Uncertainties on atomic data

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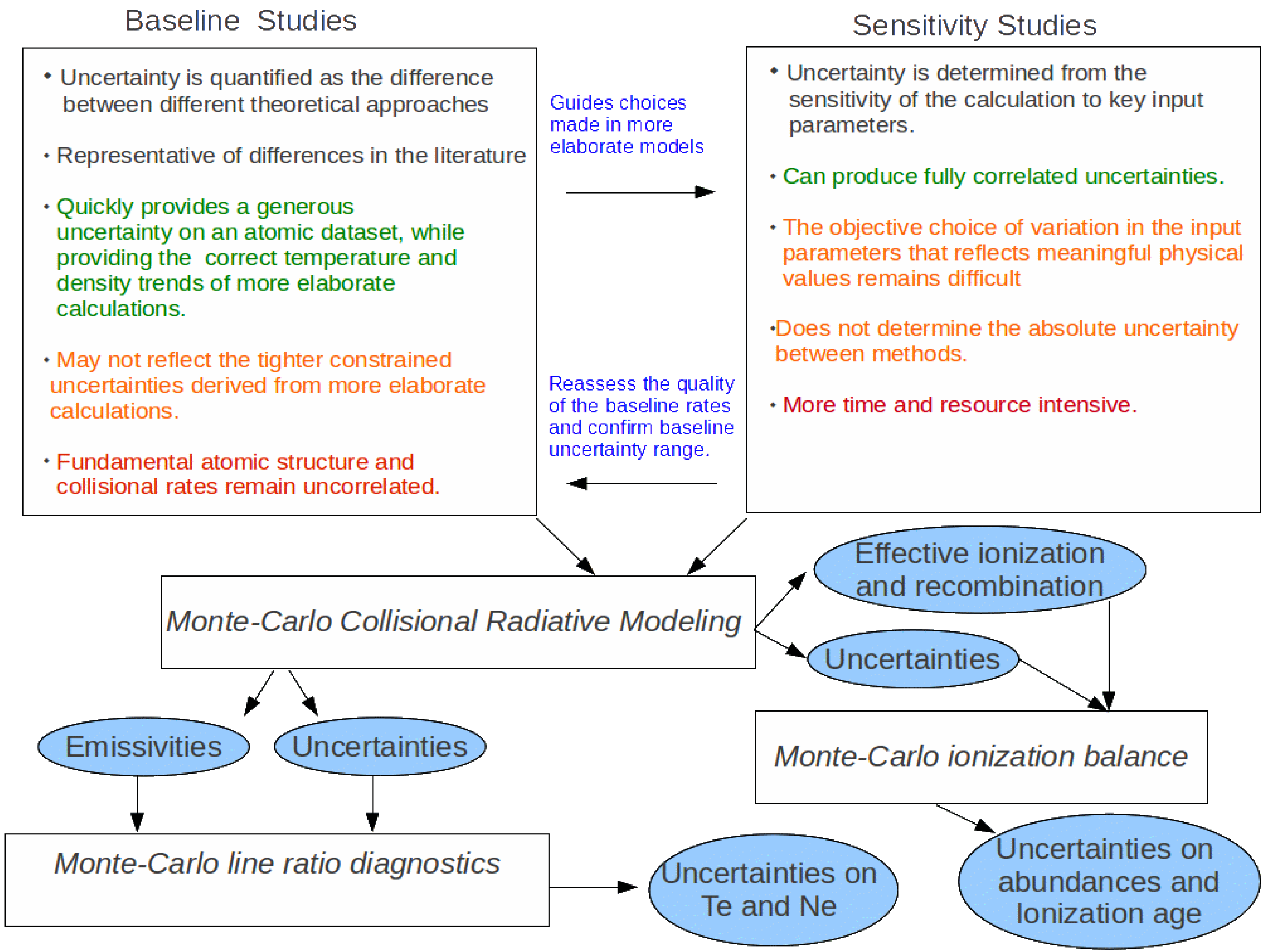
Background

- The modeling community has been asking for some time to have meaningful error bars put on atomic data.

- We would categorize the problem into 2 groups

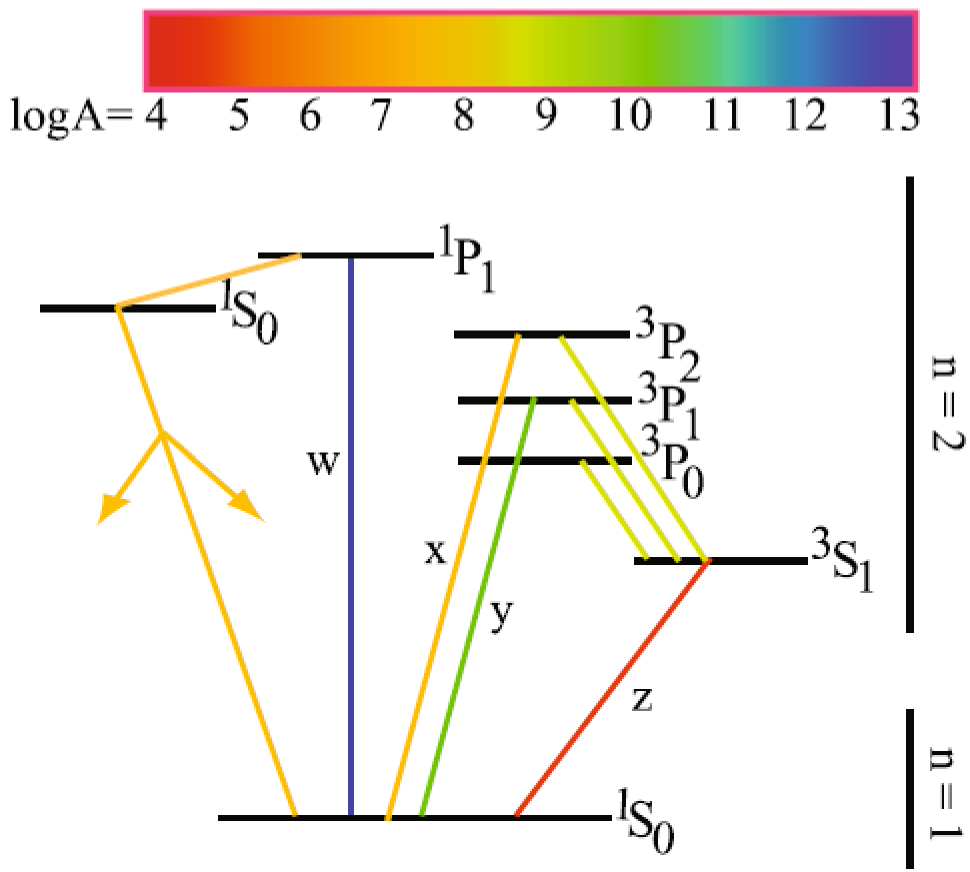
    - ***Baseline*** uncertainty data to give an indication of the parameter space.
    - ***Method sensitivity*** uncertainty data with tighter and more realistic error bars.

    - The approach is valid for both astrophysical and tokamak plasma regimes.



Baseline Studies
Sensitivity Studies
• Uncertainty is quantified as the difference between different theoretical approaches
• Representative of differences in the literature
• Quickly provides a generous uncertainty on an atomic dataset, while providing the correct temperature and density trends of more elaborate calculations.
• May not reflect the tighter constrained uncertainties derived from more elaborate calculations.
• Fundamental atomic structure and collisional rates remain uncorrelated.
Guides choices made in more elaborate models
Reassess the quality of the baseline rates and confirm baseline uncertainty range.
• Uncertainty is determined from the sensitivity of the calculation to key input parameters.
• Can produce fully correlated uncertainties.
• The objective choice of variation in the input parameters that reflects meaningful physical values remains difficult
•Does not determine the absolute uncertainty between methods.
• More time and resource intensive.
Monte-Carlo Collisional Radiative Modeling
Effective ionization and recombination
Uncertainties
Emissivities
Uncertainties
Monte-Carlo ionization balance
Monte-Carlo line ratio diagnostics
Uncertainties on Te and Ne
Uncertainties on abundances and Ionization age

He-like line ratio diagnostics

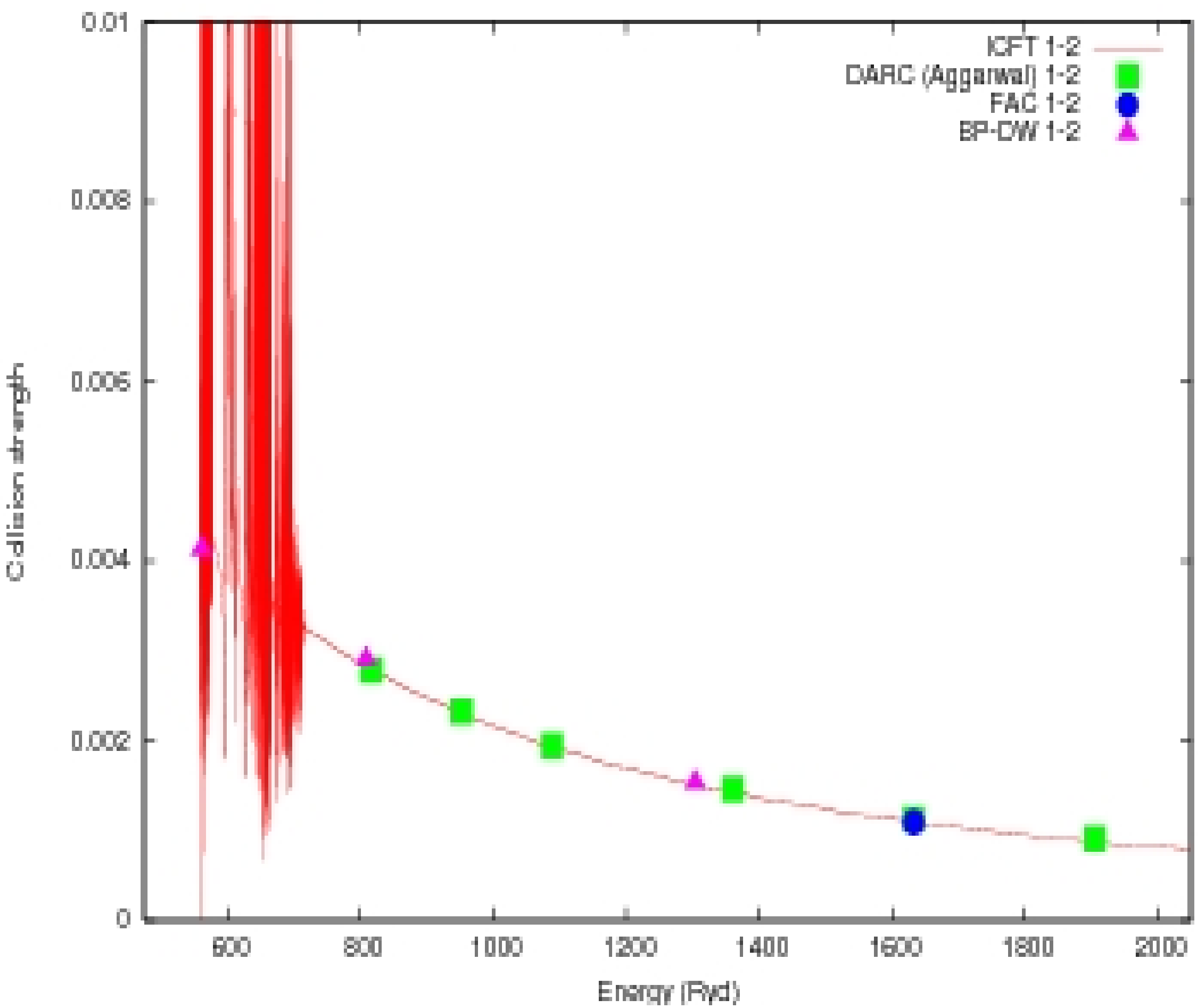


- For O^{6+}
  - The ratio of the (X+Y+Z)/W is Te dependent for Ne < 1×10^{7} cm^{-3}.
  - The ratio of the Z/(X+Y) is density dependent.

Baseline uncertainties

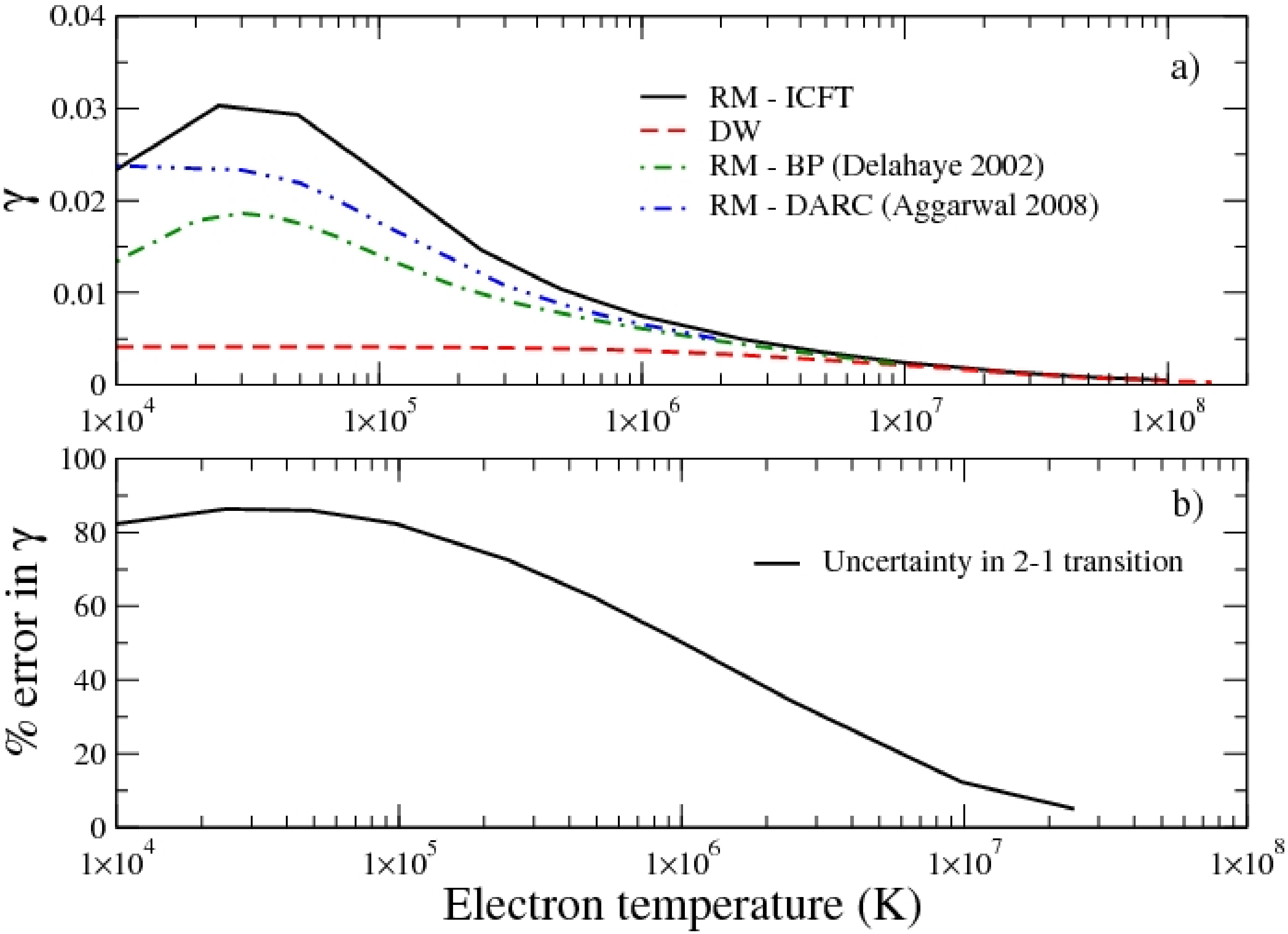
- The aim for the baseline uncertainty data is to generate a range of values that should encompass most of the currently available data in the databases.
- So we are looking for generous error bars.
- We also want uncertainties that have the correct temperature and n-shell behavior.

Uncertainties on electron impact excitation data - O^{6+}



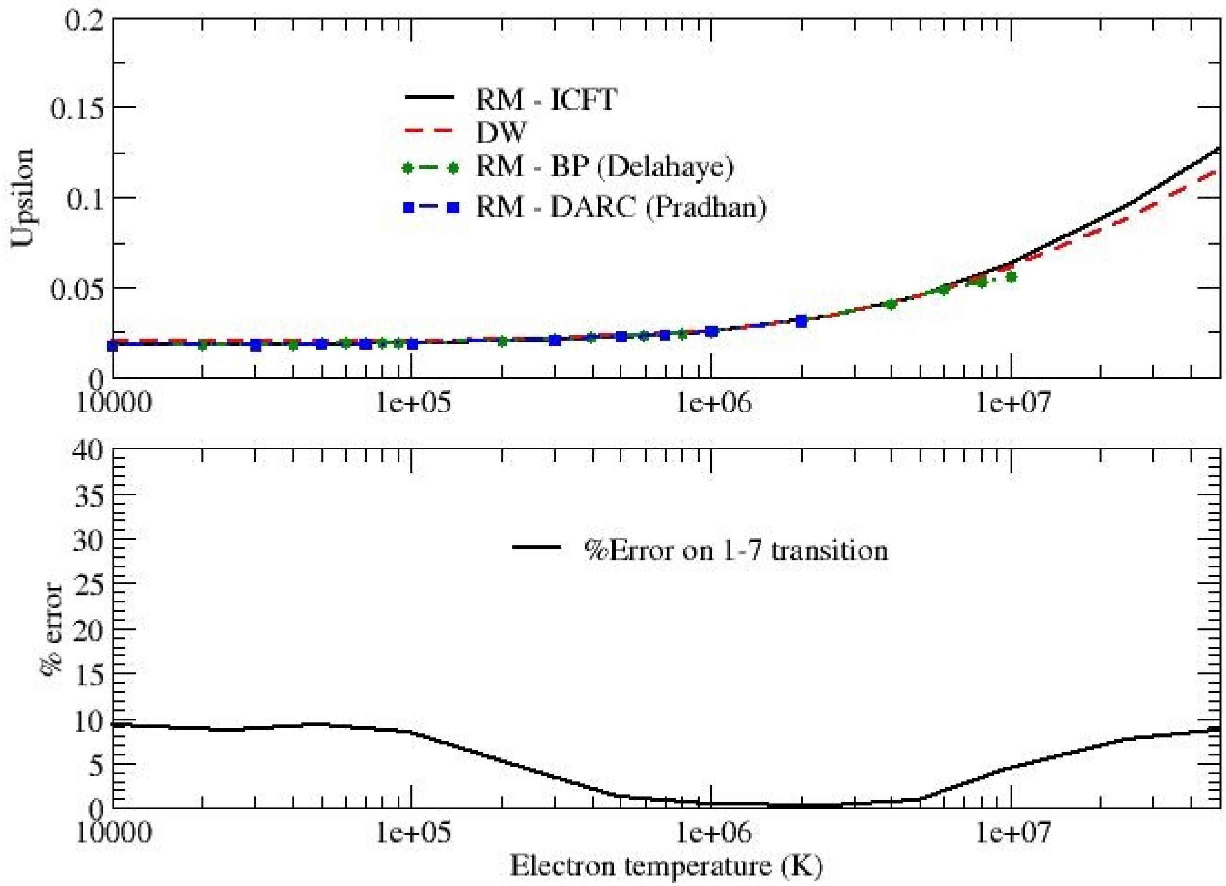
- There are two previous R-matrix calculations.
- Plus one DW calculation, we also did our own DW calculation.
- They all agree very well for the background cross section.

Effective collision strengths - forbidden transition



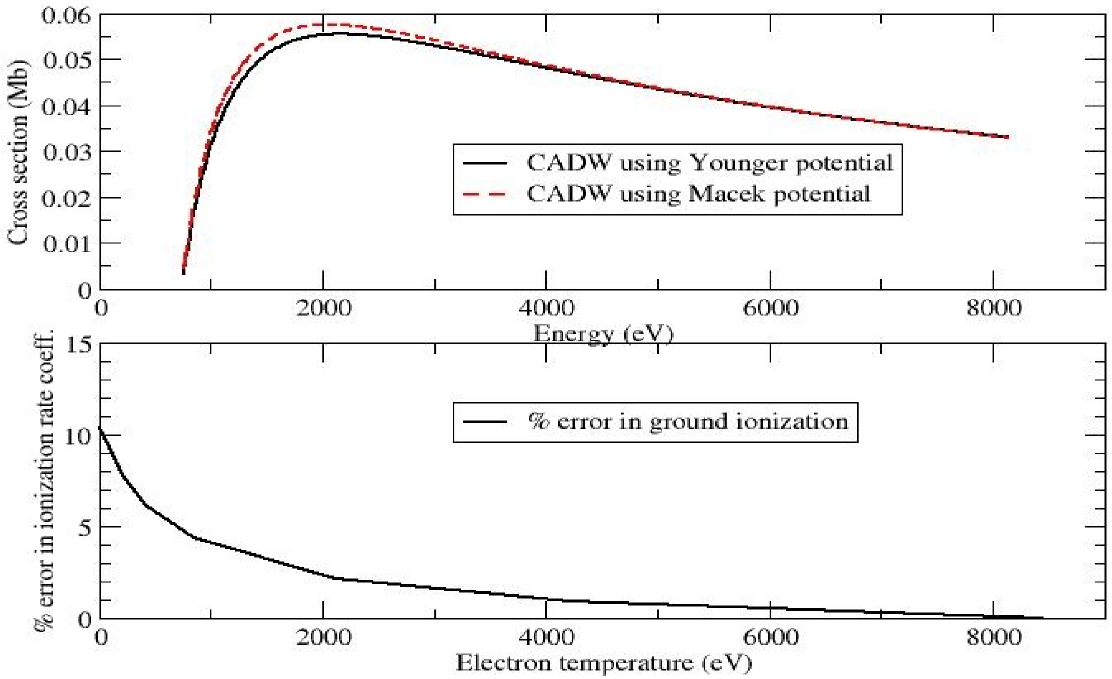
- Our baseline uncertainty data for excitation is the difference between the RM and DW upsilons.
- Shown is our baseline uncertainty data for the 1-2 transition in O^{6+}

Effective collision strengths - allowed transition



- Note that the errors are very small for the resonance line.
- The difference at the highest temperatures is due to different last energy points in the RM and DW calculations.
-

Uncertainties on ionization cross sections



- Shown is the ground state ionization of O^{6+}.
- We took the difference between a Post and Prior scattering potential calculations.
- We calculated level-resolved data for the first 4 n-shells.

Uncertainties in recombination

- The uncertainty in the RR data is the difference between a Gaunt factor calculation of ADAS and a DW calculation from AUTOSTRUCTURE.
  - ~2% error in RR.
- The uncertainty in the DR is the difference between two DW AUTOSTRUCTURE calculations. One with and one without shifts to NIST core excited energies.
  - ~8% error at low Te which decreases to close to zero for the highest temperatures.

Method Sensitivity (variation within a chosen method)

- With the advent of supercomputers we can adopt a Monte Carlo approach to R-matrix calculations, and and build up meaningful statistics from hundreds of calculations. This has been implemented within an elaborate perl script.
- This requires a rigorous and well defined output to manage perhaps a thousand calculations
- In the case of excitation, we have Maxwellian averaged collision strengths for every transition for a range of temperatures and now the associated error file.

helike_cb12#o6.dat

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helike_cb12#o6.dat

```
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    2 1S1 2S1          (3)0( 1.0)       4526947.0
    3 1S1 2P1          (3)1( 0.0)       4587888.0
    4 1S1 2P1          (3)1( 1.0)       4588243.0
    5 1S1 2P1          (3)1( 2.0)       4588974.0
    6 1S1 2S1          (1)0( 0.0)       4594943.0
    7 1S1 2P1          (1)1( 1.0)       4636124.0
    8 1S1 3S1          (3)0( 1.0)       5343184.0
    9 1S1 3P1          (3)1( 0.0)       5359516.0
   10 1S1 3P1          (3)1( 1.0)       5359615.0
   11 1S1 3P1          (3)1( 2.0)       5359816.0
   12 1S1 3S1          (1)0( 0.0)       5360831.0
   13 1S1 3D1          (3)2( 1.0)       5368693.0
   14 1S1 3D1          (3)2( 2.0)       5368728.0
   15 1S1 3D1          (3)2( 3.0)       5368792.0
   16 1S1 3D1          (1)2( 2.0)       5369321.0
   17 1S1 3P1          (1)1( 1.0)       5372722.0
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 7.00    3       9.80+03 2.45+04 4.90+04 9.80+04 2.45+05 4.90+05 9.80+05 2.45+06 4.90+06 9.80+06 2.45+07 4.90+07 9.80+07
   2   1 1.00-30 4.08-02 5.13-02 4.10-02 2.81-02 1.61-02 1.10-02 7.83-03 5.04-03 3.57-03 2.45-03 1.40-03 8.72-04 5.25-04 0.00+00
   3   1 1.00-30 3.97-03 3.83-03 3.32-03 2.90-03 2.66-03 2.57-03 2.37-03 1.91-03 1.47-03 1.03-03 5.72-04 3.39-04 1.92-04 0.00+00
   4   1 3.81+08 1.26-02 1.18-02 1.01-02 8.77-03 8.01-03 7.74-03 7.14-03 5.75-03 4.43-03 3.15-03 1.90-03 1.35-03 1.04-03-7.80-06
   5   1 1.00-30 2.21-02 2.01-02 1.70-02 1.47-02 1.34-02 1.30-02 1.20-02 9.60-03 7.38-03 5.19-03 2.87-03 1.70-03 9.61-04 0.00+00
   6   1 1.00-30 1.75-02 1.34-02 1.12-02 9.57-03 8.48-03 8.25-03 8.20-03 8.48-03 9.07-03 9.94-03 1.12-02 1.21-02 1.29-02 1.45-02
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  12   1 1.00-30 6.30-03 4.85-03 3.56-03 2.67-03 2.06-03 1.84-03 1.76-03 1.80-03 1.92-03 2.11-03 2.41-03 2.63-03 2.82-03 3.25-03
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  14   1 9.72+05 4.21-04 4.44-04 4.48-04 4.45-04 4.27-04 3.99-04 3.54-04 2.70-04 1.99-04 1.36-04 7.70-05 5.02-05 3.40-05 1.20-05
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   3   2 7.99+07 7.23-01 7.77-01 7.99-01 8.22-01 8.81-01 9.55-01 1.06+00 1.23+00 1.40+00 1.58+00 1.81+00 1.98+00 2.15+00-2.32-01
   4   2 8.14+07 2.31+00 2.40+00 2.44+00 2.49+00 2.65+00 2.87+00 3.17+00 3.71+00 4.20+00 4.73+00 5.44+00 5.95+00 6.46+00-6.97-01
   5   2 8.43+07 3.86+00 4.04+00 4.10+00 4.17+00 4.43+00 4.79+00 5.28+00 6.17+00 6.98+00 7.87+00 9.04+00 9.91+00 1.07+01-1.16+00
   6   2 1.00-30 9.75-02 6.97-02 5.75-02 5.13-02 5.27-02 5.29-02 4.64-02 3.29-02 2.35-02 1.60-02 9.02-03 5.57-03 3.33-03 0.00+00
   7   2 5.26+04 6.92-02 7.32-02 7.41-02 8.11-02 1.05-01 1.11-01 9.51-02 6.03-02 3.80-02 2.25-02 1.08-02 6.43-03 4.12-03-7.98-05
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   9   2 4.97+10 3.35-02 2.93-02 2.57-02 2.35-02 2.30-02 2.47-02 2.91-02 4.13-02 5.67-02 7.77-02 1.13-01 1.45-01 1.79-01-5.66-02
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Propagation of uncertainties

- So we have a recommended dataset, plus an uncertainty dataset.
- We initially used a Gaussian distribution about the recommended data, with the uncertainty providing the standard deviation for the Gaussian.
- We then do a Monte-Carlo set of collisional-radiative calculations (typically about 1,000,000) and produce excited populations and emissivities.
  - These are post-processed to give line ratios, with error bars