Adding uncertainties to the ADAS beam model – some questions

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Background – motivation for ADAS

The CRM for describing beam behaviour requires atomic data:

1. Re-assessing the fundamental data is always needed – the goal of this CRP.
2. How does the latest data compare to existing sets of data?
3. Is uncertainty quantification (UQ) on this data possible?
4. How does using UQ data affect interpretation of diagnostics?

Where we stand:

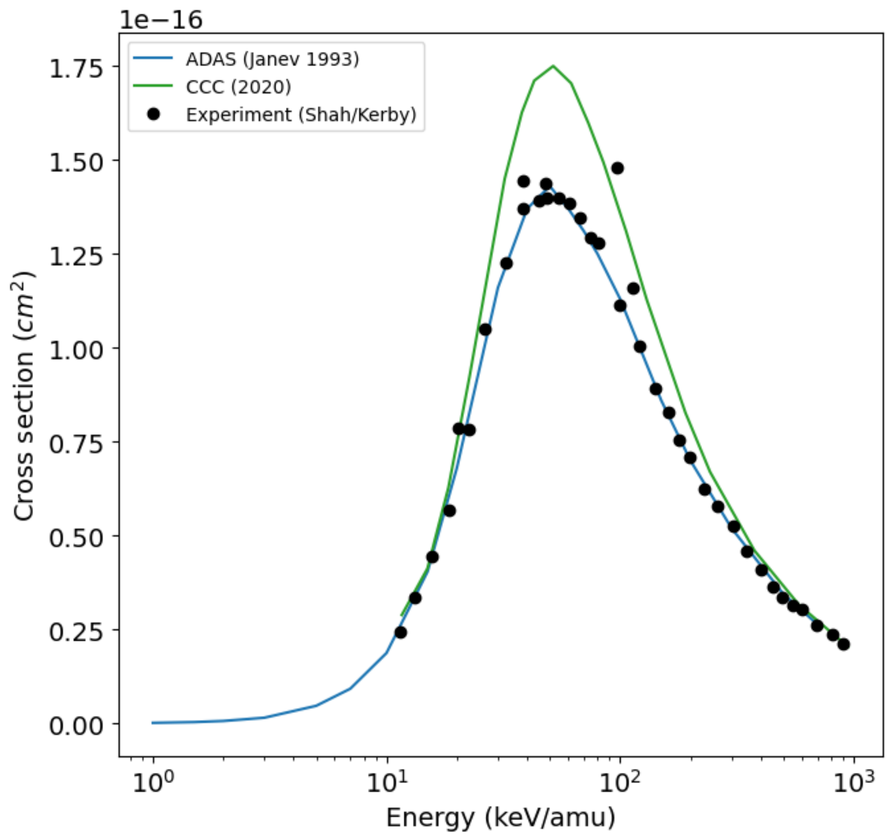
1. Is there consensus?
2. The new data make a difference.
3. This has been demonstrated.
4. It's a noticeable effect but 'atomic error' is not dominant.

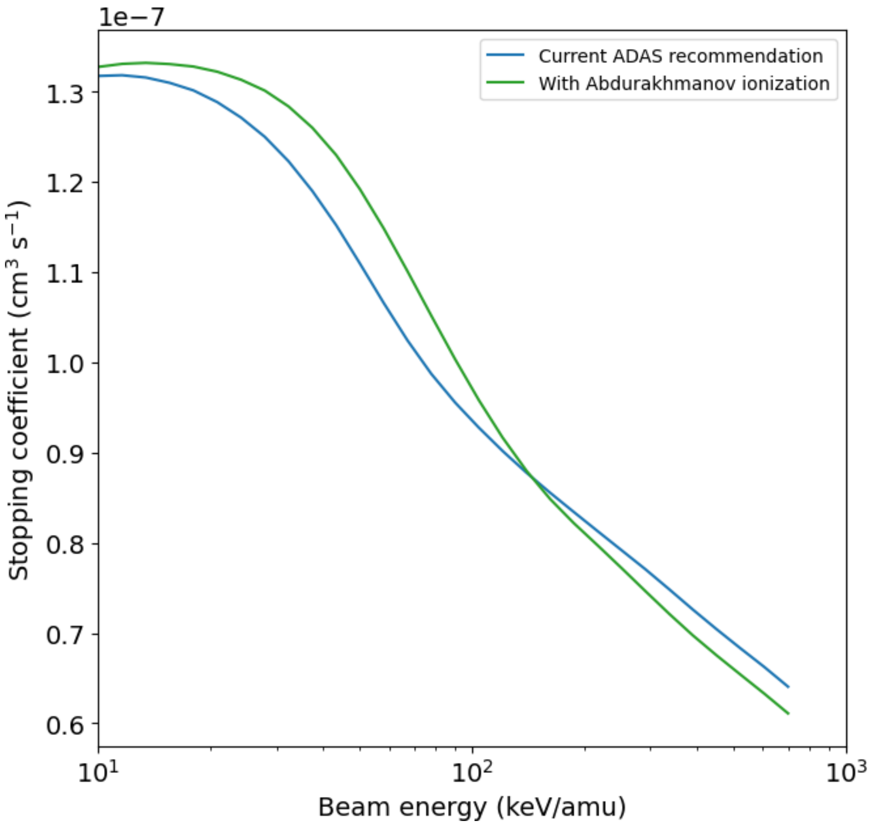
Questions:

- Should we change the fundamental data in our models?
- Can we justify making the change?
- What are the error bars?

Should we ignore experimental cross sections?

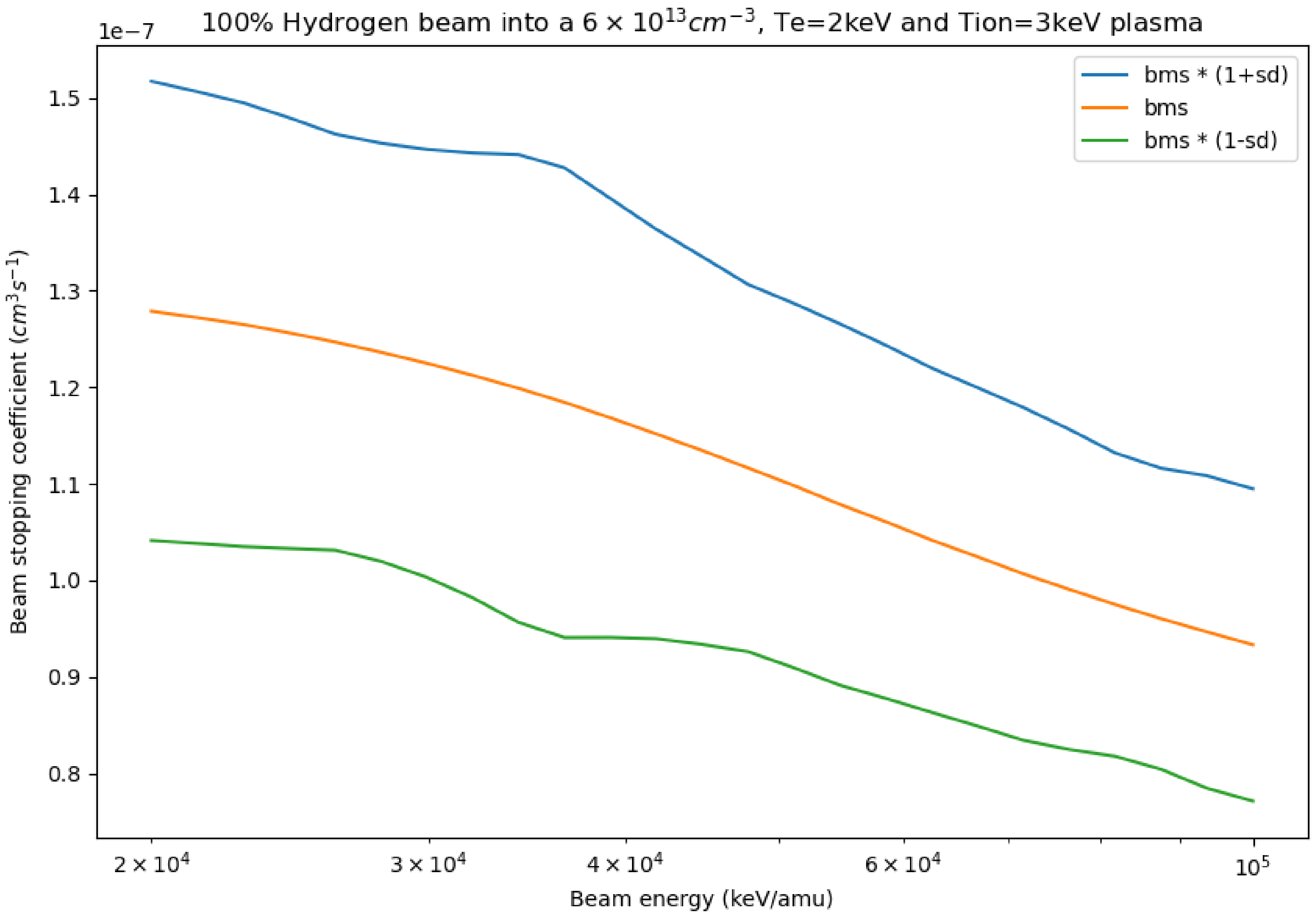
Effect of different p + H^0 ionization cross sections on the stopping coefficient





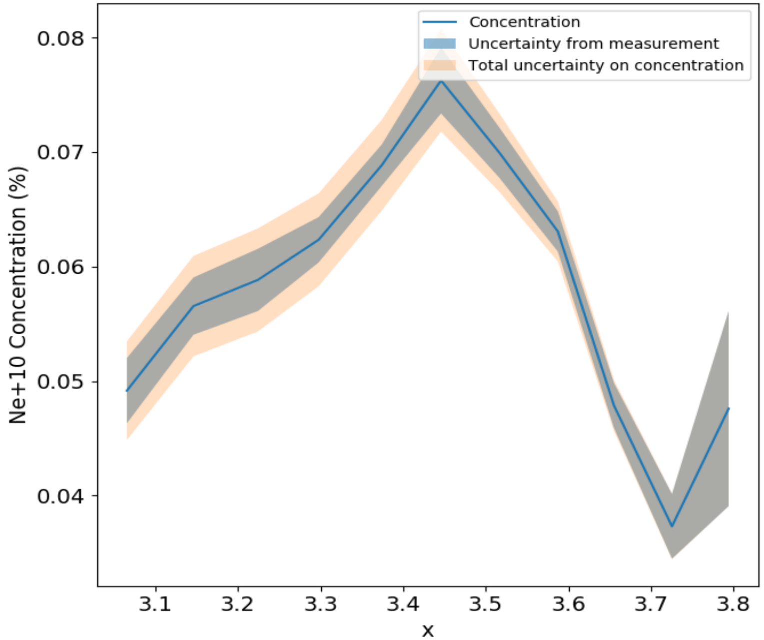
- A lesser effect at high energies – good for ITER
- Low energy difference may influence energy deposition and current profile interpretation in present day tokamaks.

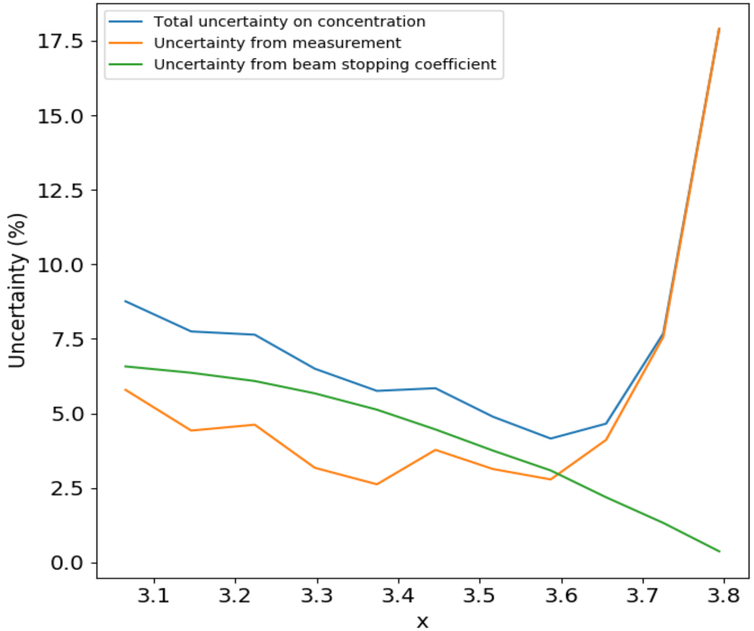
Propagated error on beam coefficients



Effect on the concentration

Apply CHEAP to Ne10+ concentration measurement with:
bms-sd bms bms+sd
and separate out the new ‘atomic error’





- Uncertainties on the diagnosed parameter due to atomic inputs are of same order as measurement errors.
- Important to properly determine this uncertainty and to reduce it as much as possible.

New fundamental atomic data

Plan to use data from:

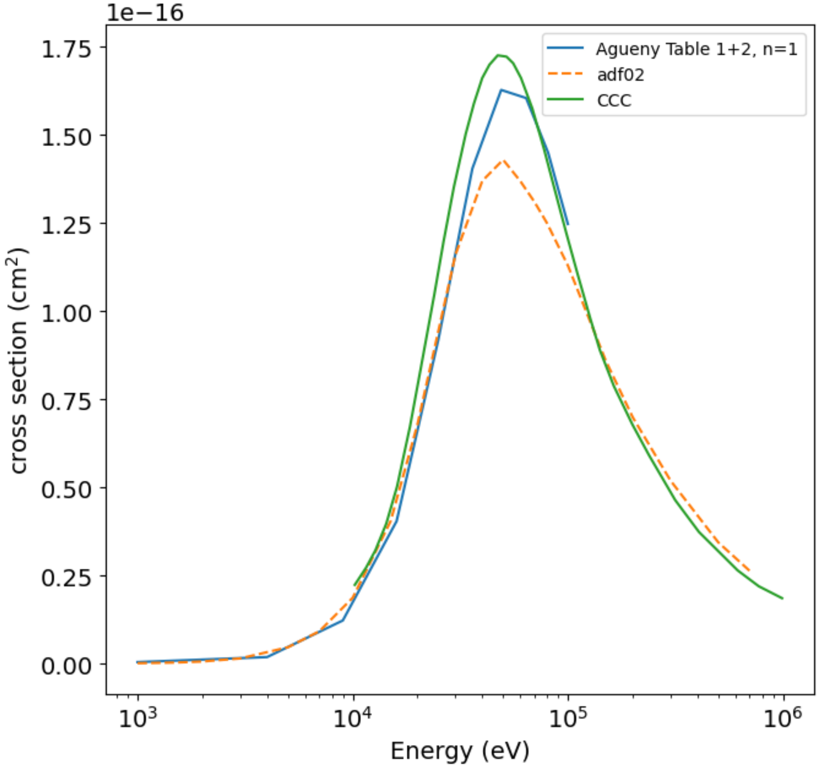
- p + H^0 ionization: I B Abdurakhmanov et al, J. Phys. B, 53 (2020) 14520
- p + H^0 excitation: H Agueny et al, Atomic Data and Nuclear Data Tables,
  129-130 (2019) 101281
- e + H^0 excitation: new R-matrix data – published as part of this work.

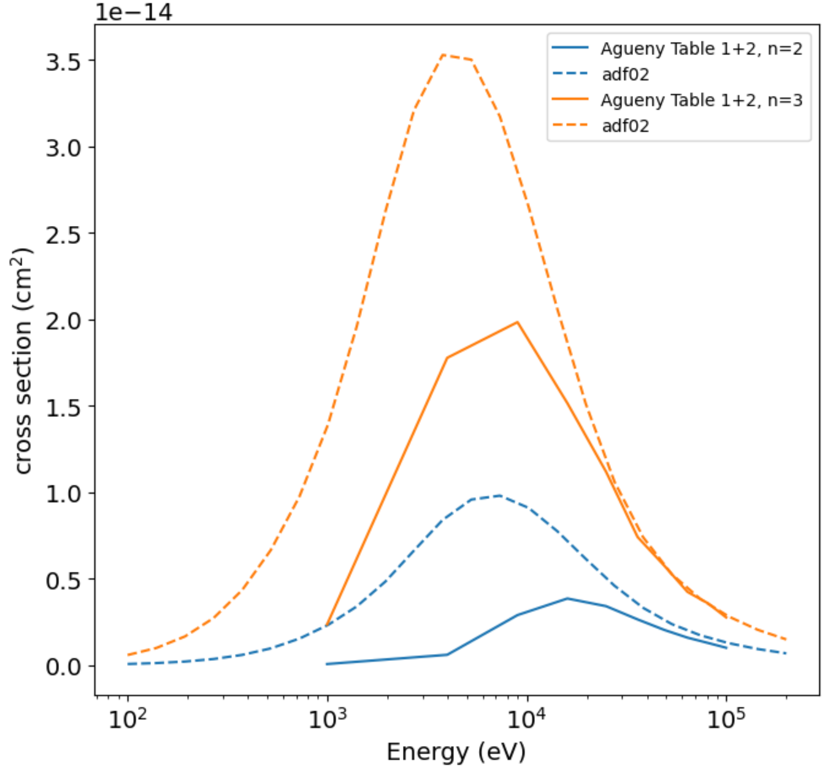
- CX emissivity – UQ propagation code need development and neon is the observation of choice for JET.

Questions:

- What are the error bars or uncertainty limits?
- Are there canonical numerical tabulations?

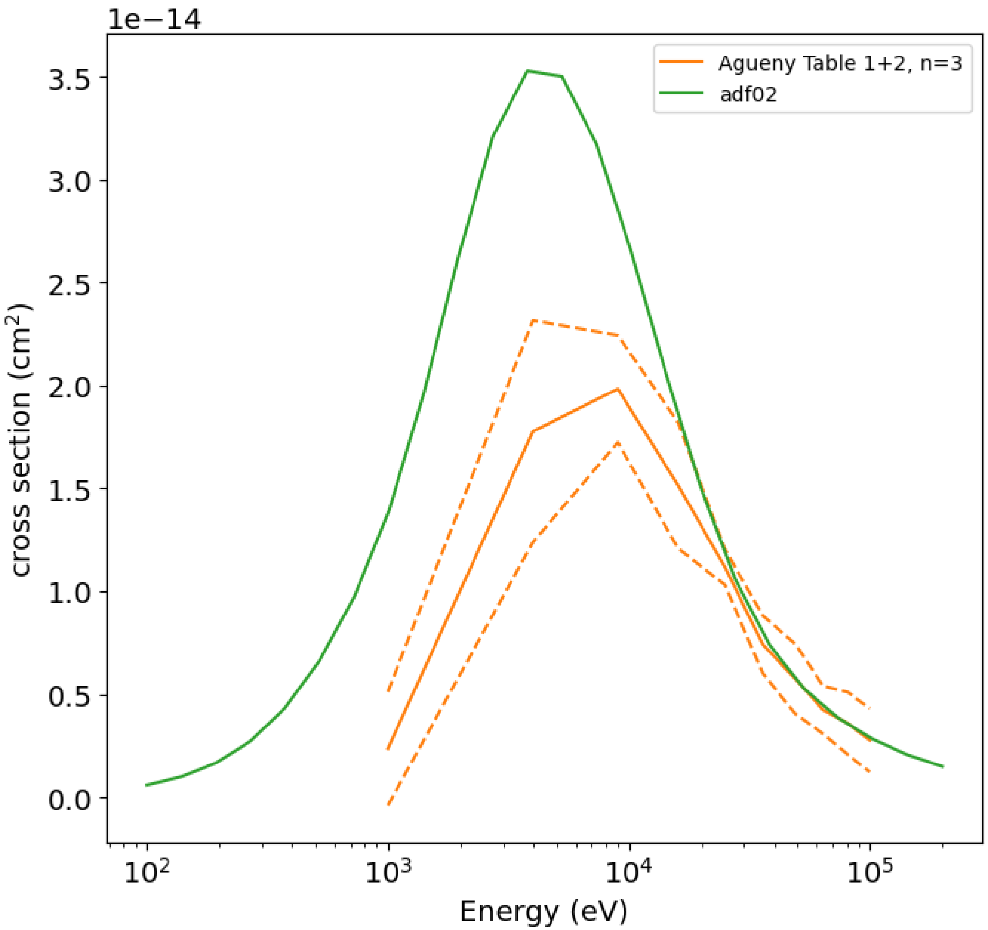
Ionization





- Large differences for n=2,3 (adf02 – Janev & Smith)
- Should we expect similar differences for n=4,5,6….?

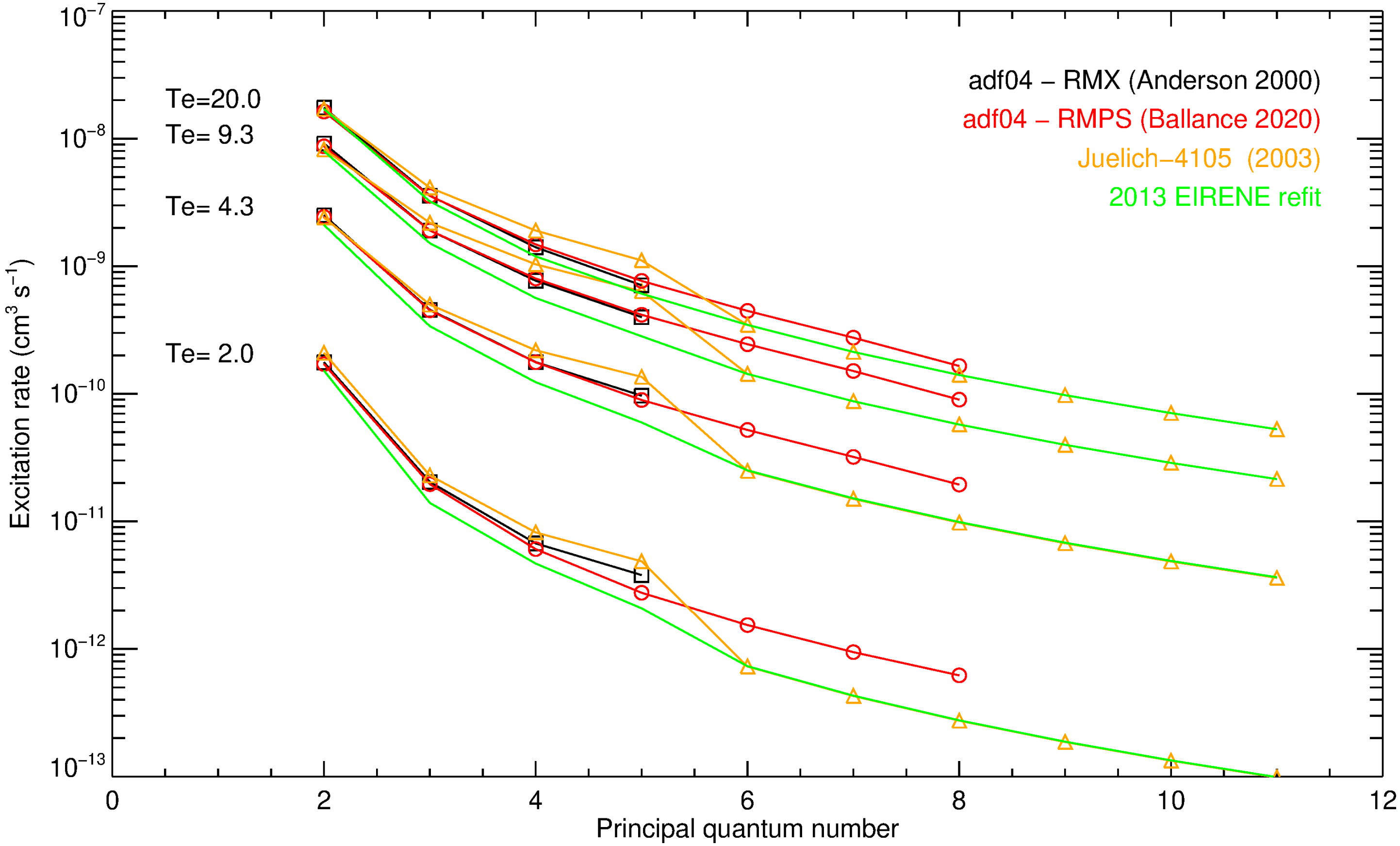
Ionization



- Is the convergence criterion a good error bar?

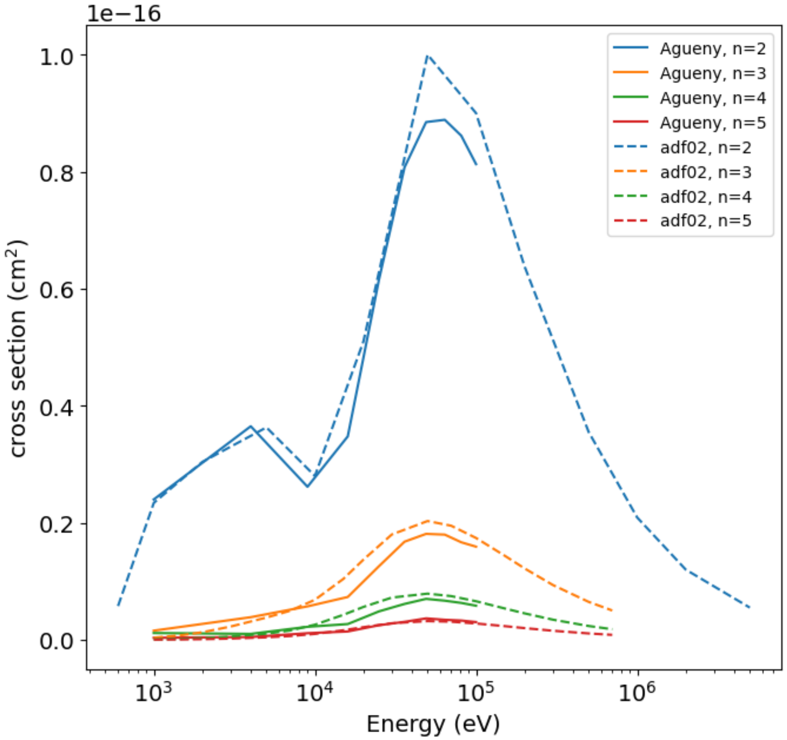
Electron-impact excitation data for H^0

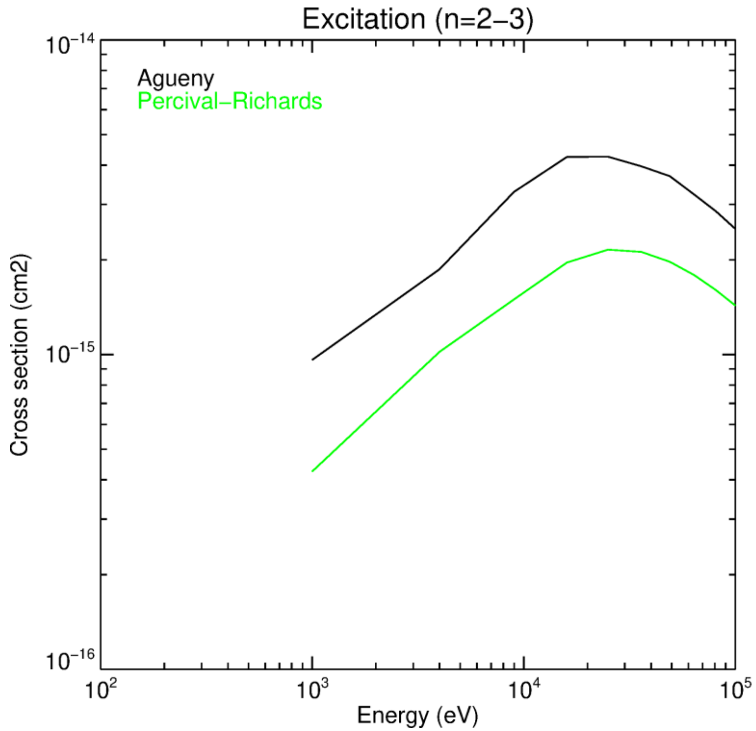
Excitation from ground to excited n-levels



- 1958 – first measurement of 2p→ground (Fite and Brackmann).
- 1963 – close coupling calculation (Burke).
- 2020 – R-matrix up to n=8 and all n-n' transitions (C Ballance, QUB)

Excitation





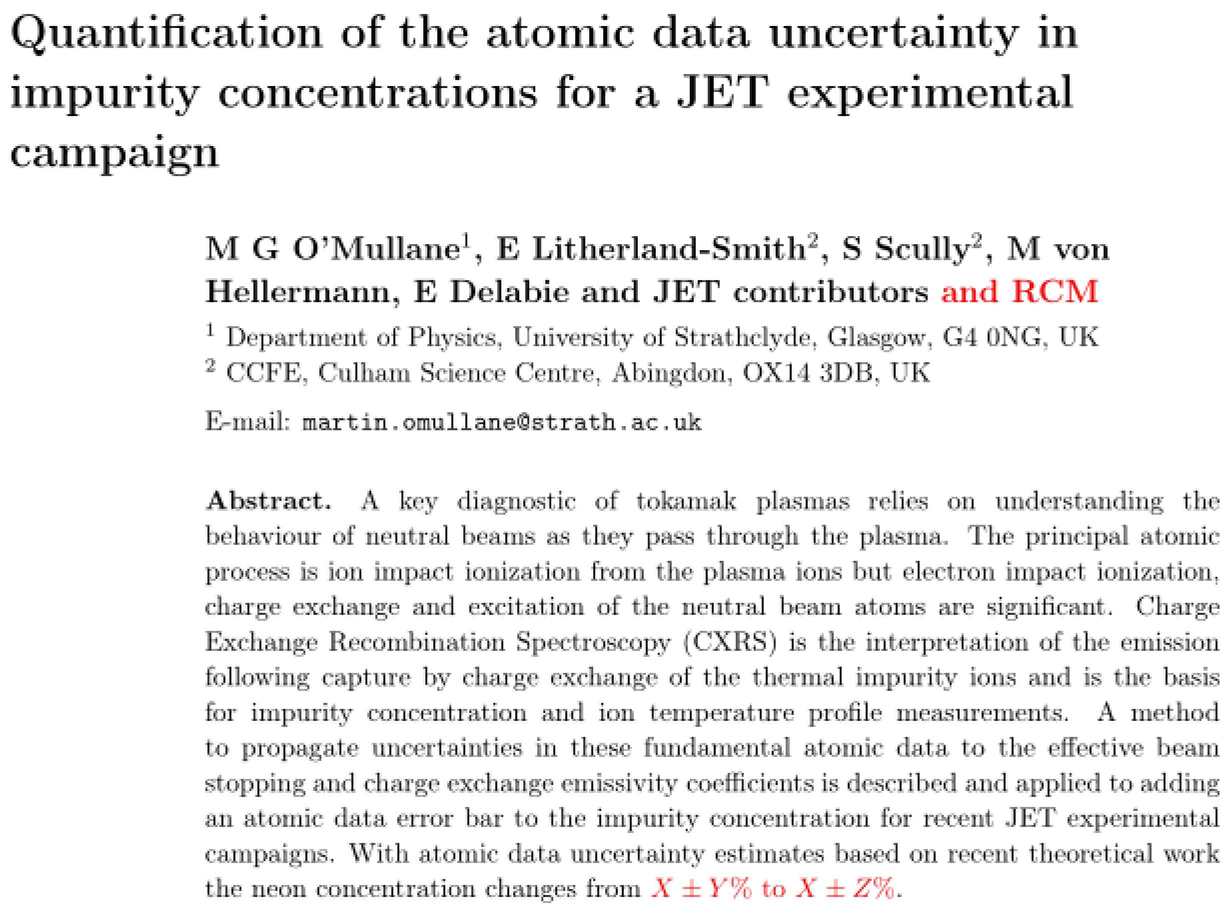
- Comprehensive coverage n=1 to n=5
- Is the convergence criterion a good error bar?
- factor of 2 difference for n=2-3 Percival-Richards – real or a bug?

Numerical data

```
LI+ 0          3          1     43489.0(1S)   516797.0(3S)
    1 1S2 2S1             (2)0( 0.5)             0.0000   {1}1.000    {2}1.500
    2 1S2 2P1             (2)1( 2.5)         14903.9000   {1}1.000
    3 1S2 3S1             (2)0( 0.5)         27206.1000   {1}1.000
    4 1S2 3P1             (2)1( 2.5)         30925.4000   {1}1.000
    5 1S2 3D1             (2)2( 4.5)         31283.1000   {1}1.000
    6 1S2 4S1             (2)0( 0.5)         35012.1000   {1}1.000
    7 1S2 4P1             (2)1( 2.5)         36469.6000   {1}1.000
    8 1S2 4D1             (2)2( 4.5)         36623.4000   {1}1.000
    9 1S2 4F1             (2)3( 6.5)         36630.2000   {1}1.000
   -1
  1.0     1       1.00+02 1.23+02  ...      1.8.11+05 1.00+06
/mt =     6.9410 /zp =   1.00 /mp =    1.0073 /  1^H  impact /
   2   1 0.00+00 2.05+01 3.55+01          6.13+05 6.45+05
   3   1 0.00+00 2.62-01 6.56-01  ...     8.55+03 8.77+03
   4   1 0.00+00 5.61-01 1.38+00          3.40+03 3.42+03
   5   1 0.00+00 4.23-01 1.07+00          1.39+04 1.40+04
   6   1 0.00+00 1.51+00 2.03+00          1.93+03 1.99+03
                                   .
                                   .
                                   .
   9   7 0.00+00 1.49+06 1.51+06          2.59+06 2.60+06
   9   8 0.00+00 1.33+07 1.37+07  ...     5.22+07 5.39+07
S  1  +1         5.82+02 9.33+02          8.95+04 9.28+04
S  2  +1         1.50+04 1.84+04          4.33+05 4.55+05
S  3  +1         1.56+04 1.89+04          1.96+05 1.98+05
S  4  +1         2.65+04 3.21+04          9.32+05 9.83+05
S  5  +1         3.86+04 4.71+04  ...     1.58+06 1.65+06
S  6  +1         5.79+04 6.39+04          4.04+05 4.26+05
S  7  +1         7.92+04 9.15+04          1.38+06 1.45+06
S  8  +1         1.00+05 1.18+05          2.41+06 2.50+06
S  9  +1         1.38+05 1.62+05          3.30+06 3.43+06
  -1
  -1  -1
C-------------------------------------------------------------------------------
C
C  Ion (proton) impact collision strengths for excitation and ionisation of neutral lithium,
C  suitable for use in modelling lithium beams. The collision strength includes a mass
C  factor mu=(m_p * m_t / (m_p + m_t)) where m_p is the mass of the proton and m_t is the
C  mass of the Li0 target. The quantity stored here is:
C       omega_exc = mu * g_i * (E_i/I_H) * (sigma / pi * a0^2)
C  where g_i is the statistical weight of the lower level, E_i the energy of the proton,
C  I_H=13.6m and sigma the cross section in cm^2. For ionisation the definition is similar.
C
C  The data is used in Asdex Upgrade modelling and was assembled by J Schweinzer and
C  E Wolfrum and supplied to ADAS by K Igenbergs.
C
C  The data is described in: J Schweinzer et al, 'DATABASE FOR INELASTIC COLLISIONS OF
C  LITHIUM ATOMS WITH ELECTRONS, PROTONS, AND MULTIPLY CHARGED IONS', Atomic Data and
C  Nuclear Data Tables, vol 72, p 239 (1999)
C  DOI: 10.1006/adnd.1999.0815
C
C  Assembled for ADAS : Martin O'Mullane
C  Date               : 01-09-2018
C
C-------------------------------------------------------------------------------
```

- In my ideal world the p-impact data would be in an *adf06* file
- And it would have a companion *.err* file.

Reporting on work


Quantification of the atomic data uncertainty in impurity concentrations for a JET experimental campaign

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Abstract. A key diagnostic of tokamak plasmas relies on understanding the behaviour of neutral beams as they pass through the plasma. The principal atomic process is ion impact ionization from the plasma ions but electron impact ionization, charge exchange and excitation of the neutral beam atoms are significant. Charge Exchange Recombination Spectroscopy (CXRS) is the interpretation of the emission following capture by charge exchange of the thermal impurity ions and is the basis for impurity concentration and ion temperature profile measurements. A method to propagate uncertainties in these fundamental atomic data to the effective beam stopping and charge exchange emissivity coefficients is described and applied to adding an atomic data error bar to the impurity concentration for recent JET experimental campaigns. With atomic data uncertainty estimates based on recent theoretical work the neon concentration changes from $X \pm Y\%$ to $X \pm Z\%$.