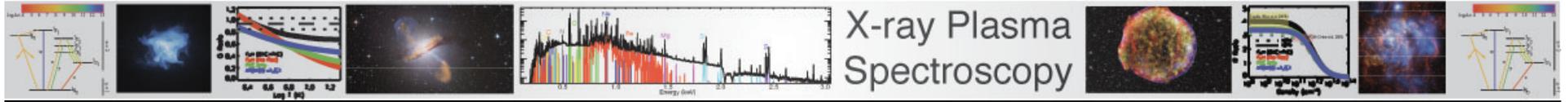
- Emission line intensity tables
- Spectral energy distributions (SEDs)
- 3D (gas &/or dust) temperature distributions
- 3D ionization structures
- Emission line(s), continuum band projections through any line of sight



## Comparison of (some) photoionization models

	<b>Xstar 2.1kn4</b>	<b>Xstar <math>\beta</math> 2.1In2</b>	<b>Warm- abs</b>	<b>Warmab s 2.1In2</b>	<b>Moca ssin</b>	<b>Titan</b>	<b>Cloudy</b>
Xspec interface	Tables	Tables	Analytic	Analytic	?	?	None
Atomic Data	KB01	KB01, K04, Chianti	KB01	KB01, K04, Chianti	Chianti, ?	Chianti, ?	Ferland
Real slab	Y	Y	N	N	Y	Y	Y
Self-consistent SED	Y	Y	N	Y	Y	Y	Y
NLTE	Y	Y	Y	Y	Y	Y	Y
Radiative Transfer	N	N	N	N	Y	Y	N (coming)
Dynamics	N	N	N	(Y?)	N	N	N





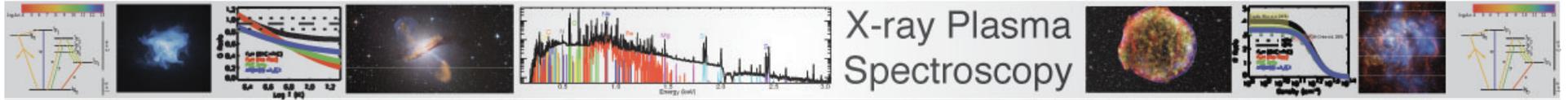
# Comparing photoionization codes

## Main photoionization codes used for X-ray irradiated media

- XSTAR (Kallmann & Krolik)
- Cloudy (Ferland)
- ION (Netzer)
- TITAN (Dumont & Collin)

## Pros and Cons

- **Atomic data:** TITAN is worse, with “only” 1000 lines treated (19000 in XSTAR)
- **Transfer treatment:** TITAN is better (exact transfer for continuum and lines); other codes use “escape probability” formalism for the line transfer and RC
- **Computation time:** TITAN models are very time consuming (up to ~30h for pressure equilibrium models, ~90h for cold/hot solutions with all printouts)
- **TITAN unique features:** selection and self-consistent modeling with the hot/cold solutions; also accurate modeling in total pressure equilibrium



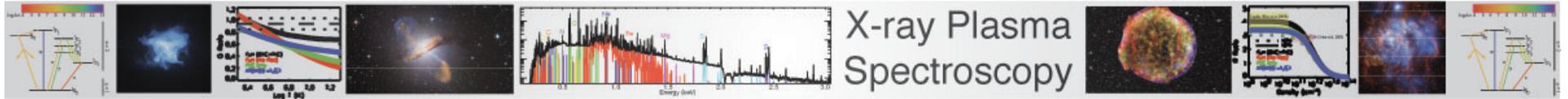
## Atomic Codes

**HULLAC** (Hebrew University / Lawrence Livermore Atomic Code) : Fast, used for many APED calculations, not generally available.

**R-Matrix** : Slow, used for detailed calculations of smaller systems of lines, available on request but requires months to learn.

**FAC** (Flexible Atomic Code) : Fast, based on HULLAC and written by Ming Feng Gu. Available at

<http://www.atomdb.org/fac>



## Ions of Importance

*All ions are equally important.*

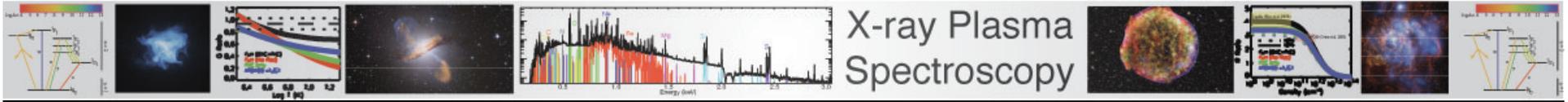
*...but some are more equal than others.*

In collisional plasmas, three ions are of particular note:

**H-like** : All transitions of astrophysically abundant metals (C→Ni) are in the X-ray band. Ly $\alpha$ /Ly $\beta$  is a useful temperature diagnostic; Ly $\alpha$  is quite bright.

**He-like**:  $\Delta n \geq 1$  transitions are all bright and in X-ray. The  $n=2 \rightarrow 1$  transitions have 4 transitions which are useful diagnostics, although  $R=300$  required to separate them.

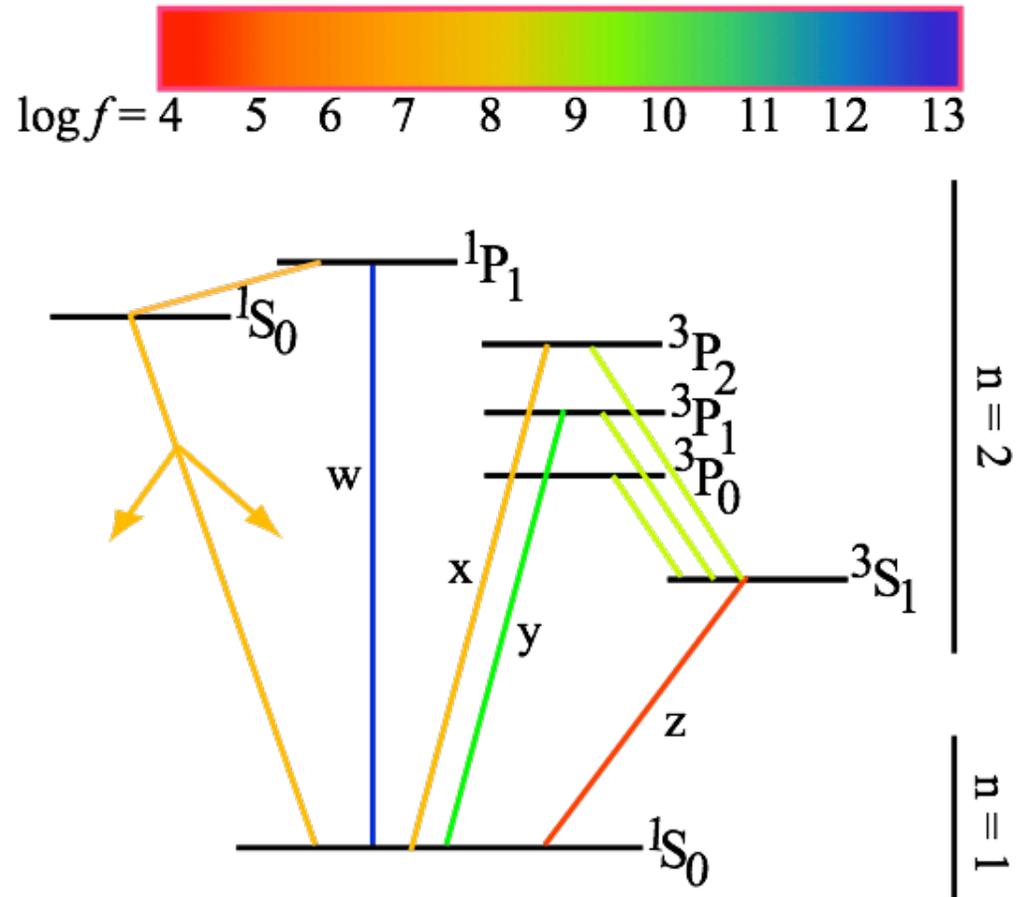
**Ne-like**: Primarily Fe XVII; two groups of bright emission lines at 15Å and 17Å; ionization state and density diagnostics, although there are atomic physics problems.



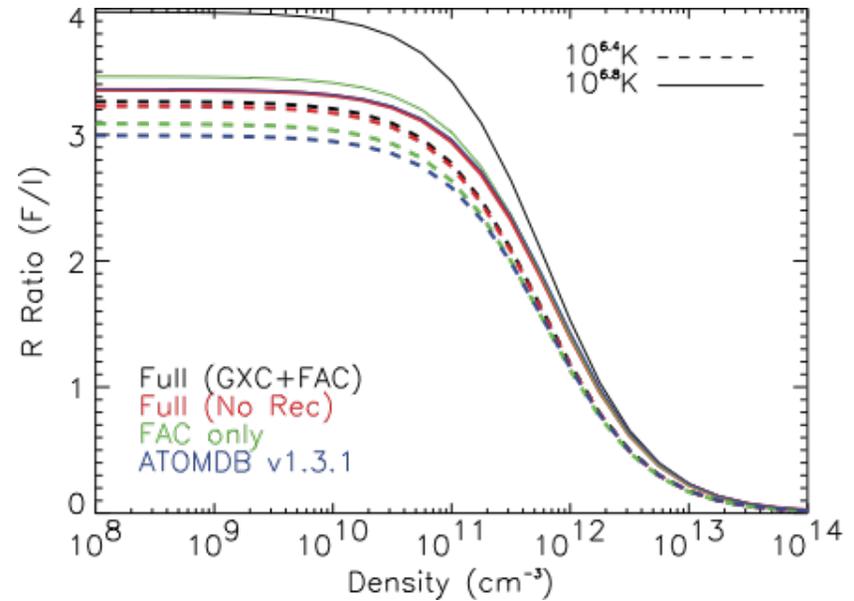
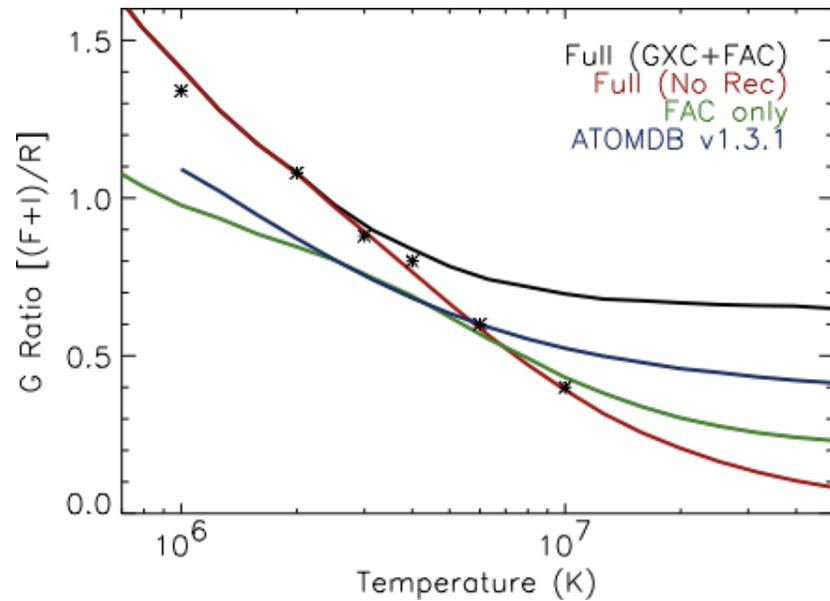
# X-ray Plasma Spectroscopy

## He-like Systems

- All strong transitions
- Different  $f$  ( $A$ ) values lead to line diagnostics



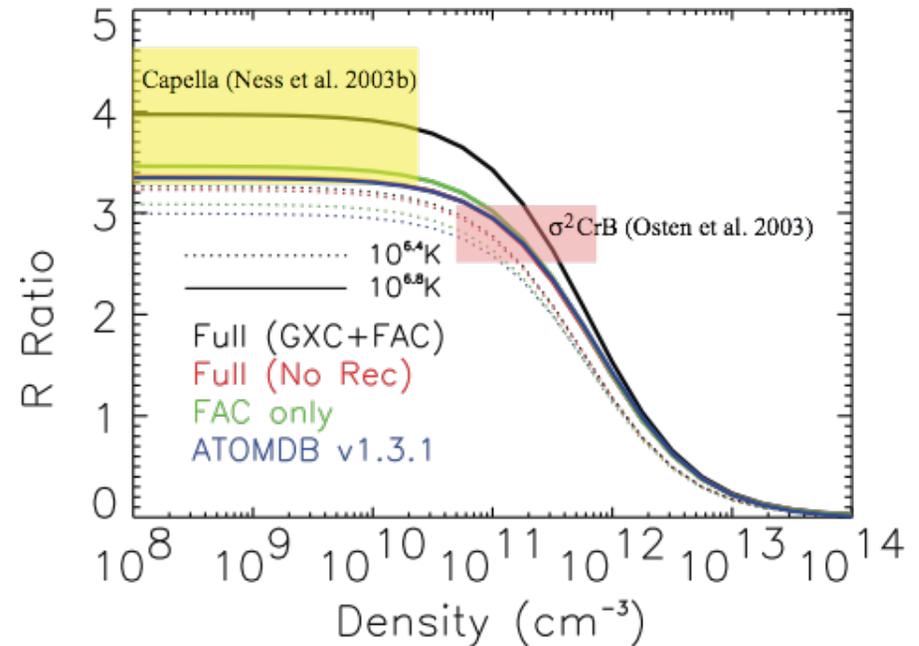
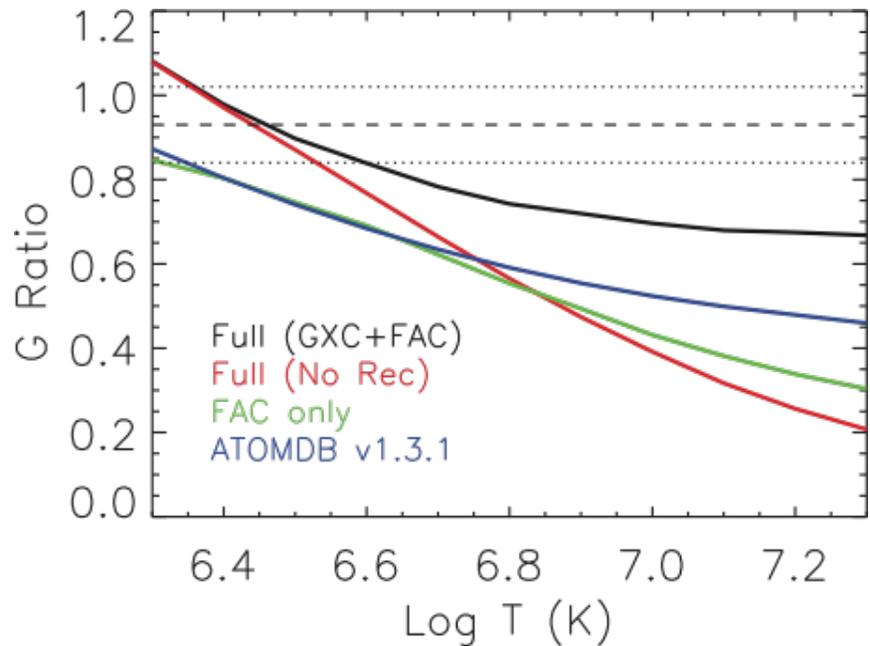
# Line Ratio Calculations



[Left] Temperature diagnostic (triplets/singlet)

[Right] Density diagnostic (forbidden/intercomb)

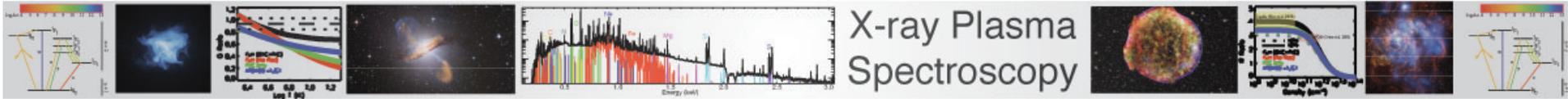
# Line Ratio Uses



[Left] Temperature diagnostic (triplets/singlet)

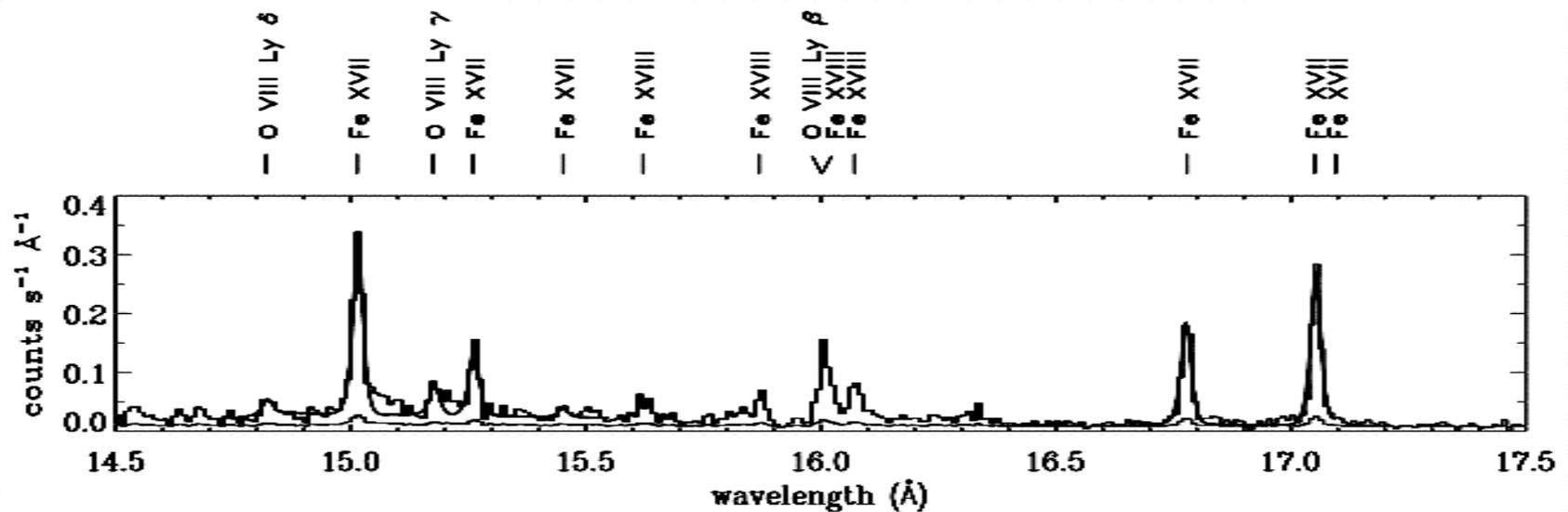
[Right] Density diagnostic (forbidden/intercomb)



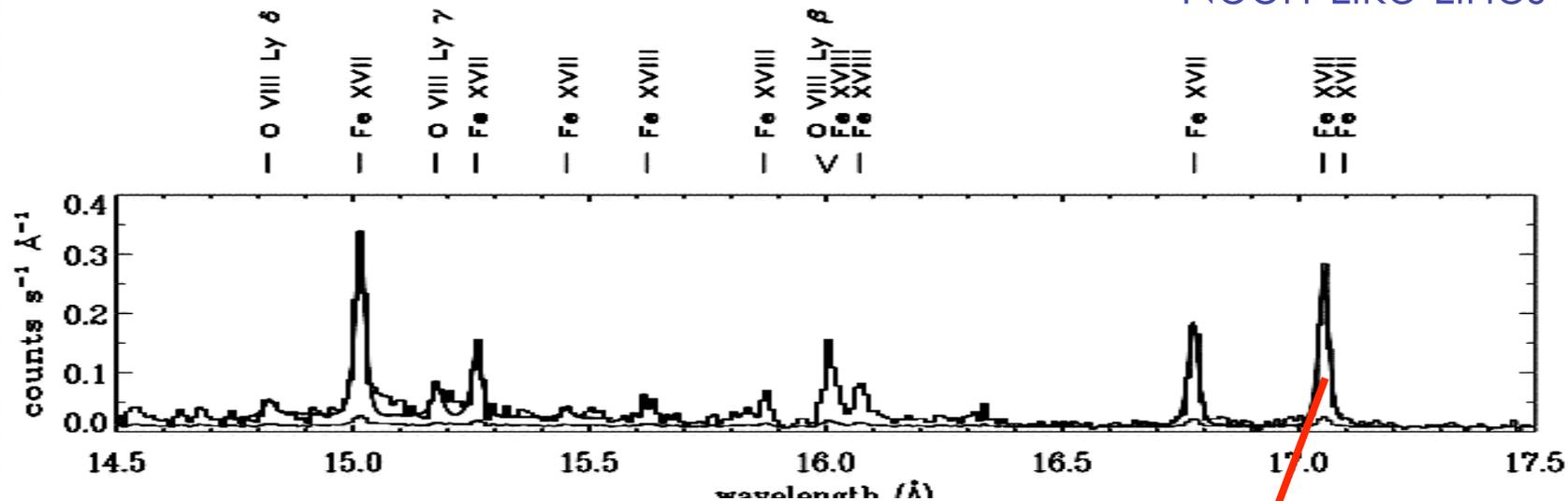


## Neon-Like Lines

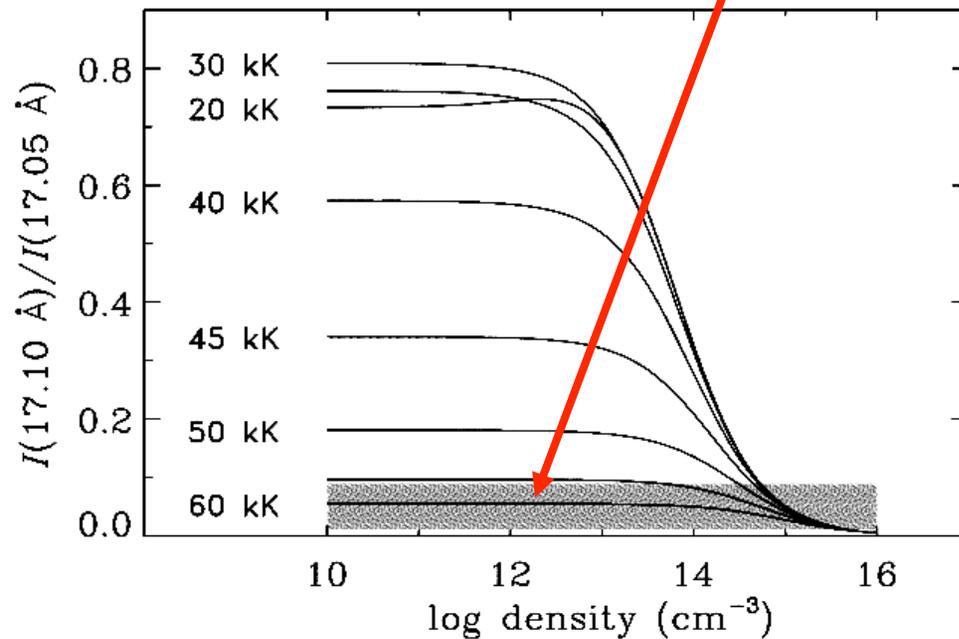
Fe XVII is the most prominent neon-like ion; Ni XIX is 10x weaker simply due to relative abundances. There are a number of diagnostic features, as can be seen in this grating spectrum of the WD EX Hya (Mauche *et al.* 2001):



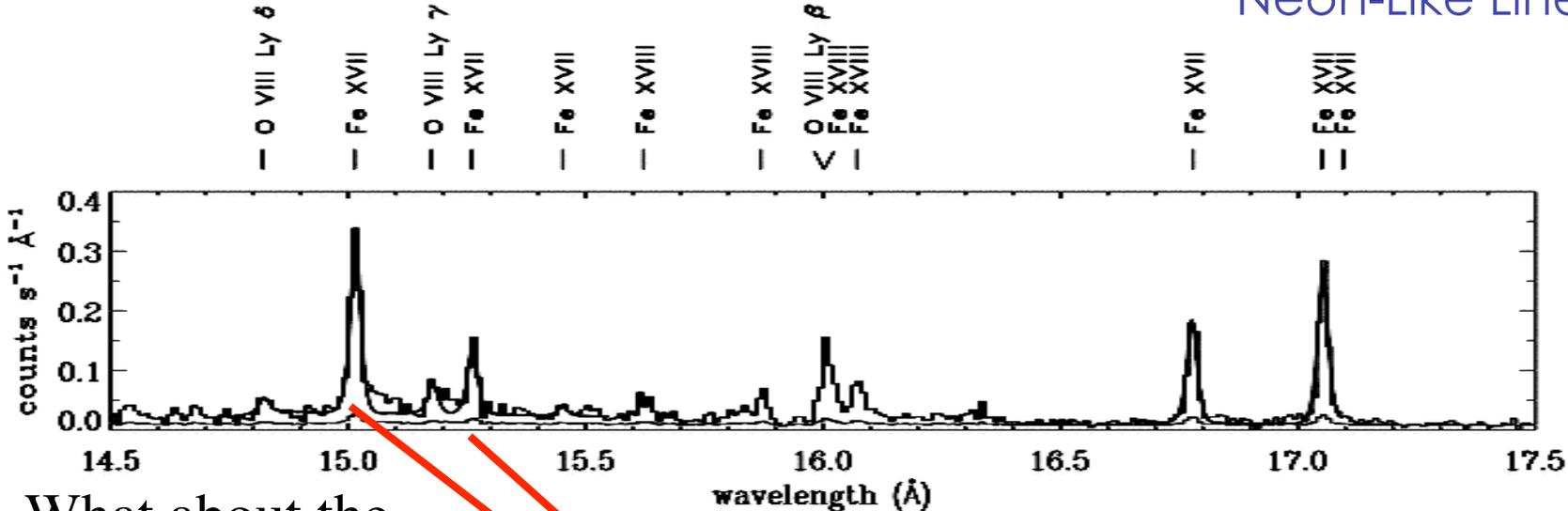
Neon-Like Lines



Here they have extracted the ratio of two very closely spaced Fe XVII lines, which are a density or a UV flux diagnostic

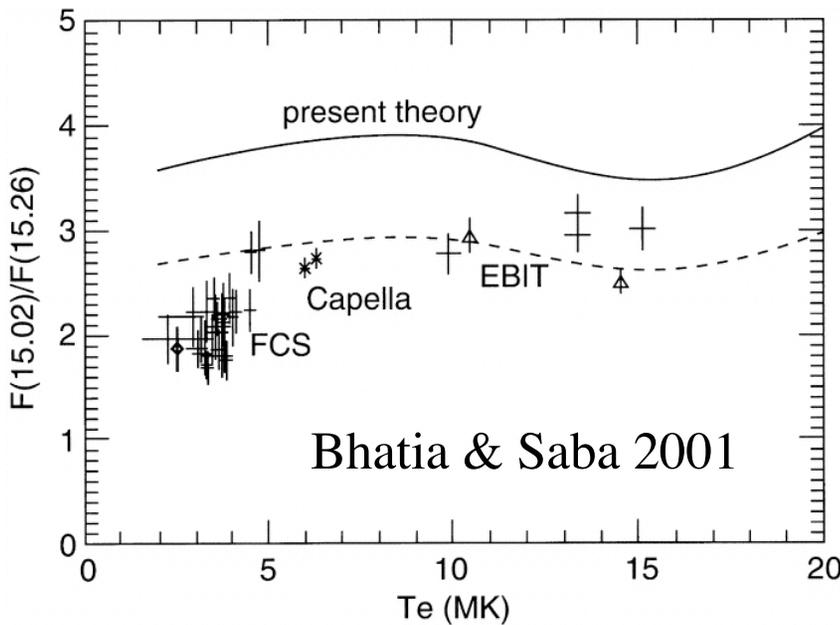


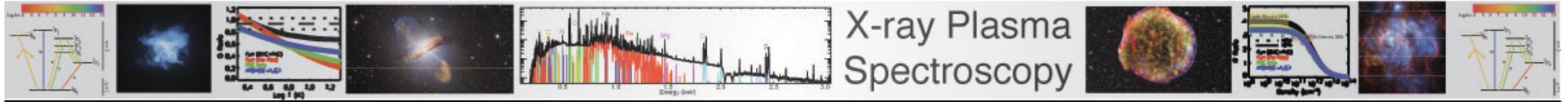
Neon-Like Lines



What about the strong 15.02Å and 15.26Å lines?

They should be useful diagnostics, but right now we're still debating their proper ratio...stay tuned





## Conclusions

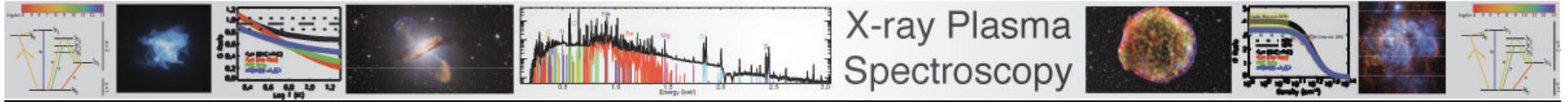
So you've got the spectrum of a plasma: what do you do?

- If high resolution data are available, line-based analysis allows the best control of errors, both atomic and data/calibration.
- If CCD (or worse) is all that you have, remember Clint Eastwood's admonition:

**A spectroscopist's gotta know his or her limitations.**

Keep in mind that :

- (a) only the strongest lines will be visible,
- (b) they could be blended with weaker lines,
- (c) plasma codes have at least 10% errors on line strengths,
- (d) the data have systematic calibration errors, and finally:
- (e) the goal is understanding, not  $\chi^2_n \sim 1$  fits.



## A few words from a code author

- Writing one of these codes is time-consuming, difficult work.
- You may well have a need of some code with ‘a few changes’
- I strongly urge you to
  - Discuss the problem with the code author
  - Offer to collaborate: you’ll make the changes after learning about the code, and include the author in the work!