Organizing Notes

Slack

Slack is designed for “coffee break” type chat. Live questions are answered in the session. Any follow up can occur later on Slack.

This is probably especially useful in the tutorial sessions – if you work on a problem or similar, you can share the results.

Feel free to make whatever channels etc you wish – it is for you to use.

Will be deleted about 2 weeks after the meeting- Some time after 21st August.

AtomDB Training/Questions

If you have detailed AtomDB questions or issues, please get in touch on Slack. I will be available 8-11am on Thursday and Friday.

Talks

Please remember to send slides of your talks to me so I can share them: afoster@cfa.harvard.edu

Updates to AtomDB

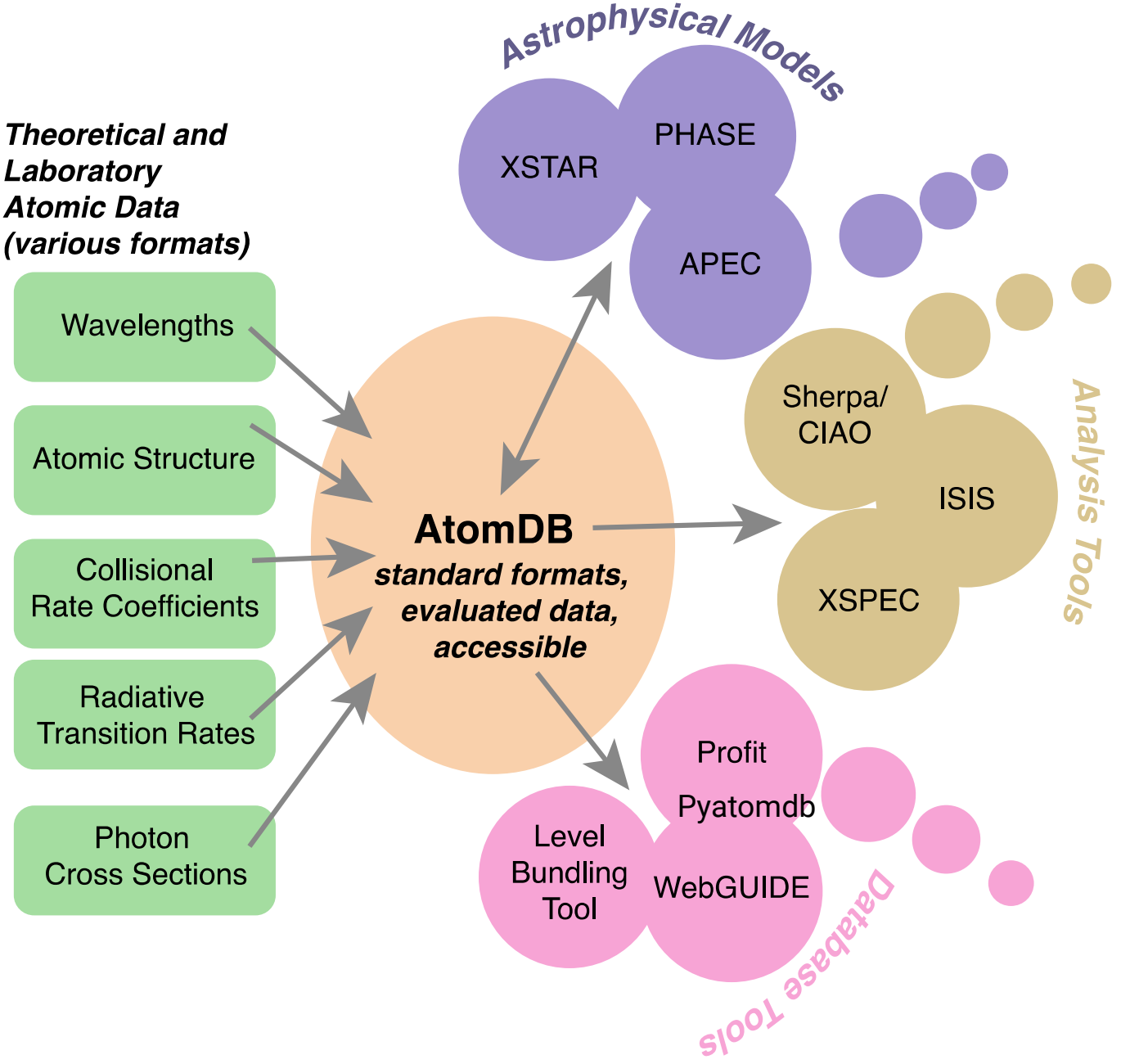
Adam Foster
Smithsonian Astrophysical Observatory
afoster@cfa.harvard.edu

With contributions from:
Randall Smith
Keri Heuer
Lots of people who filed bug reports...

What is AtomDB?

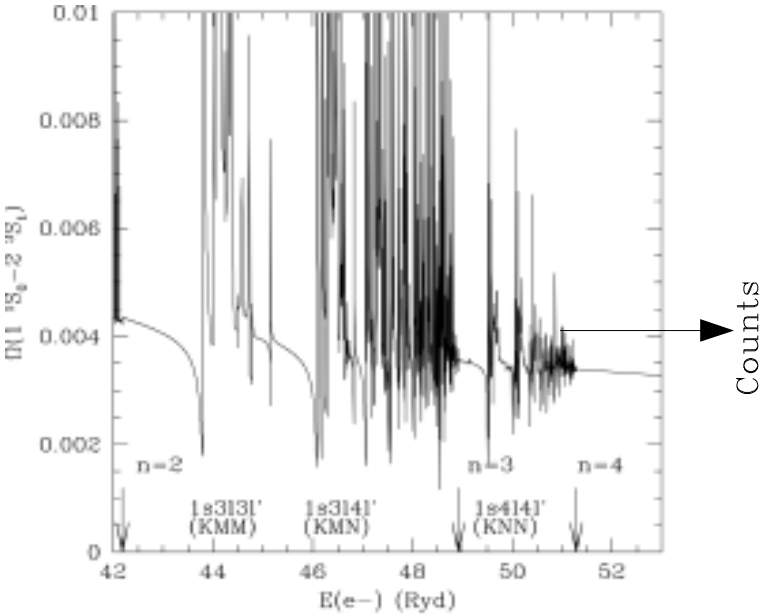
Large collection of atomic data used to model a range of X-ray emitting plasmas

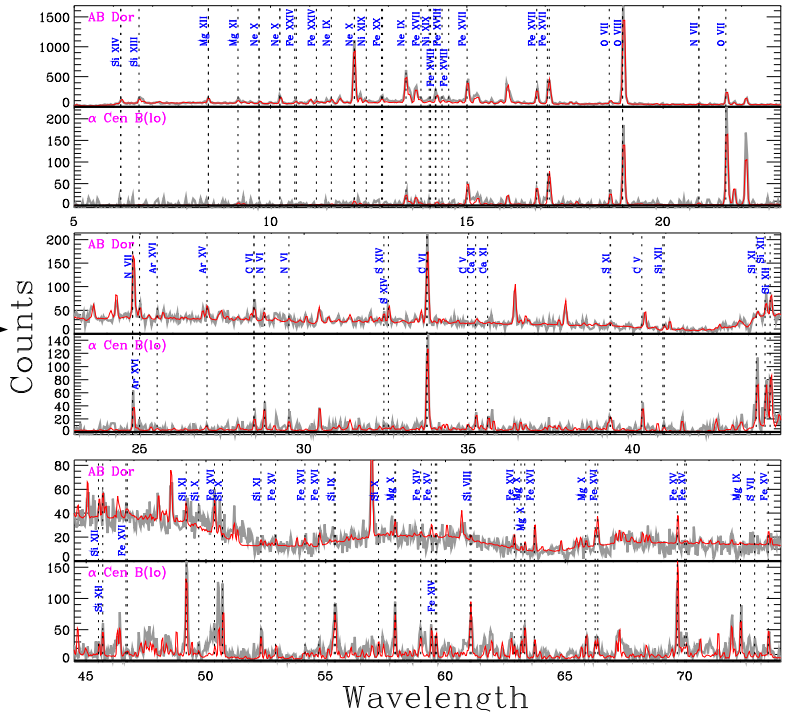
- Create **useful** spectra for data analysis
- Ensure tight **integration** into modeling tools
- Provide **open access** to all the data and the models
- Ingest and **update** models with new atomic data
- Identify atomic data needs and **communicate** them to data producers



What AtomDB does

APED (database) → APEC (plasma code) → Emissivity Files → XSPEC (etc) apec model






```
>xspec
XSPEC12> model apec
XSPEC12> fit
```

O6+ collision strengths

Stellar Spectra

Simple input!

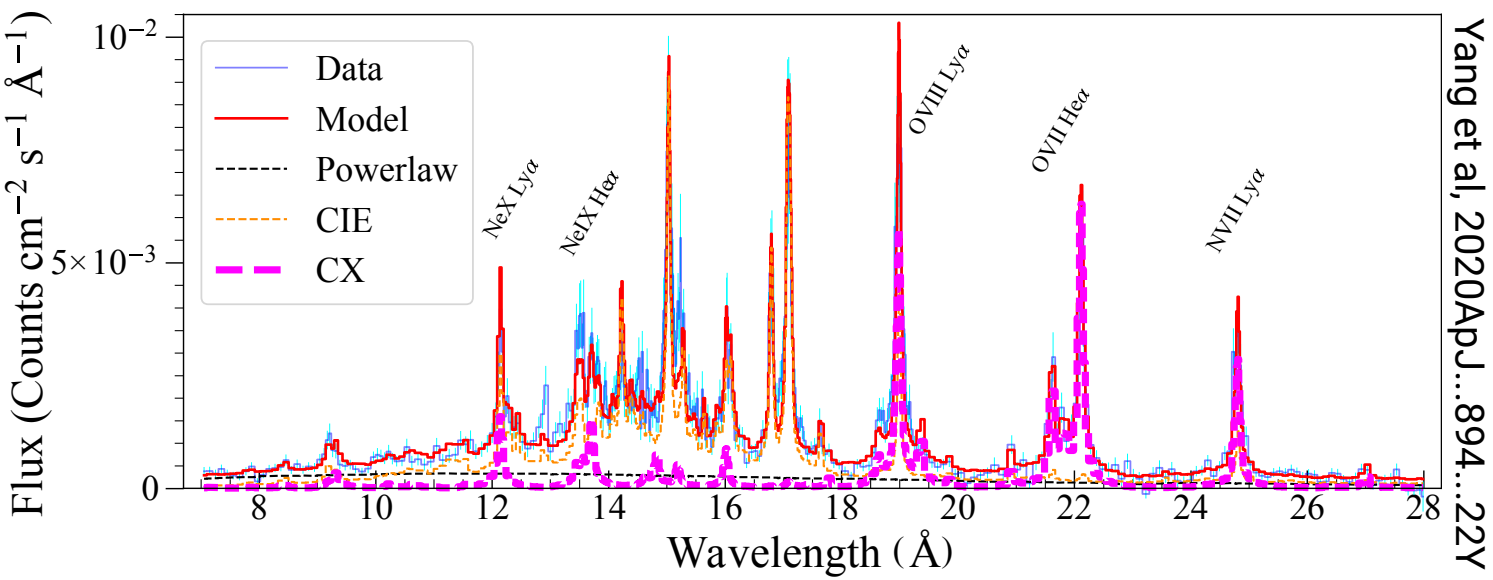
What's new in 2020 [ish]

- Mostly Usability, Software and Models:
  - PyAtomDB
  - Charge Exchange
  - Non-Maxwellian Electrons
  - XSPEC/Sherpa integration
  - Website updates
- Upgrades and new work on Uncertainties

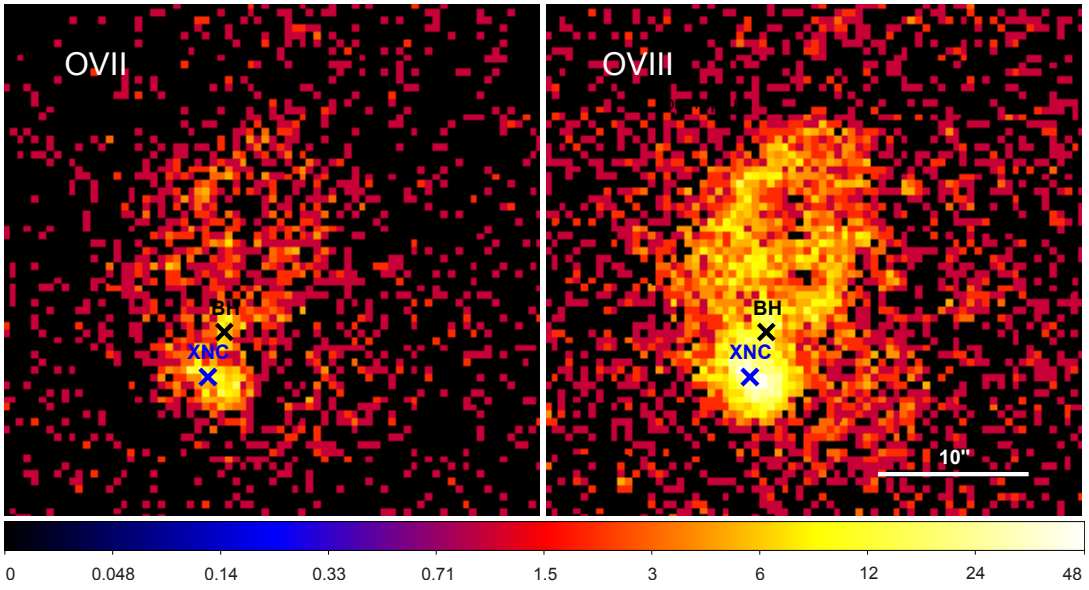
Charge Exchange Models

CX Models updated to include real cross sections from U.GA Kronos database.

Released as ACX2



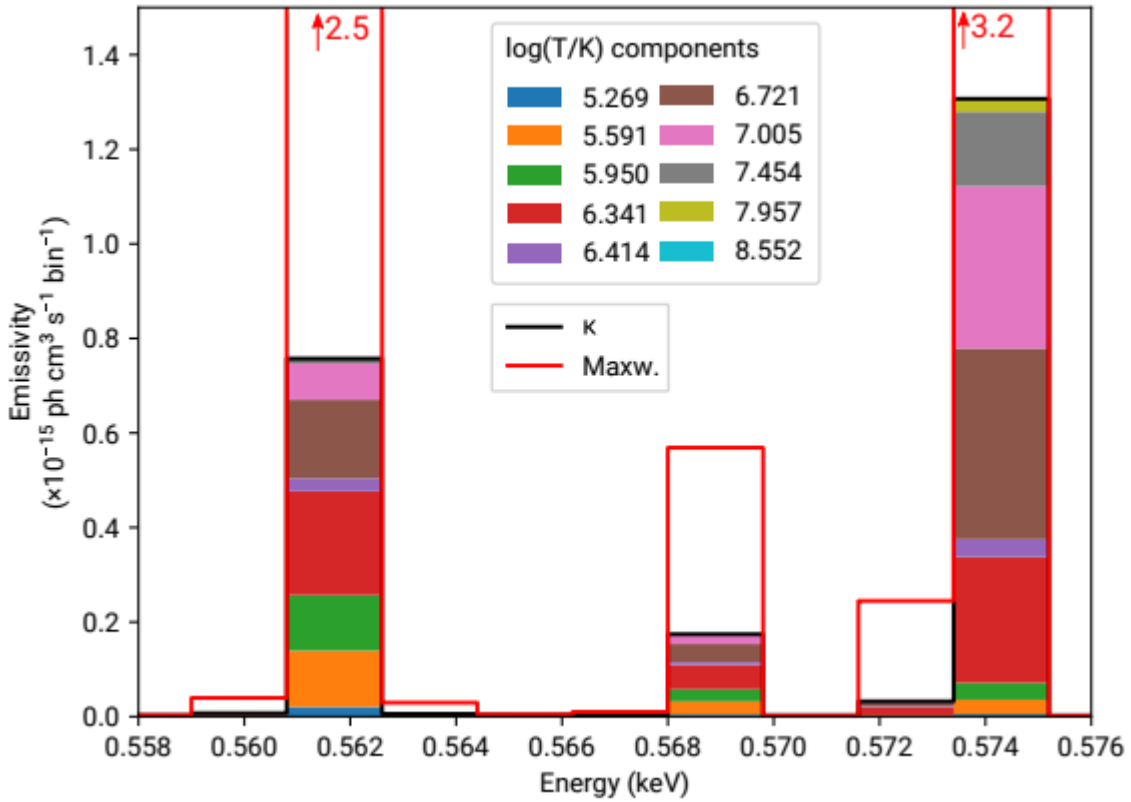
Used to model M51 emission, locating interaction of AGN jet and quantifying interaction region



http://www.atomdb.org/CX/

Non-Maxwellian Modeling

K=2 vs Maxwellian plasma @0.2keV



Kappa model created based on sum-of-Maxwellians (2015ApJ...809..178H) to approximate non-thermal electron distributions. Devised by 2019ApJ...887..182C

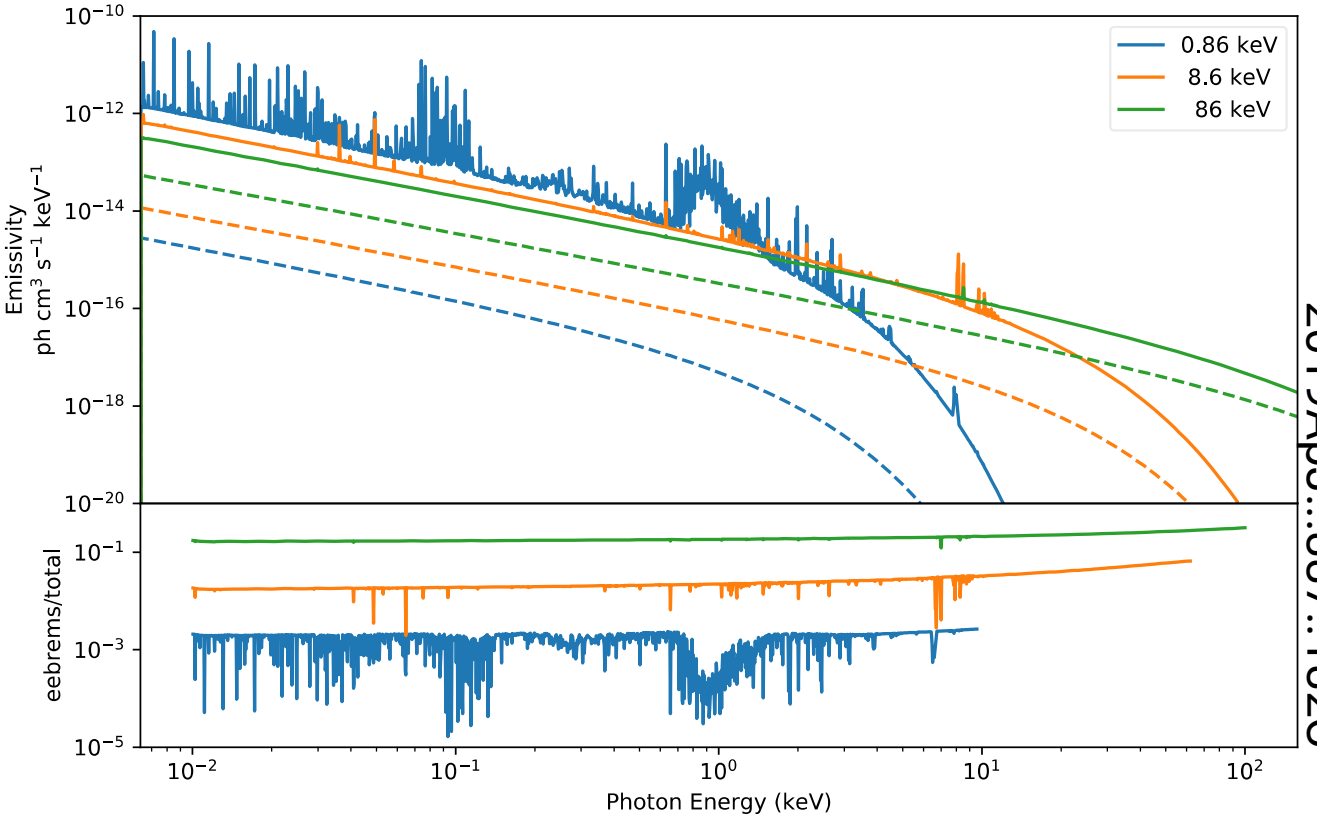
Non-Maxwellian plasma model published 2019ApJ...887..182C
And released as a stand-alone XSPEC model (http://atomdb.org/kappa/)

Electron-Electron Bremsstrahlung

- At high energies (kT~>10keV), electron-electron interactions create an additional intense Bremsstrahlung component.

As electrons approach relativistic speeds, the electron-electron brems is at least equal to the electron-proton brems.

Now included in PyAtomDB, will be in XSPEC apec model after next release



PyAtomDB

Ongoing project to open source all the atomic codes and models within AtomDB, while providing easy access to the underlying data.

Python 3 module on Github: https://github.com/AtomDB (or "pip install pyatomdb")

Documentation: https://atomdb.readthedocs.io/

- Basing all the models on the same sets of atomic data and access routines
  - Consistency
  - New data is applied to all models simultaneously
- Modules (the interesting ones):
  - apec: the plasma code, converting atomic data to thermal plasma emissivities.
  - atomdb: tools for interacting with the database, downloading and extracting atomic data.
  - spectrum: converting the outputs of apec into an assortment of plasma spectra, for equilibrium, non-equilibrium, and other spectra.
- All models comes with wrappers allowing them to be used in XSPEC; Sherpa coming soon.

Online Tools

Transition information for Ne VIII, from level 7 to 1

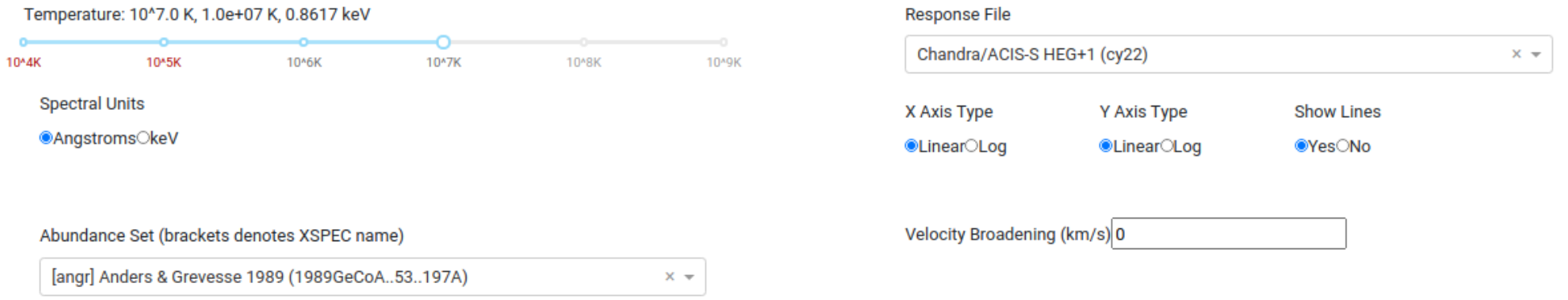
Energy level 7	
Electron configuration	1s2 3d1
Energy above ground (eV)	142.2529
Quantum state	n=3, L=2, S=0.5, degeneracy=4, parity=0
Energy Level Data Source	NIST ASD 5.3
Photoionization Data Source	Clark, Cowan, and Bobrowicz 1986

Energy level 1	
Electron configuration	1s2 2s1
Energy above ground (eV)	0.0
Quantum state	n=2, L=0, S=0.5, degeneracy=2, parity=0
Energy Level Data Source	2011A&A...528A..69L
Photoionization Data Source	Verner and Yakovlev 1995

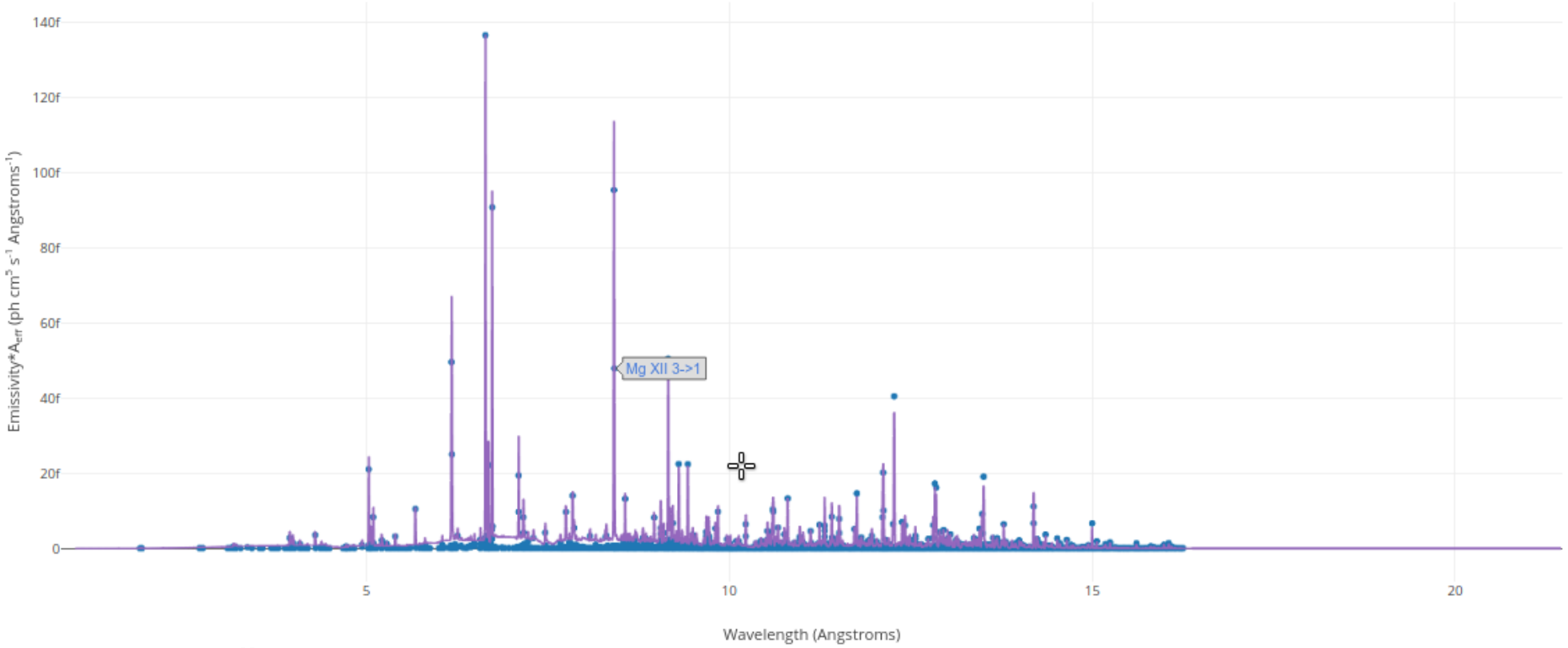
Level 7 → 1 Interactions	
Electron collision rate	Nonzero
Electron collision reference	2011A&A...528A..69L
Wavelength (theory)	87.157623Å
Transition rate/Einstein A	2.07e+07 s^{-1}
Transition type*	M1
Oscillator Strength $f_{1 \rightarrow 7}$	4.714898e-05
Wavelength (theory) reference	NIST ASD 5.3
Wavelength (lab/observed) reference	
Transition rate reference	2011A&A...528A..69L

http://www.atomdb.org/Webguide/

Online Tools



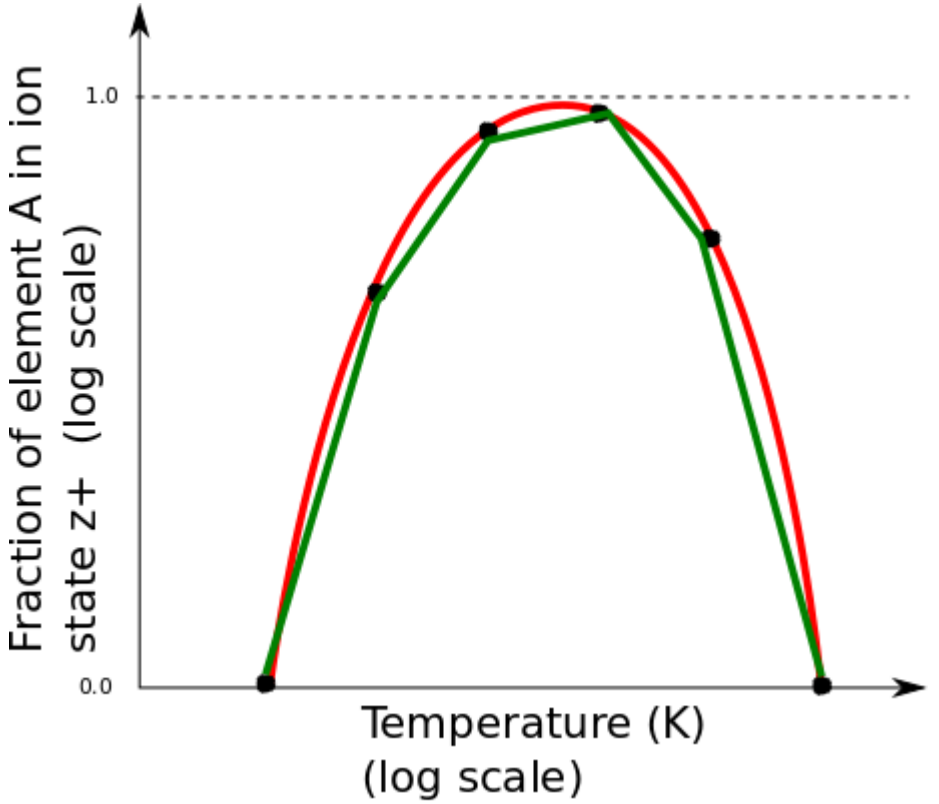
Replace a popular apple AtomDB App
with a web based solution



http://app.atomdb.org

Change to the standard temperatures

- AtomDB Emissivity files for APEC model are stored at 51 temperatures from 10^4 to 10^9K.
- To get emission at intermediate temperatures, XSPEC interpolates between them.
- In some edge cases, the knots become apparent



Solutions:

1) Update to 201 temperature grid (done, now default in XSPEC). Variations now in the few % range.
2) Prefer use of rnei model ("done", but is ~6 times slower than APEC)
3) Change simple continuum emission (e.g. Brems) to be done on the fly instead of tabulated (still in the thinking stage)

Uncertainties on Atomic Data

Uncertainties on atomic data are a serious underlying issue

Complex spectra rely on millions of individual pieces of atomic data

But which matter the most?

Start small – ionization and recombination rates

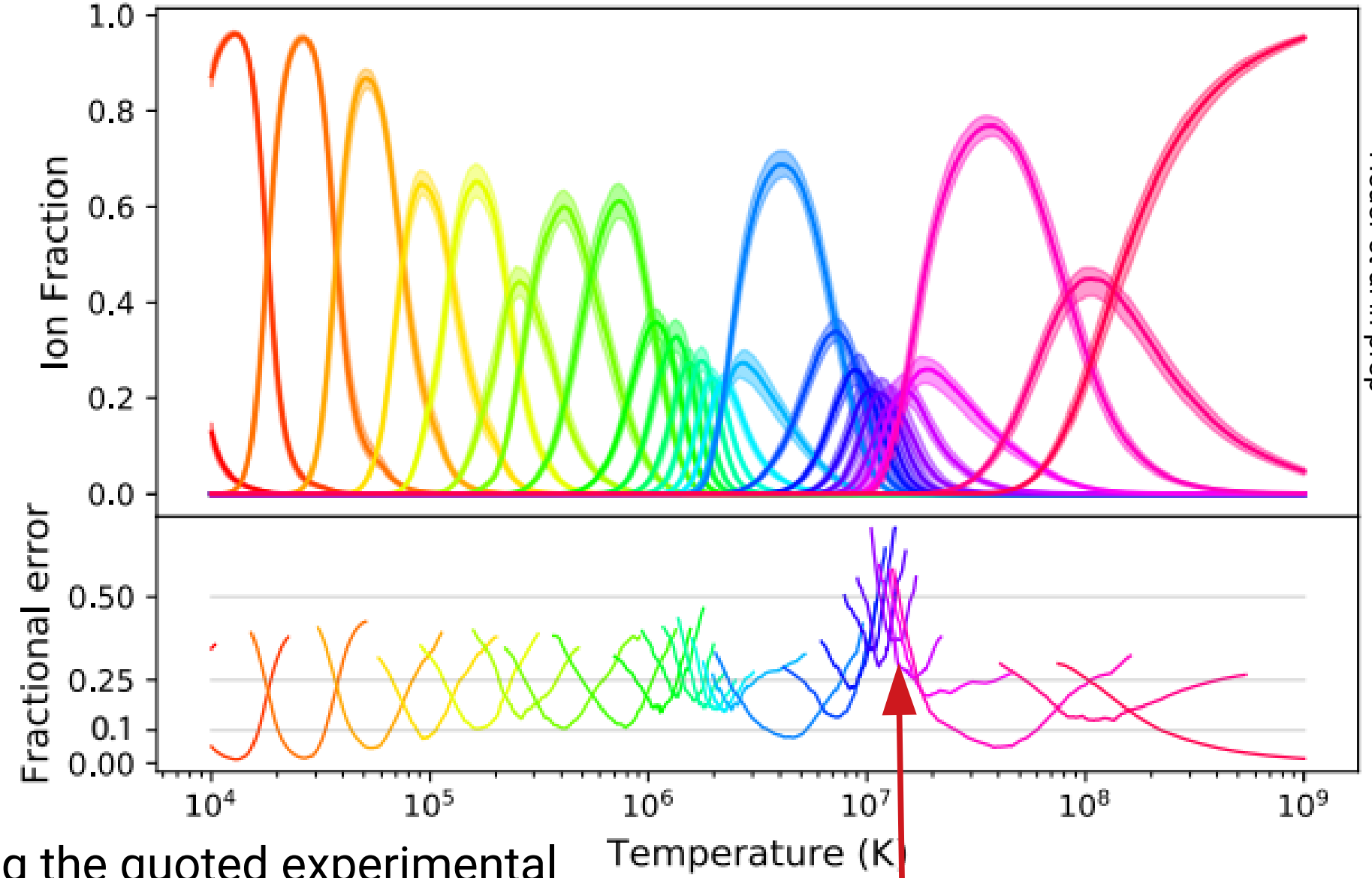
Table 2. Systematic uncertainties for experimentally measured recombination rate coefficients.

Ion	Error	Type[a]	Method[b]	Reference	ΔR	Comparison
O 7+	25%	DR		Kilgus et al. 1990	20%	Bell and Bell 1982.
	18%	RR	cb	Andersen et al. (1990)		
O 6+	20%	DR		Andersen et al. (1990)		
O 5+	11%	DR	cb	Böhm et al. (2002)		
	20%	DR		Andersen et al. (1990)		
	35%	DR	cb	Dittner et al. (1987)		
	18%	RR	cb	Andersen et al. (1990)		
O 4+	30%	DR	cb	Dittner et al. (1987)		
Fe 24+		DR	cb	Schmidt et al. 2006		

Looked through all currently and recently available data to assemble uncertainties on experimental ionization and recombination rates

Find average of roughly 25% uncertainty on recombination rates and 15% on ionization rates.

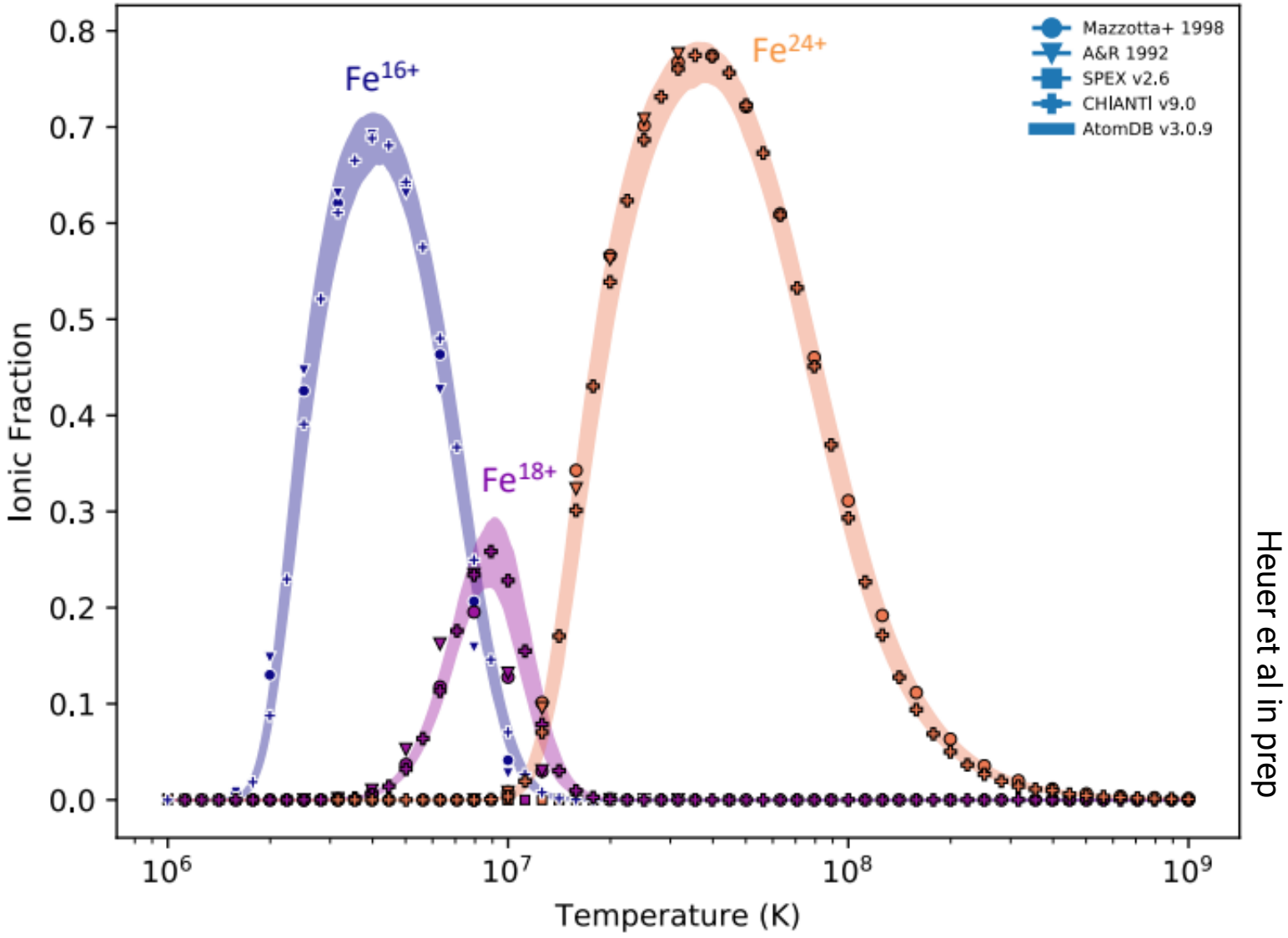
Uncertainties on Ionization & Recombination Rates



Applying the quoted experimental uncertainties has a huge effect on underlying rates!

Minimum 30%!

Comparison with Published Collections

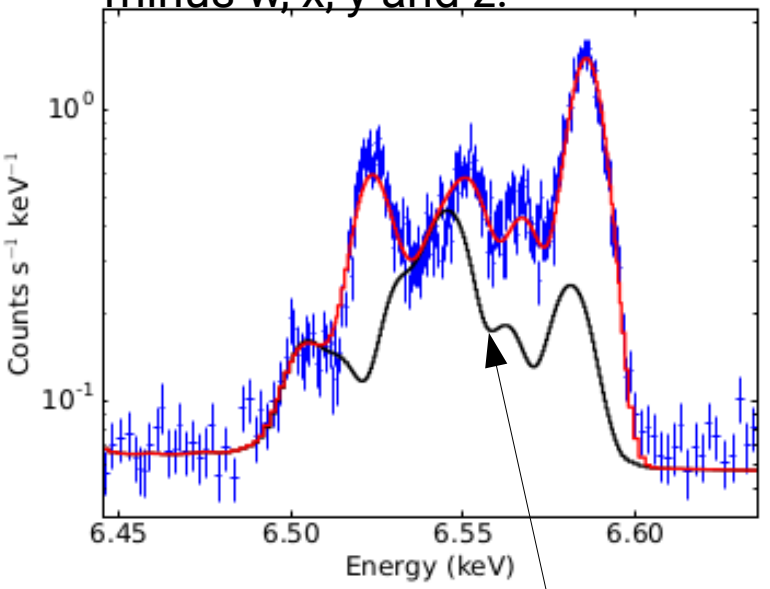


The end result of most of the updates to ionization and recombination rates in recent history lie within the error range of experimental values

Li-like ions are important

Large quantities of emission in He-like bands are dependent on neighboring ion populations

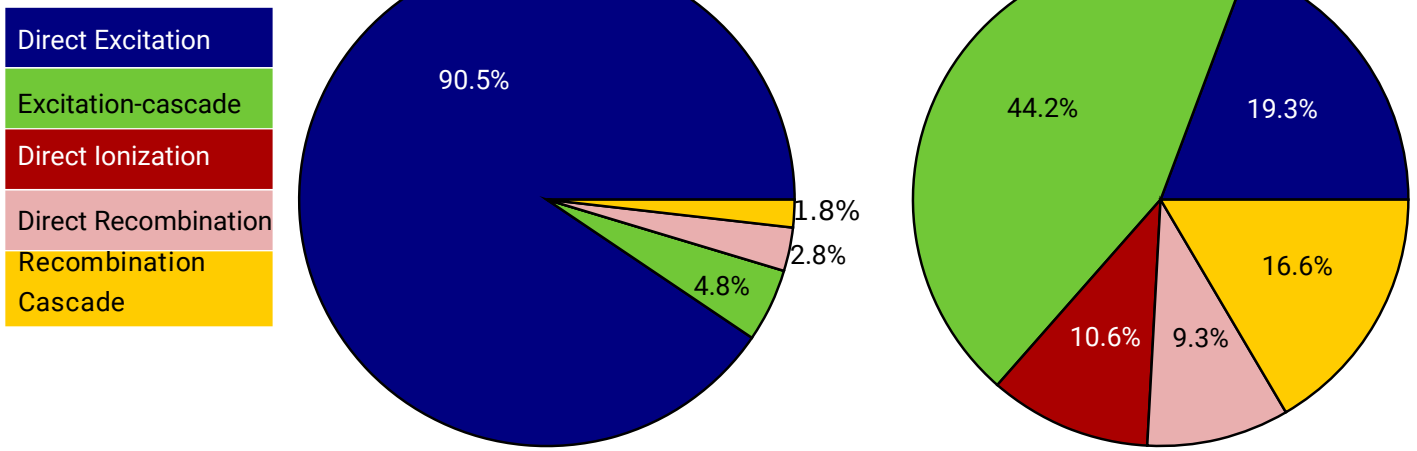
SXS Perseus He-like Fe band, minus w, x, y and z.



20-30% of the flux!

1s 2p $^1P_1$ resonance line

1s 2s $^3S_1$ forbidden line



Upcoming Plans

- Release of AtomDB 3.1 (this year)
  - Change of ionization rates to Urdampilleta
  - Inclusion of ee-brems as standard, 201 temperature bins
- Interface work
  - Fold in CX and Kappa work into PyAtomDB
  - Improve code speed
  - Rewrite APEC module to improve performance
- Uncertainties work
  - Line diagnostic sensitivities to underlying atomic data
  - Estimating uncertainties on fundamental atomic data
- Density sensitive diagnostics
  - Simple models for density sensitive line ratios and ionization balance calculations
- Atomic Data
  - L shell ions will be the next priority for update

Feedback drives development!

Please let us know what you want/what you have