Evaluating uncertainties on atomic data for X-ray spectral diagnostics

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AtomDB workshop
November 3rd 2017

Outline

- Motivation for uncertainties to be used in astrophysical diagnostics
- An overview of uncertainties propagating from fundamental atomic data through to spectral diagnostics.
- Baseline uncertainties on atomic data.
- Correlation in fundamental atomic data.
- The planned modeling tools & call for suggestions.

Motivation

- Uncertainties on fundamental data (*energies, A-values, excitation, ionization, recombination*) would allow uncertainties on:
  - Emissivities for line intensities & spectral comparisons, line ratios.
  - Fractional and elemental abundances.
- This would allow:
  - Uncertainties to be put on diagnostics (T_e, n_e, abundances etc.)
  - The source of differences between atomic databases would be easier to identify.
  - Provide feedback to atomic physicists on which processes need to be calculated with more accuracy.

Increasing interest & demand for uncertainties

- Interest in uncertainties has been growing.
  - NIST has a long history of assigning A-value uncertainties.
  - Conference: “Uncertainties in Atomic Data and How They Propagate in Chemical Abundances”, Proc. of the Int. Astr. Union, IAU Symposium, **283**, p. 139-143 (2011)
  - IAEA conference series: https://www-amdis.iaea.org/meetings/UQ2016/
- Recent papers include:
  - Foster et al., Space Science Review **157** : 135 (2010)
  - Bautista et al., ApJ **770** : 11 (2013)
  - Juan de Dios & Rodriguez, MNRAS 469 : 1036 (2017)
  - Loch et al., AIP conference proceedings **1545** 242 (2013).
  - Wang et al., MNRAS **469** : 1225 (2017)

Planetary Nebulae: An Eye to the Future
Proceedings IAU Symposium No. 283, 2011
A. Manchado, L. Stanghellini & D. Schönberner, eds.
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Report on the Tenerife Workshop on Uncertainties in Atomic Data and How They Propagate in Chemical Abundances

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Summary Report of the 3rd Biennial Technical Meeting

IAEA Headquarters, Vienna, Austria

6–8 May 2013

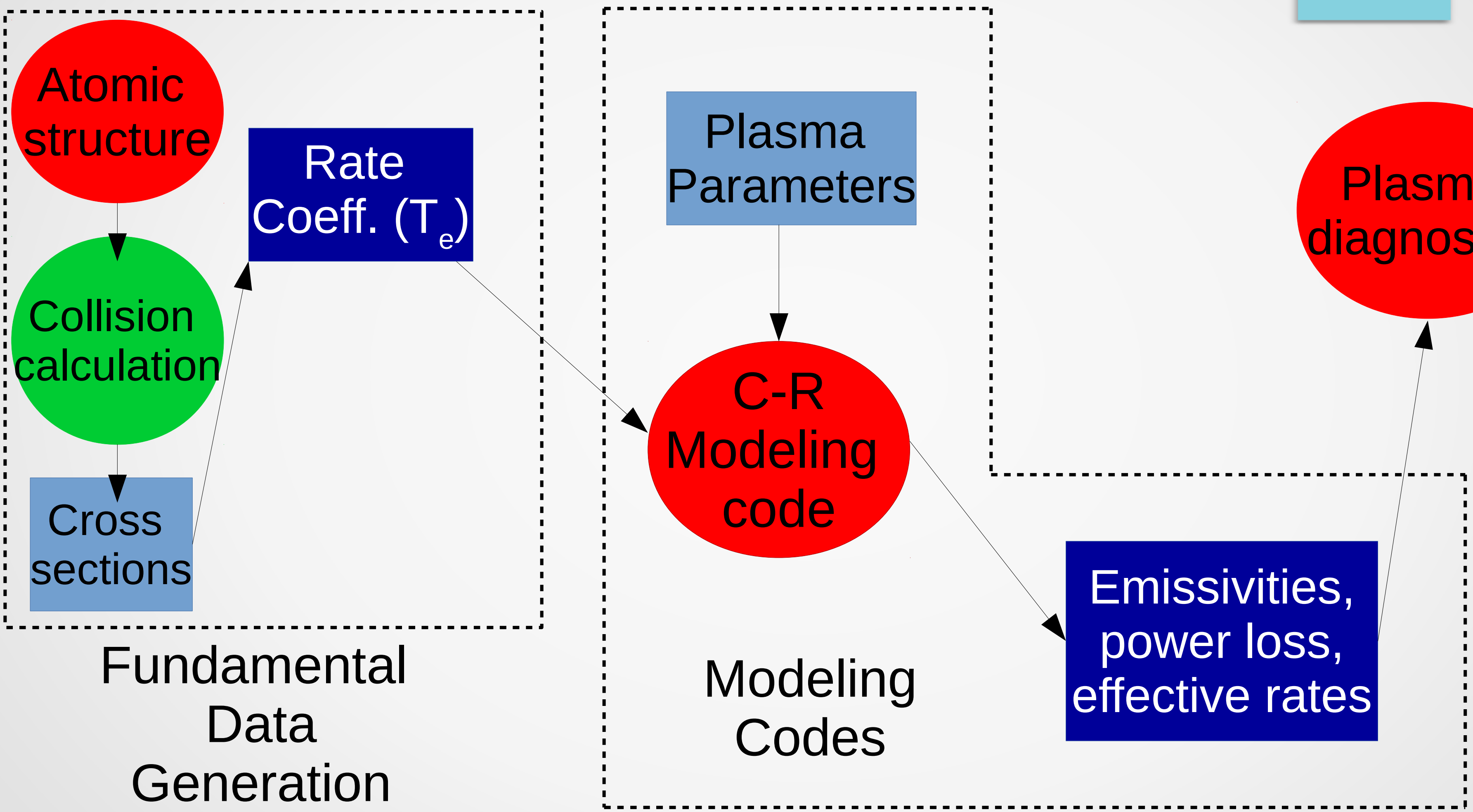
Prepared by

Hyun-Kyung Chung

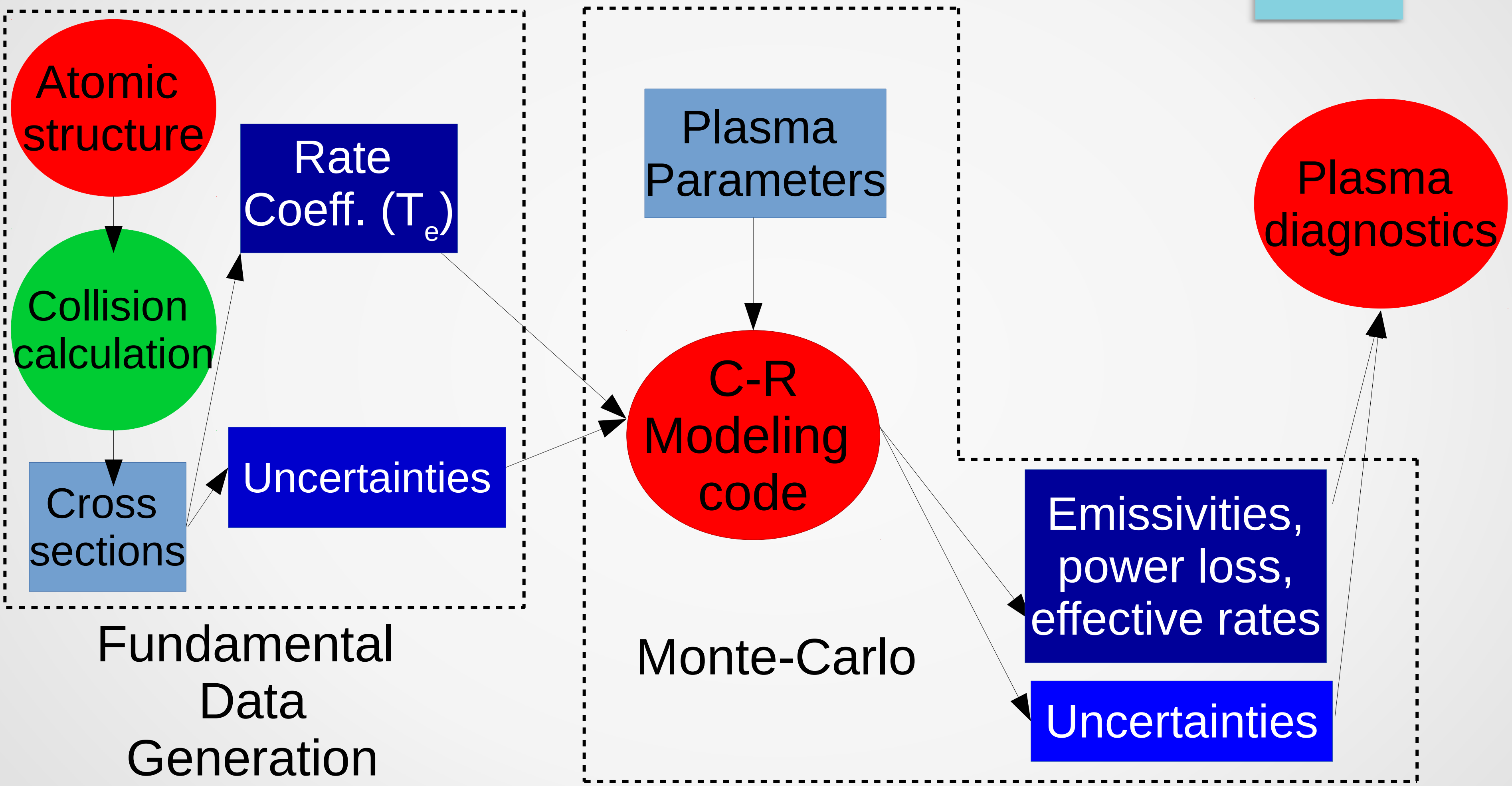
Abstract

This report summarizes the proceedings of the third Technical Meeting of the International Code Centres Network held on 6-8 May in 2013. Ten experts from seven member states and four IAEA staff members attended the three-day meeting held at the IAEA Headquarters in Vienna to discuss issues on uncertainty estimates of theoretical atomic and molecular data. The report includes discussions on data issues, meeting conclusions and recommendations for the IAEA Atomic and Molecular Data Unit.

Big Picture Overview



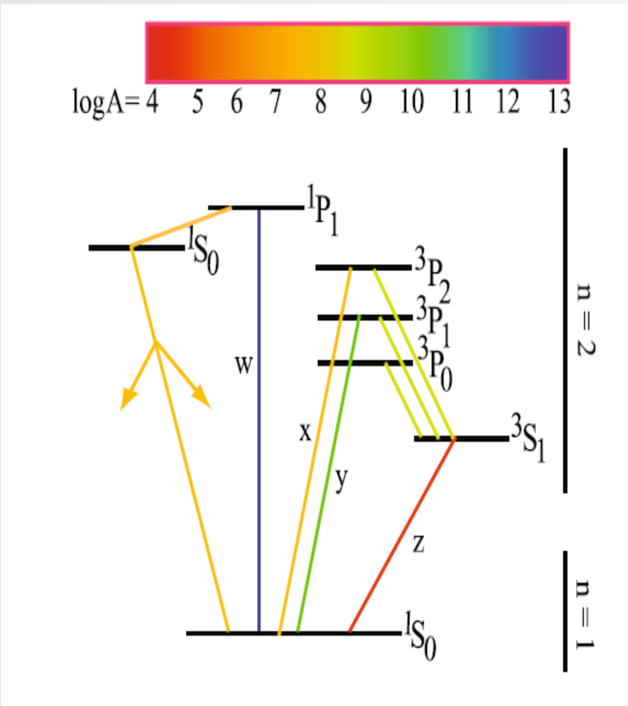
We would like to move to the following



Scope of this study

- Focus on uncertainties on **<u>theoretical atomic data</u>**
  - Other studies investigated uncertainties using multiple theoretical datasets, and comparing with observations [e.g., Bautista et al. (2013)].
- We will initially consider atomic systems for which existing theoretical methods should be accurate.
  - i.e., no missing physics or convergence limitations.
- The role of experimental measurements will be to constrain and guide the range of values in the theoretical calculations.
- We seek to <u>automate</u> the production of uncertainties.
  - First ***baseline*** methods to cover many systems.
  - Then ***method sensitivity*** approaches which would include correlation.

Example 1 : The problem with uniform uncertainties
The G- and R-ratios in He-like O



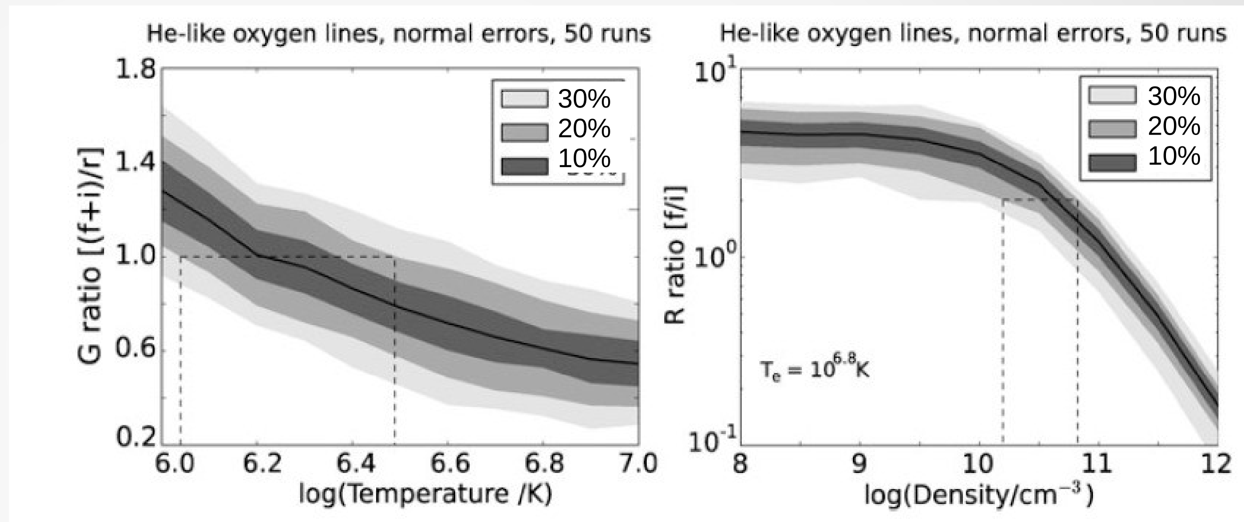


Figure from Foster et al. *Space Science Review* **157** : 135 (2010)

Flat uncertainties

- *Can lead to large uncertainties in diagnosed quantities.*
- Not very physically meaningful.
  - They don’t have any temperature-dependence
  - It is not right to assign a fixed uncertainty (even to a whole class of transitions).

Example 2 : Can you be sure of your physical interpretation?

Mon. Not. R. Astron. Soc. **415,** 244–250 (2011) doi:10.1111/j.1365-2966.2011.18695.x

Unveiling the spatial structure of the overionized plasma in the supernova remnant W49B

Xin Zhou,[1,2★] Marco Miceli,[2,3] Fabrizio Bocchino,[2] Salvatore Orlando[2] and Yang Chen[1,4]

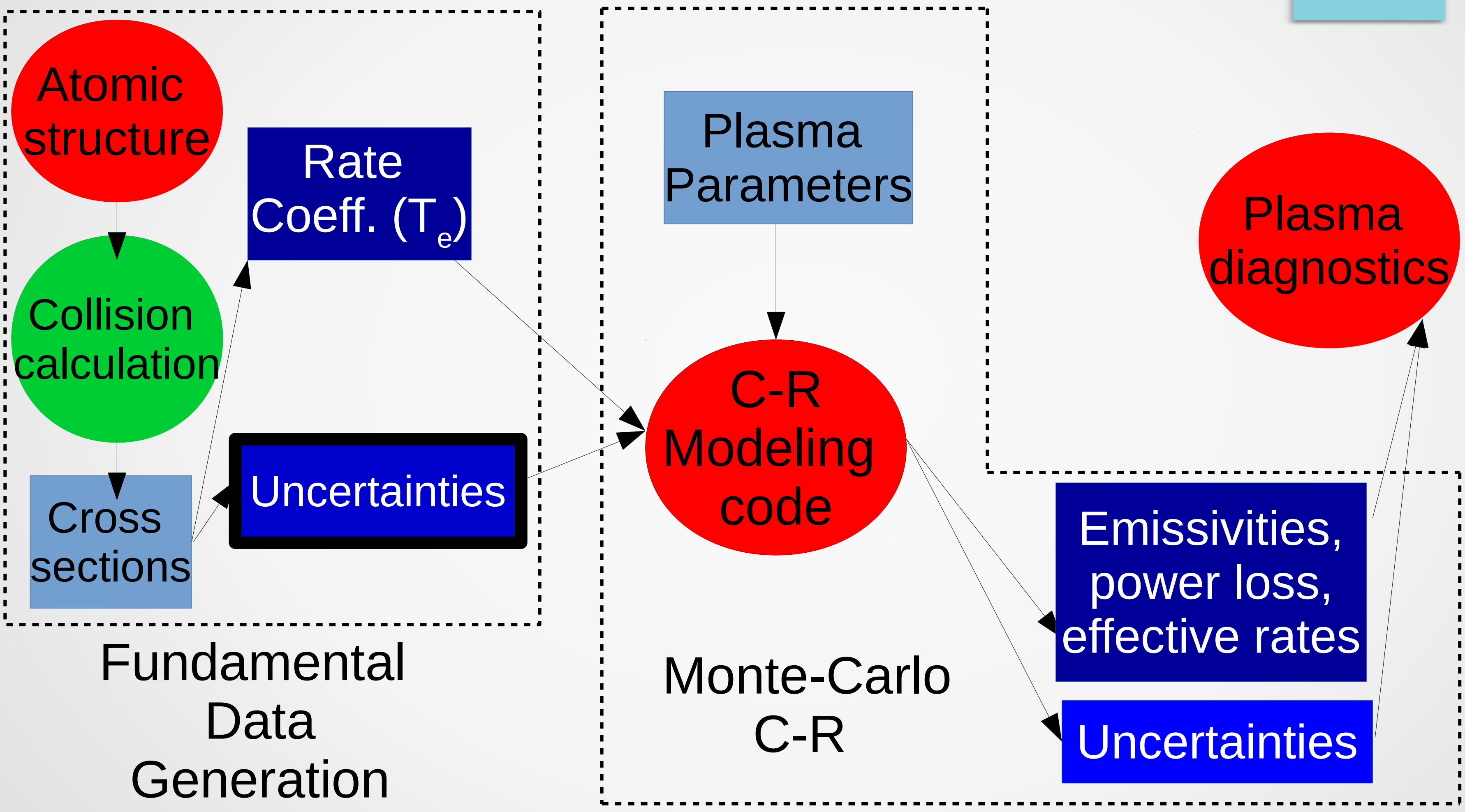
The Astrophysical Journal, 777:145 (6pp), 2013 November 10 doi:10.1088/0004-637X/777/2/145

UNRAVELING THE ORIGIN OF OVERIONIZED PLASMA IN THE GALACTIC SUPERNOVA REMNANT W49B

Laura A. Lopez[1,5,6], Sarah Pearson[2], Enrico Ramirez-Ruiz[3], Daniel Castro[1], Hiroya Yamaguchi[4], Patrick O. Slane[4], and Randall K. Smith[4]

- Supernova Remnant plasma W49B is well known to be ‘overionized’
  - It has an overabundance of H-like ions, compared to He-like ions.
  - This is thought to be due to adiabatic cooling of the electrons.
- This conclusions is likely to be sound.
- Uncertainties on ionization and recombination rates would
  - Give added confidence that this is a real effect and help in testing the explanation.

Baseline uncertainties

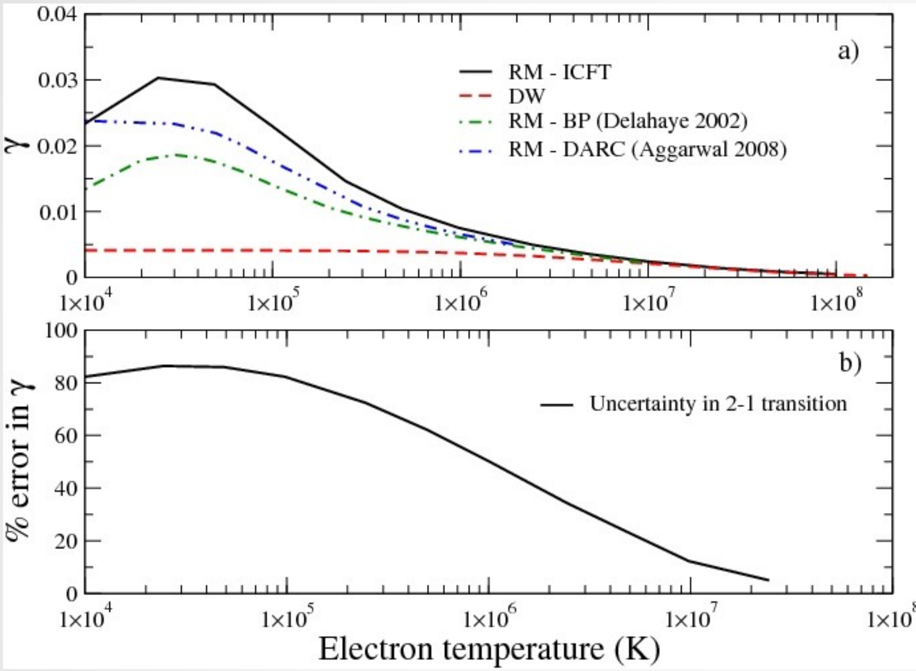


Overview of Baseline uncertainties

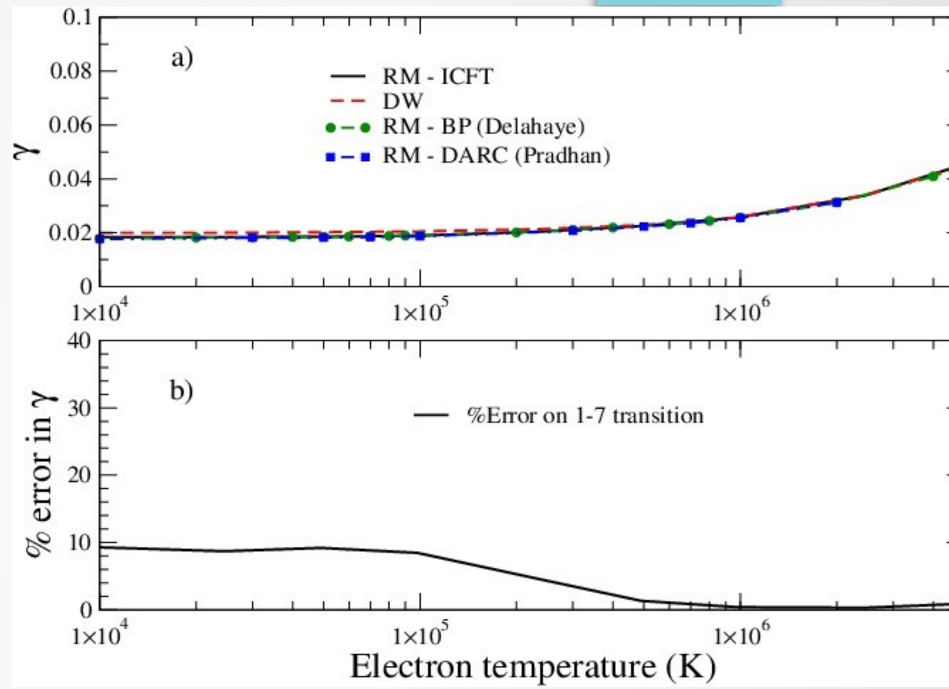
- More details given in Loch et al., ICAMDATA 2012, AIP conference proceedings, **1545** 242 (2013).
- Methods were developed to put approximate uncertainties on ***electron-impact excitation, ionization and recombination.***
- ***Guiding Principles***
  - Reflects the dominant source of uncertainty.
  - Correctly scales with temperature and process type.
  - Be relatively easy to automate

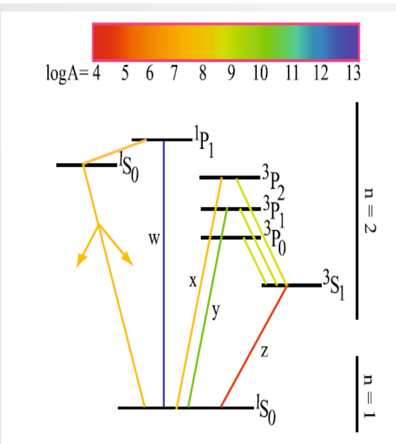
Effective collision strengths

$1s^2\ (^1S_0) \rightarrow 1s2s\ (^3S_1)$



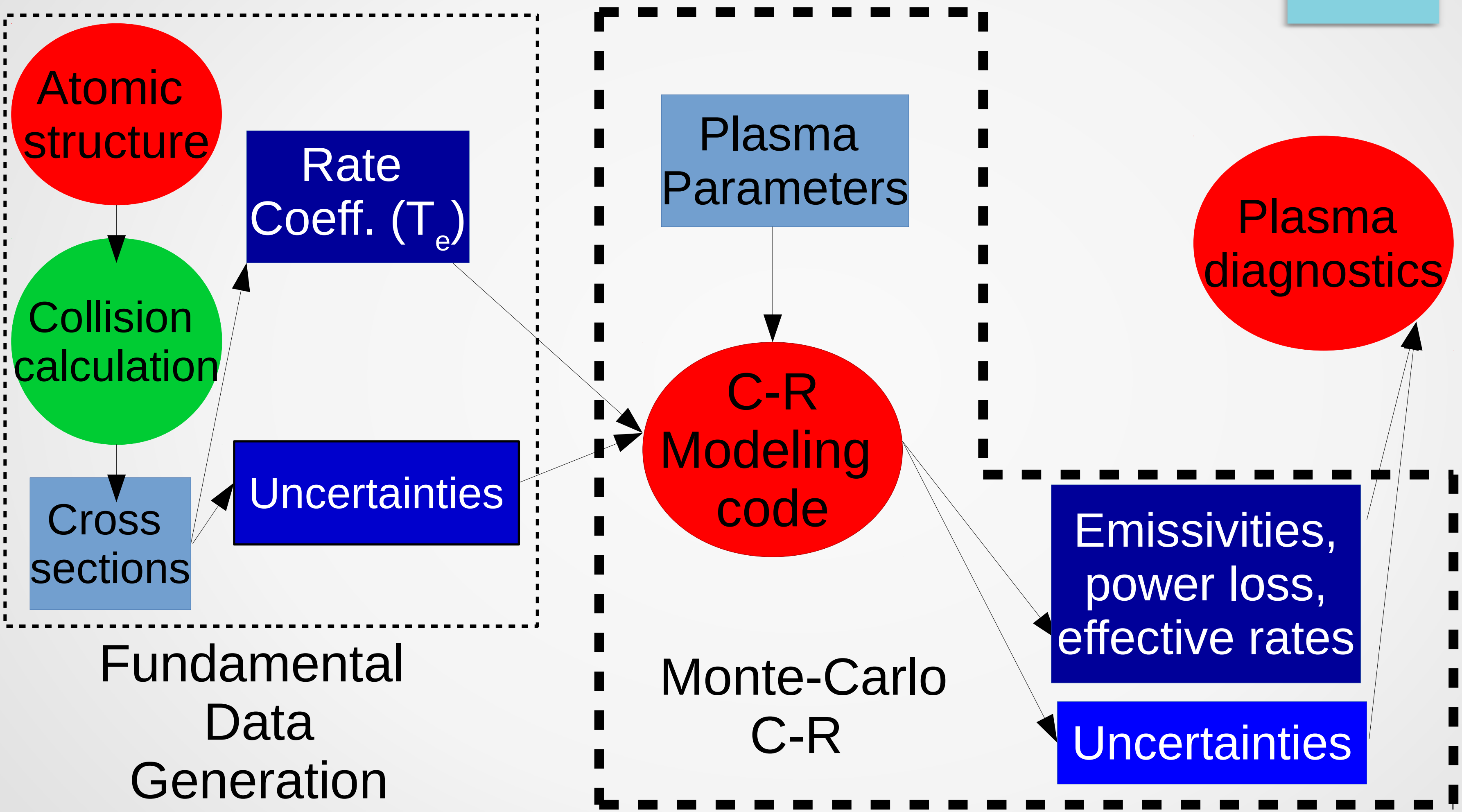
$1s^2\ (^1S_0) \rightarrow 1s2p\ (^1P_1)$





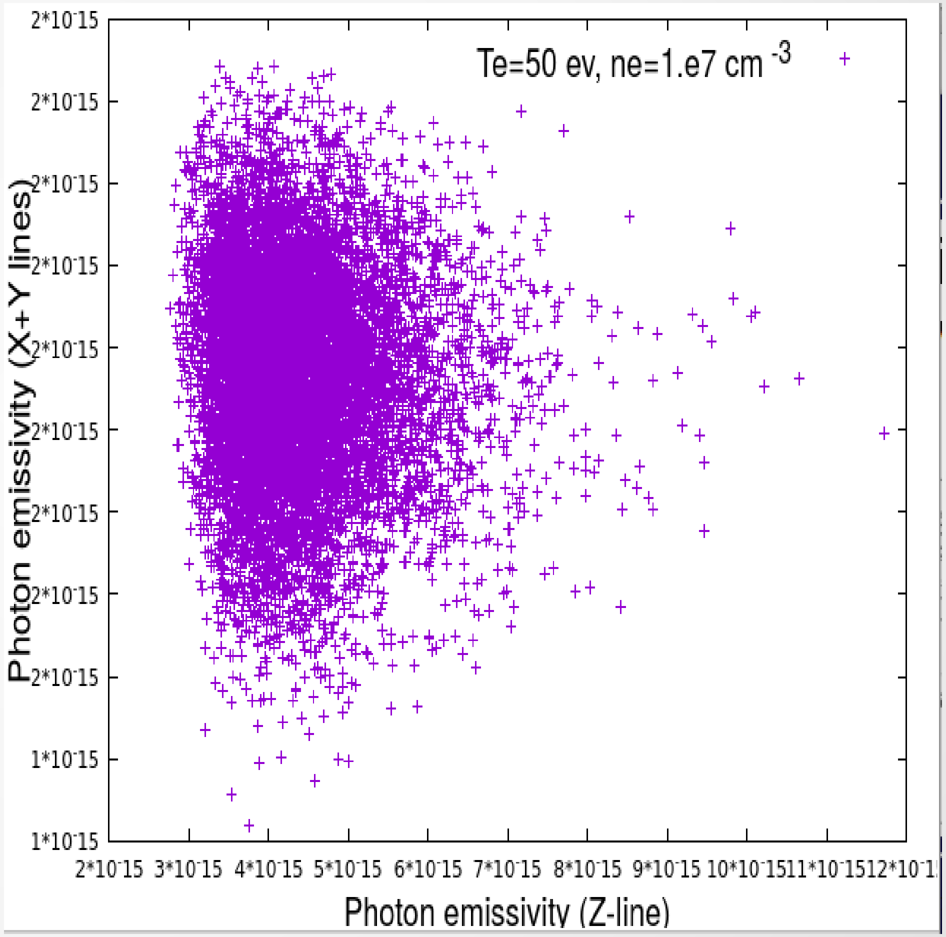
- For electron-impact excitation we use the total resonance contribution as crude estimate of the uncertainty.
- It has the right physical trends
    - It reduces at higher temperatures.
    - It is larger for forbidden transitions.

Propagation through C-R codes

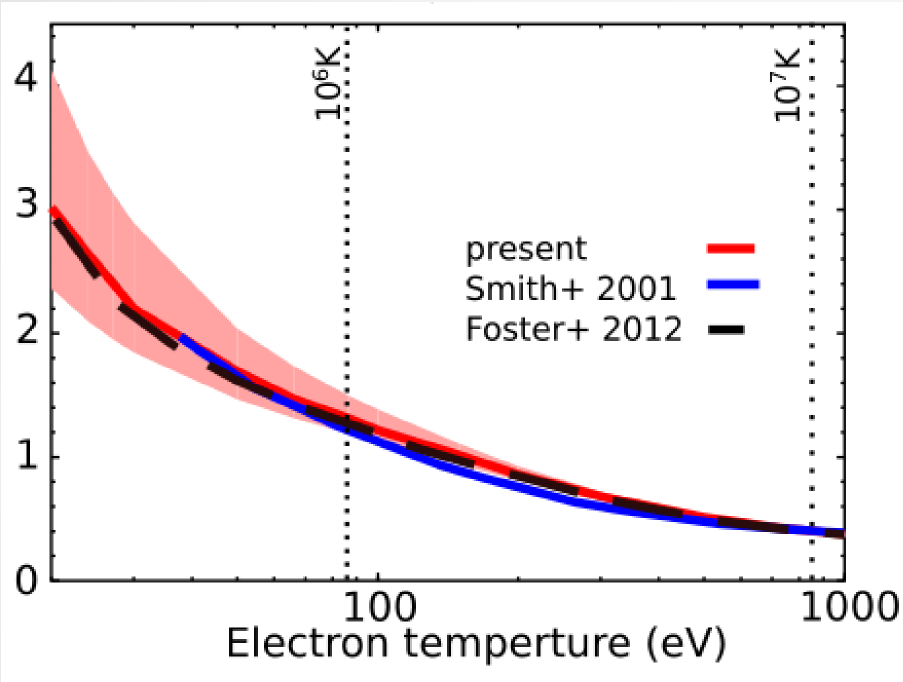


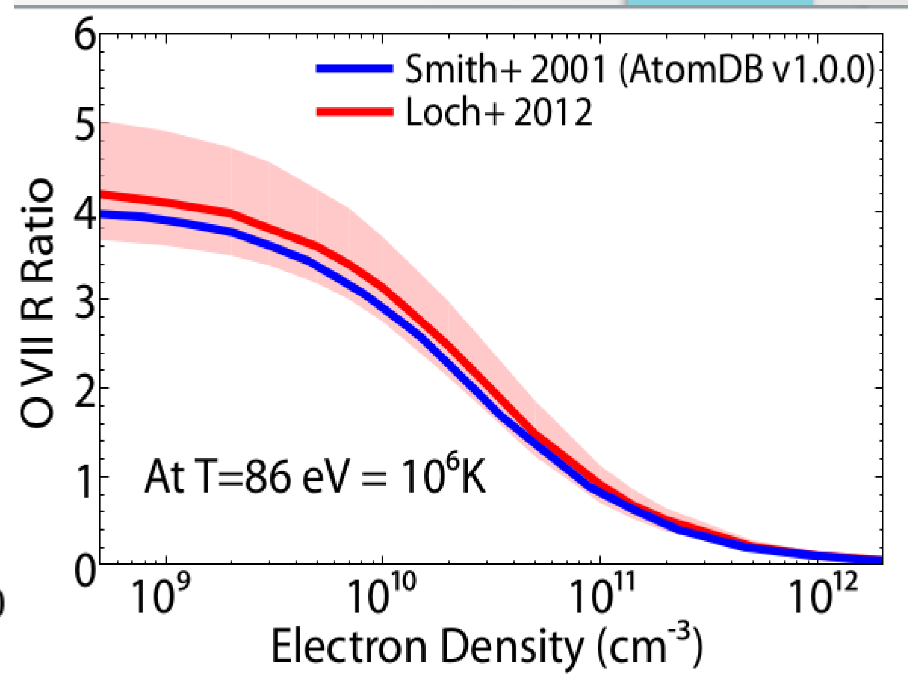
Propagating of uncorrelated uncertainties through a collisional-radiative model

- Generate sets of random numbers in an ***appropriate distribution.*** Use this to make a set of rate coefficients, within the calculated uncertainty.
- Monte-Carlo collisional-radiative approach, keeping track of the statistics of important output parameters (relative populations, emissivities, etc).
- Determine the average values and distributions for the output data (hence an uncertainty).



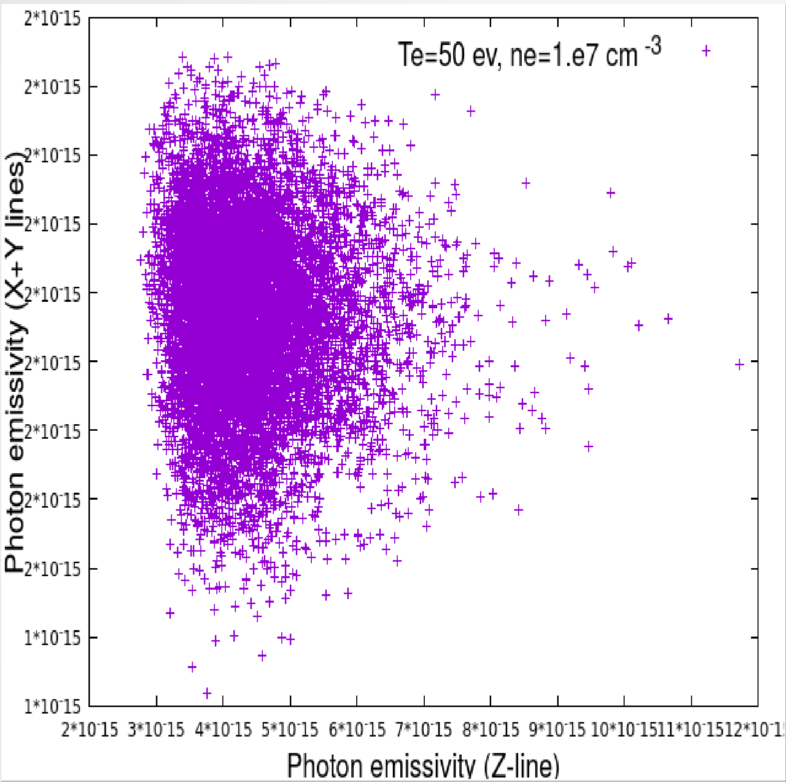
Line ratio results for O^{6+} [Baseline uncertainties]

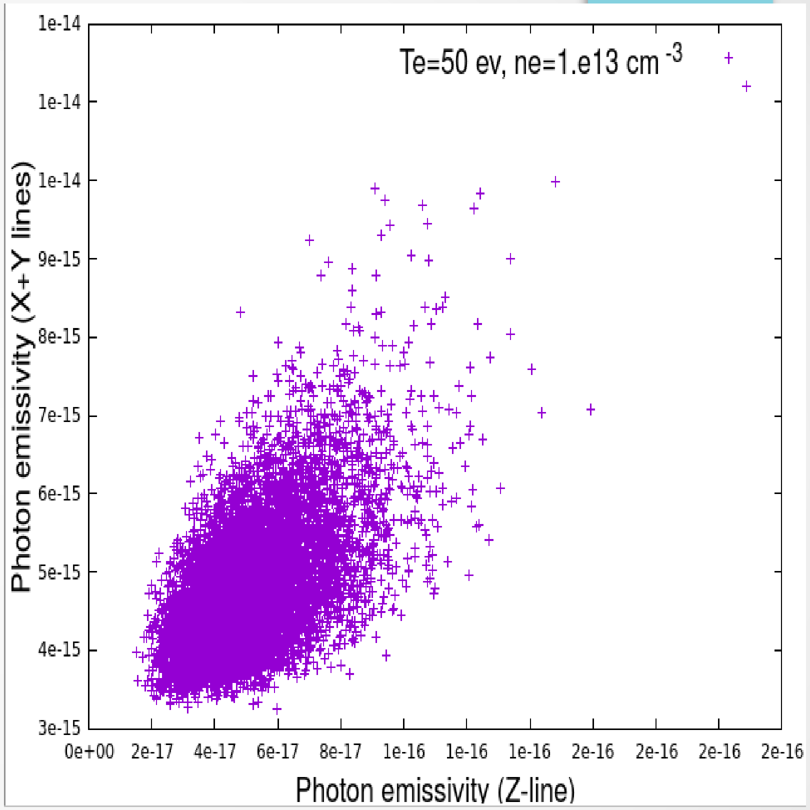




- The emissivities can be used to ***generate line ratios, with associated uncertainties.***
  - ***Collisional-radiative correlation*** information is included in the line ratio.
- This has proven to be a useful tool for finding the reason for differences between different databases.

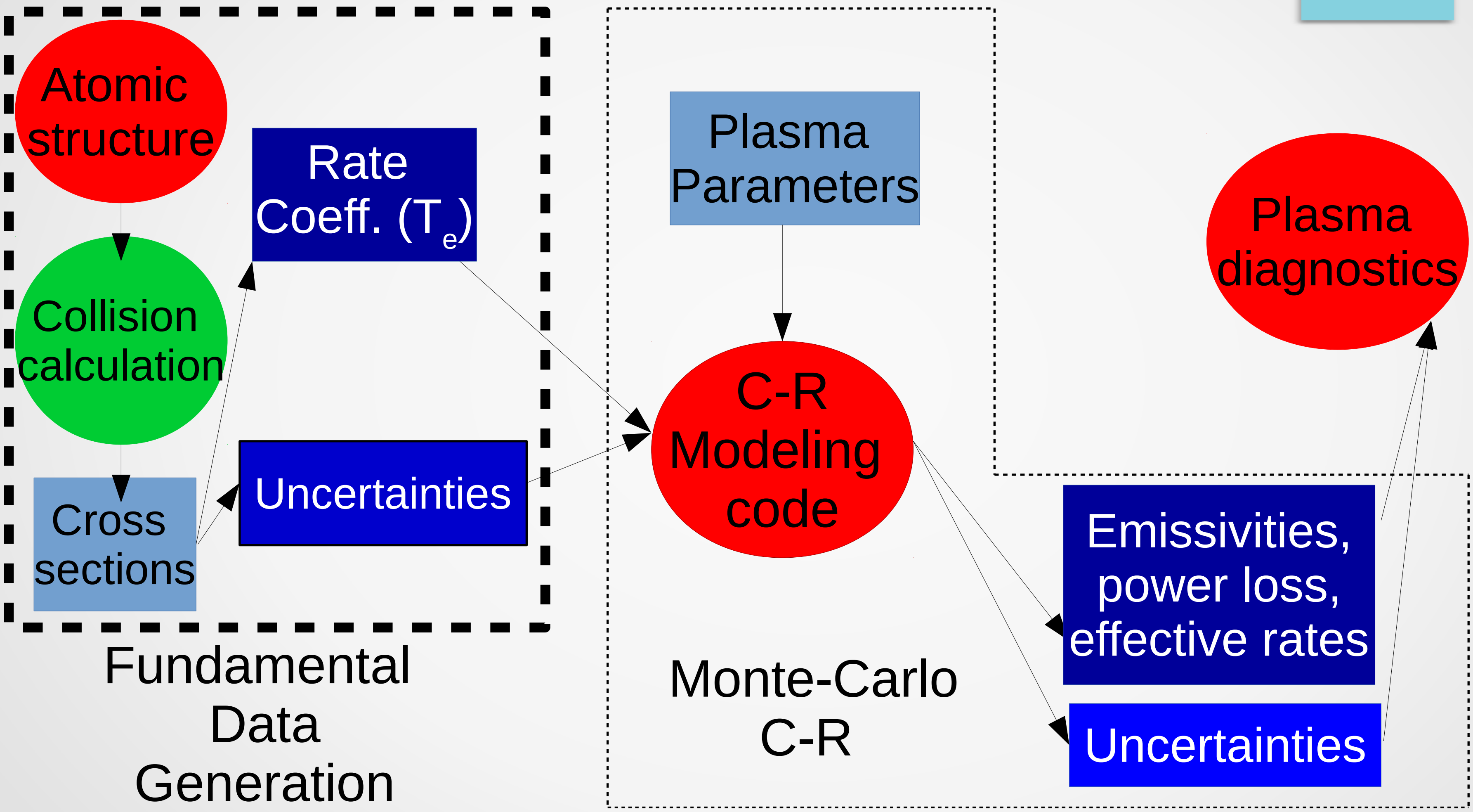
Collisional-Radiative Correlation in emissivities





- As n_e increases the emissivities in the R-ratio become more correlated.
- Note that there is still no correlation in the input atomic data.

Correlated uncertainties in fundamental data

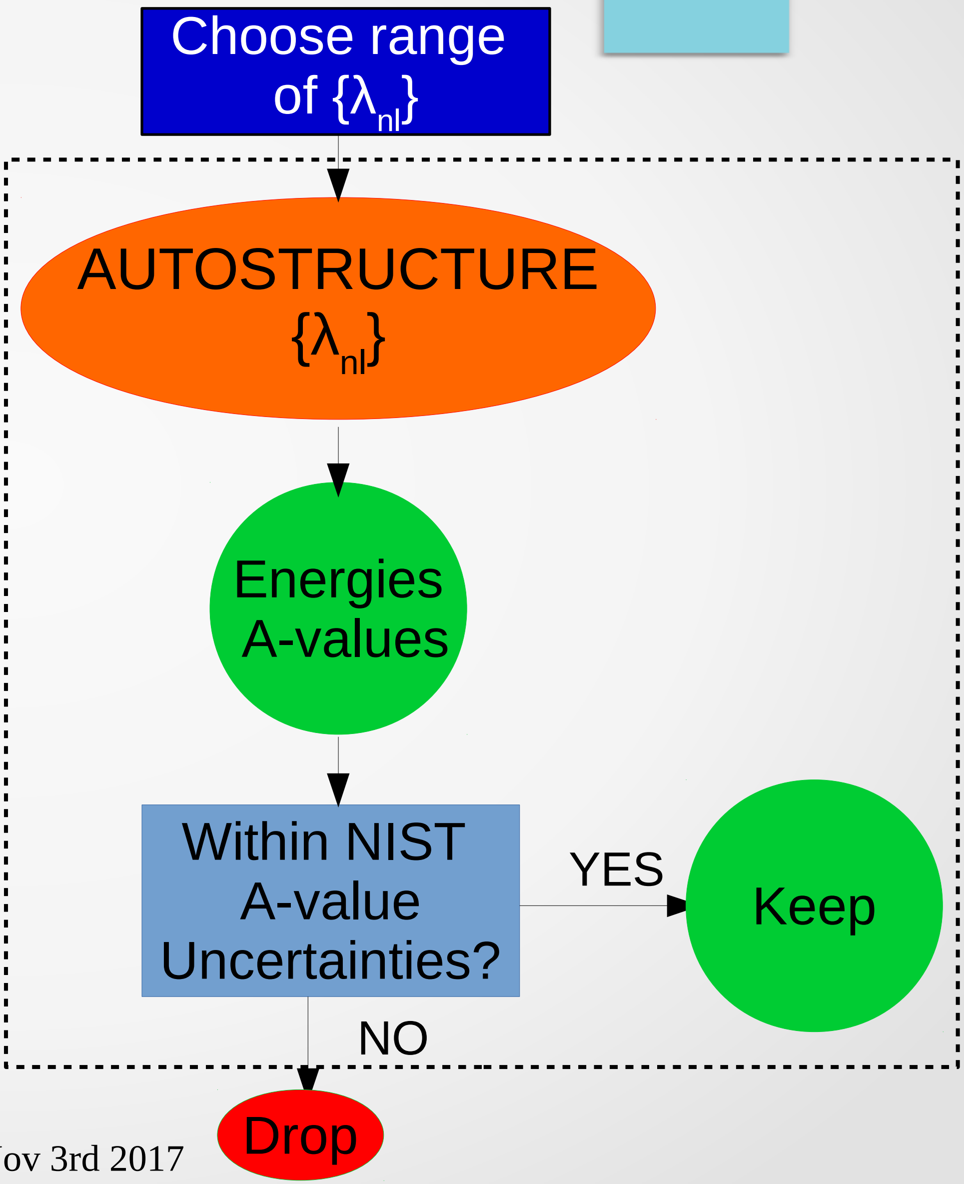


Generation of Correlated Uncertainties

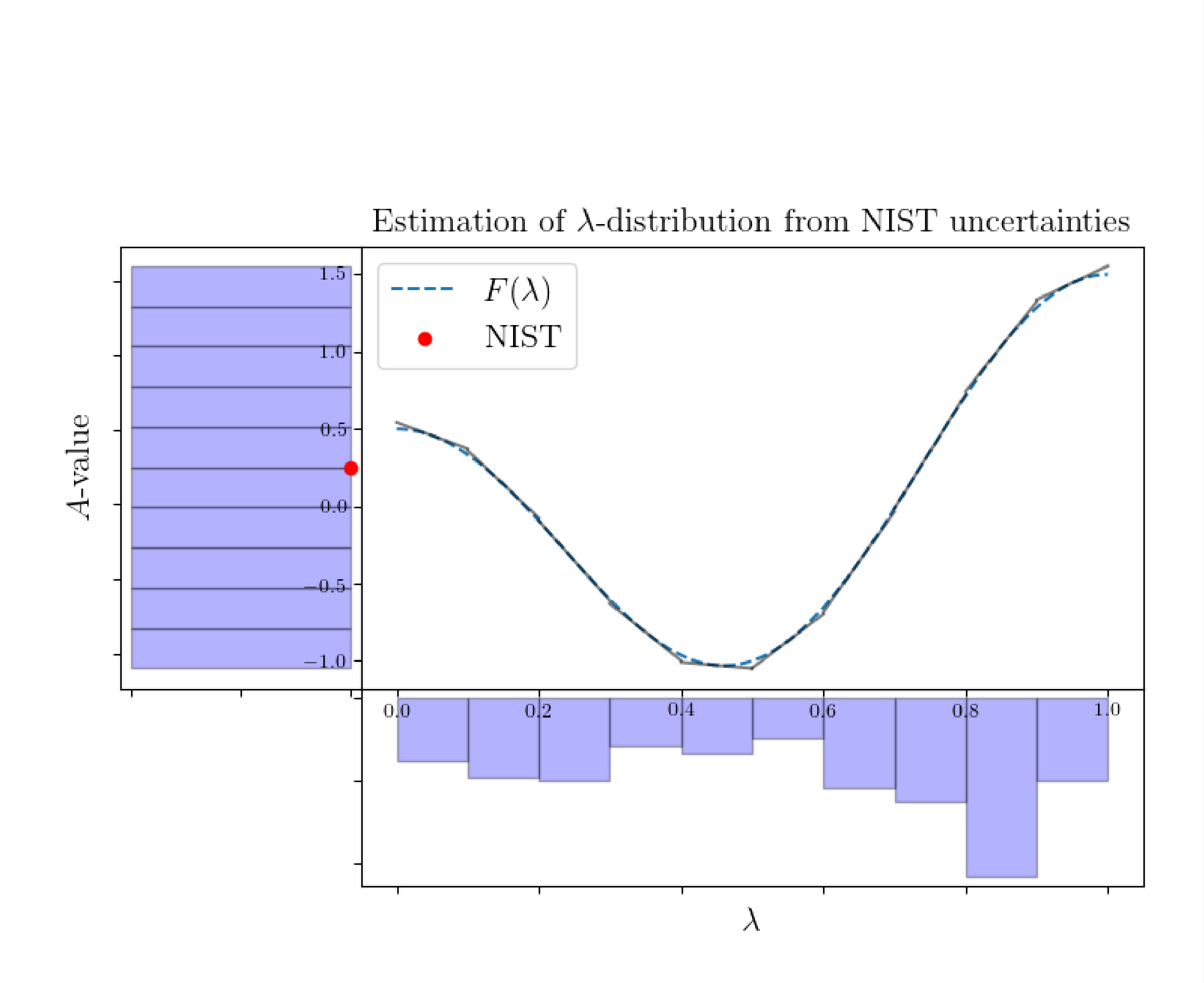
- We consider **<u>electron-impact excitation</u>** as an initial case.
  - Work is underway to for the other atomic processes.
- Our framework is that "**Uncertainties in the target description carry through to the largest uncertainties in the calculations.**"
  - Calculations using a scripted form of the ICFT *R*-matrix codes.
  - We vary the "***<u>orbital scaling parameters</u>***" (λ_{nl}) as a method of varying the underlying wavefunctions.
  - ***<u>Experimental comparison</u>***: The range of λ_{nl} values would be chosen such that the energies and A-values are within the NIST ranges.
  - These wavefunctions are carried through to differences in the energies, A-values, and collision strengths.

Determining the lambda parameters

- We use NIST energies and A-value uncertainties to select λ_{nl} values
- We immediately have correlation information on the A-values.
  - O^{6+} shows a positive correlation for configurations that share a common orbital
  - Fe^{16+} 3C and 3D A-values show a negative correlation.



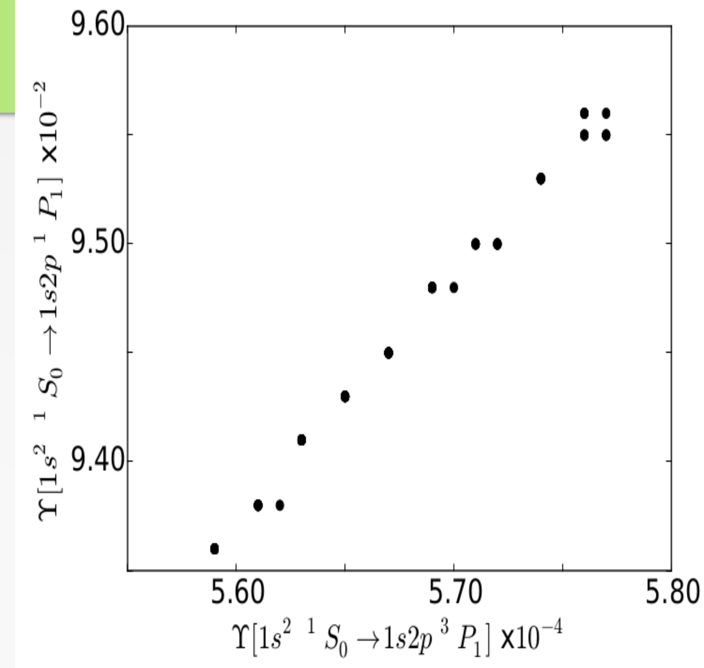
Determining the lambda distribution

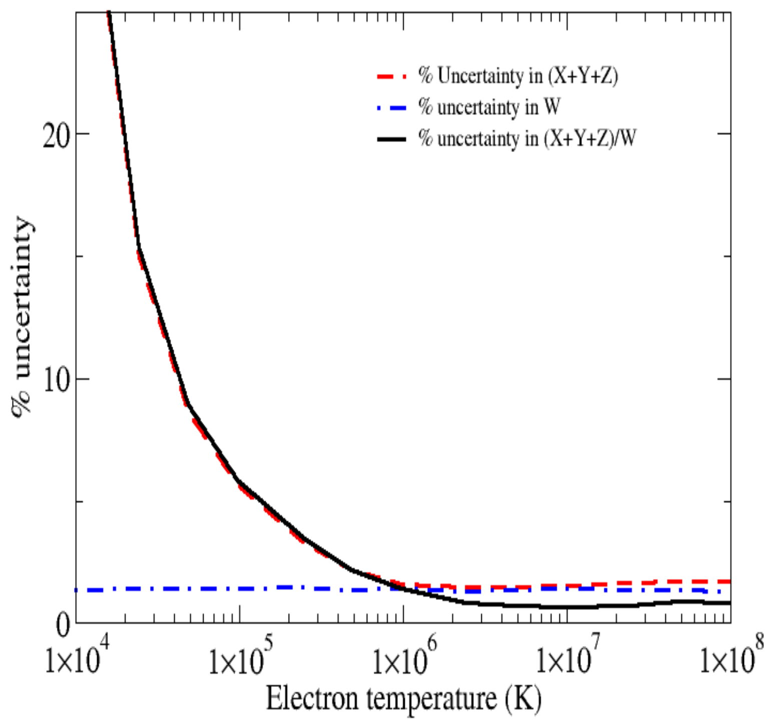


It is possible to infer what the distribution function lambda values using a Bayesian analysis.

Preliminary results for O^{6+}

- We varied the λ_{nl} parameters from 0.8 – 1.2. This led to 81 ICFT R-matrix calculations.
- We are developing a Bayesian method to determine the probability distribution function for the λ_{nl}.

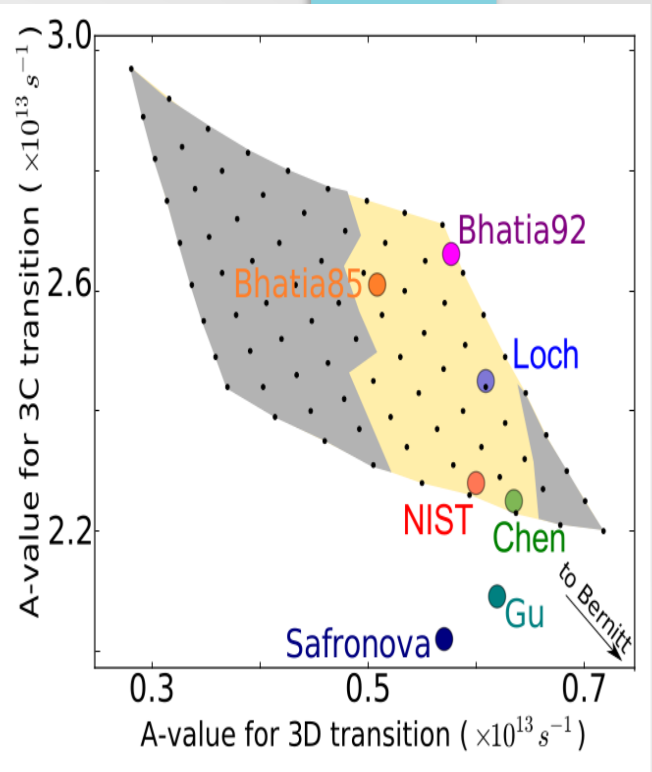


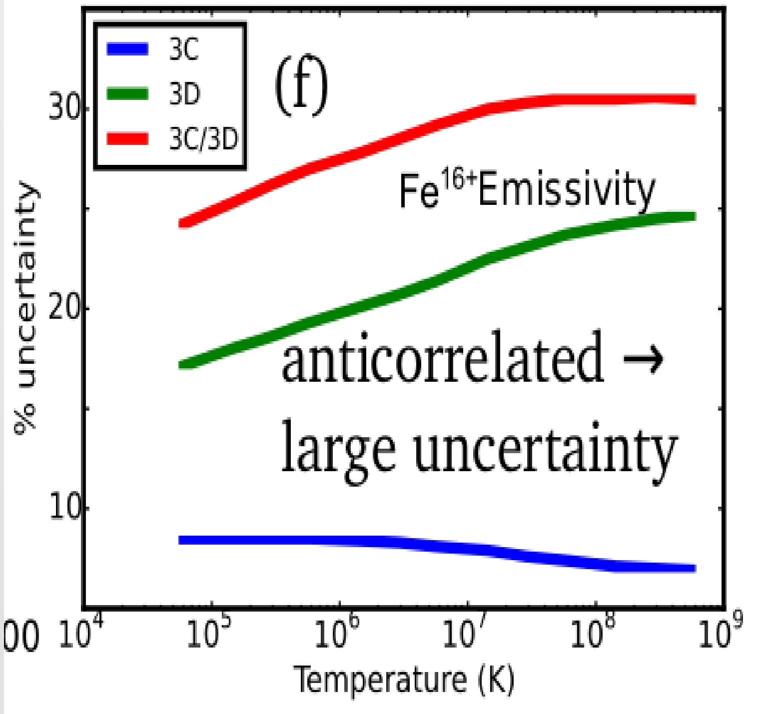


- The uncertainty in the line ratio is **<u>reduced</u>** because of the **<u>positive correlation</u>** in the excitation data.
- Such line ratios make excellent diagnostics!
- ***<u>We plan to categorize the most trustworthy diagnostics using this method.</u>***

Preliminary results for Fe^{16+}

- λ_{nl} varied from 0.8 – 1.2 for the 2p & 3d orbitals.
- A ***strong negative correlation*** in the A-values for the controversial 3C and 3D transitions.
  - Also present in the effective collision strengths.





- The 3C/3D line ratio amplifies the uncertainties.
- This calculation is just a small test case.
- ***However, as a general conclusions, such negatively correlated line ratios would not be good diagnostics.***
  - They would be good to test atomic data.

Deliverables and Diagnostic Tools

- Deliverables
  - ***Uncertainties on A-values, collision rate coefficients, photon emissivities, power loss, abundances.***
    - The data (and correlation) will be archived in AtomDB. Others could also use it directly in their own modeling codes.
  - The most commonly used line ratio diagnostics could be categorized into positive and negative correlation.
- Diagnostics tools that could be developed:
  - A **line ratio code** where the user selects a set of lines and the code returns a line ratio along with an uncertainty.
  - ***Ionization balance codes*** (NEI and EI) for fractional abundances.
  - Other idea?

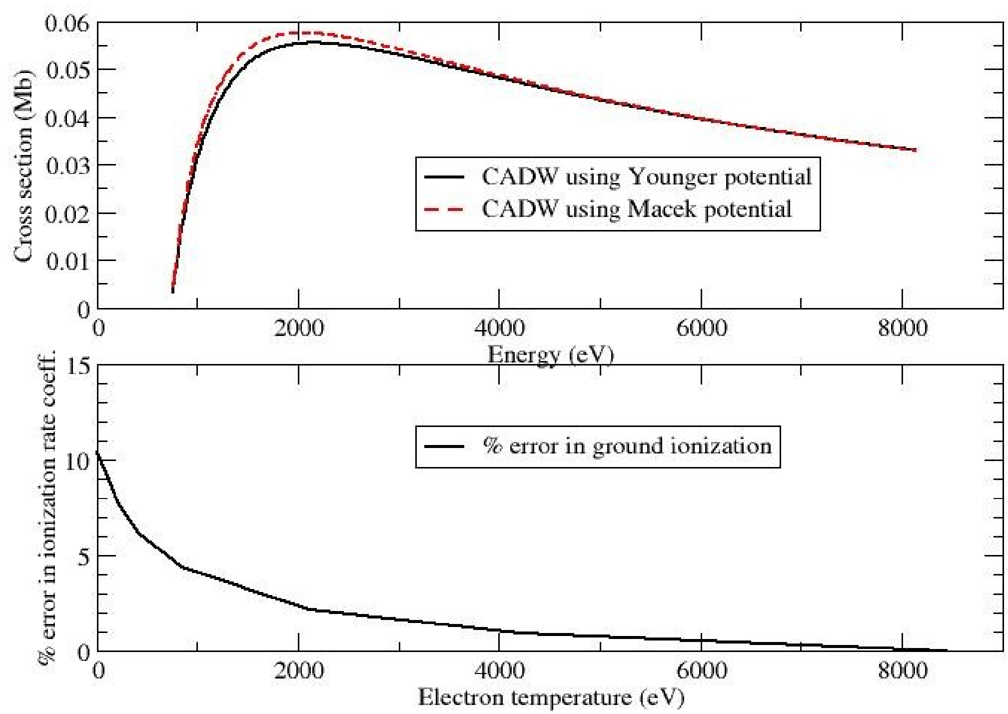
Conclusions

- A project has been started to assign uncertainties to fundamental atomic data.
  - Baseline uncertainties will be generated (iso-electronic)
  - Higher accuracy uncertainties with correlation will be generated for electron-impact excitation. Other processes covered later.
    - Probably first for O, then Si, then Fe.
    - Correlation is likely to be an important consideration (both in the fundamental data and collisional-radiative correlation).
  - A set of diagnostic tools will also be developed.
- If you have particular elements or tools that you are interested in, let us know.

EXTRA SLIDES

Baseline Uncertainties for ionization

Ground state ionization of O^{6+}



- We took the difference between a Post and Prior scattering potential calculations.
  - Has an appropriate energy scaling and n-shell scaling
- We calculated level-resolved data for the first 4 n-shells.