Data and code updates in ADAS and OPEN-ADAS and ensuring data traceability

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and many ADAS contributors

Outline

ADAS is a set of computer codes and a reaction database oriented to the needs of magnetic confined fusion and astrophysics research.

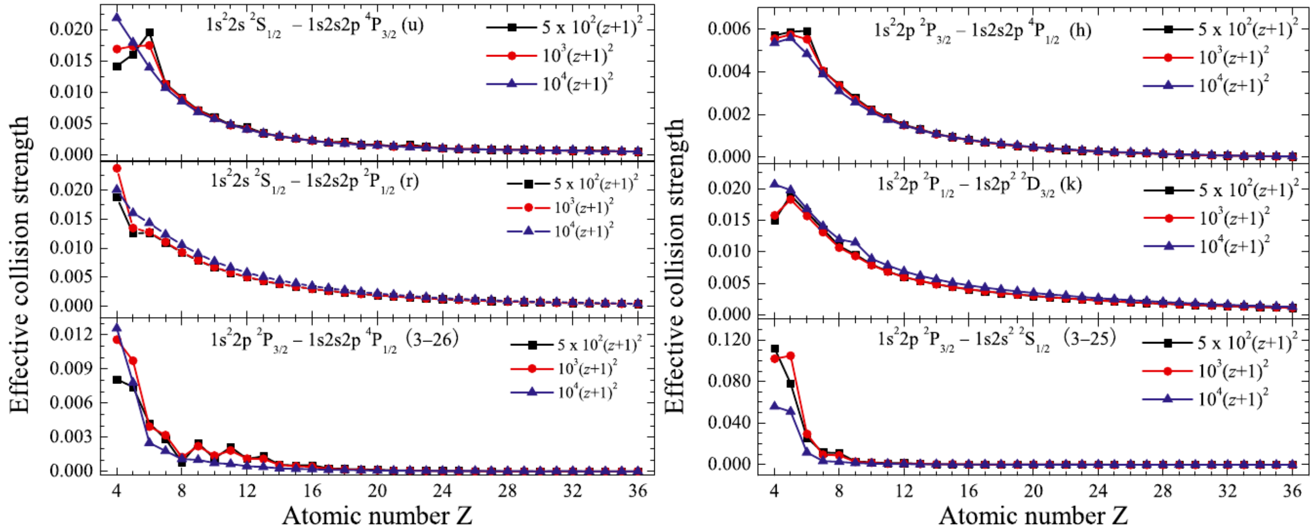
Effective coefficients, characterizing finite density conditions, are required for modelling and diagnostic interpretation. Collections of fundamental, individual process data, are needed to produce the derived, effective data.

OPEN-ADAS is the pathway for ADAS data and support software to be made publicly available and is an agreed and shared project between ADAS and IAEA.

- New data in ADAS
    - Iso-electronic sequences of excitation data
    - Radiated power
    - Beam stopping
- New codes in ADAS
    - Ion impact and inclusion in ionisation balance
    - Spectral features and fitting
- Provenance and traceability of data
    - Maintaining relevance and correcting data
    - Use of data in other systems

New data – iso-electronic sequences

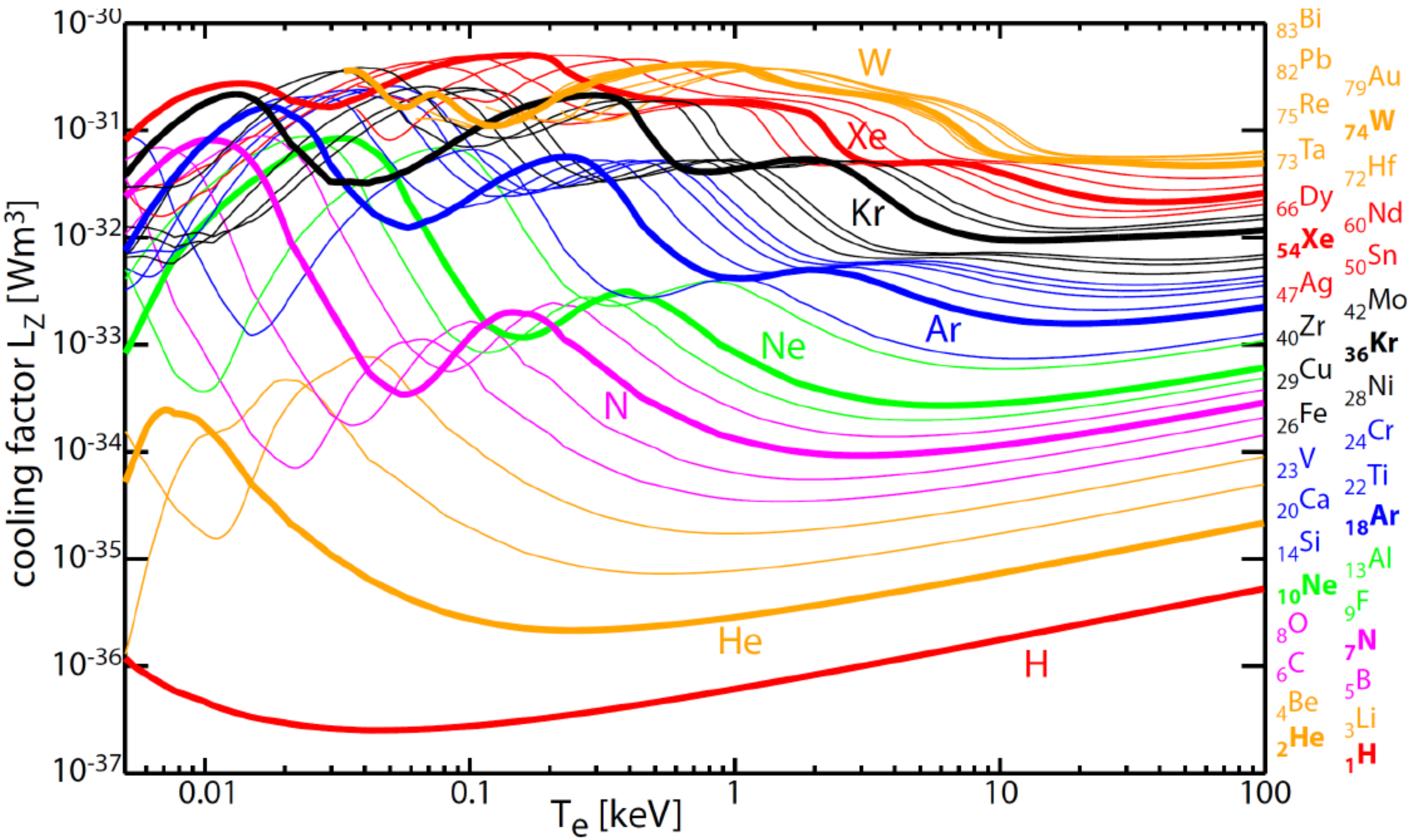
- Corpus of distorted wave excitation data
  - H-like to Ar-like for Hydrogen to Zinc (Mo, Sn, Xe and W)
  - produced with AUSTOSTRUCTURE
  - cross-section (t1) and effective collision strength (t3) data
- R-matrix sequence work
  - He-, Li-, Be-, B-, F-, Ne-, Mg-like sequences
  - N Badnell, L Menchero, G Liang, M Witthoeft
- Baseline of Cowan code PWB produced as needed but this is being replaced by distorted wave.



G Liang & N R Badnell, Astron. Astrophys. 528,A69 (2011)

New data – radiated power

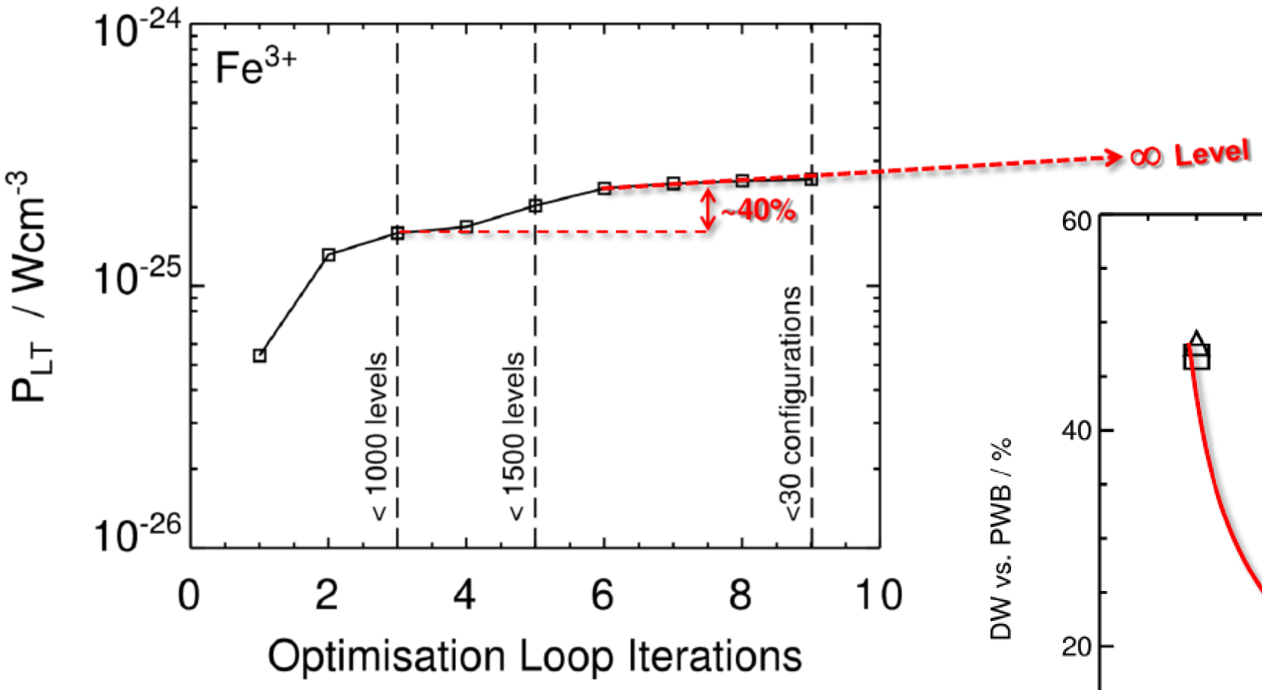
A self-consistent set of enhanced baseline fractional abundance and radiated power data for 35 elements between Hydrogen (Z=1) and Gold (Z=79)

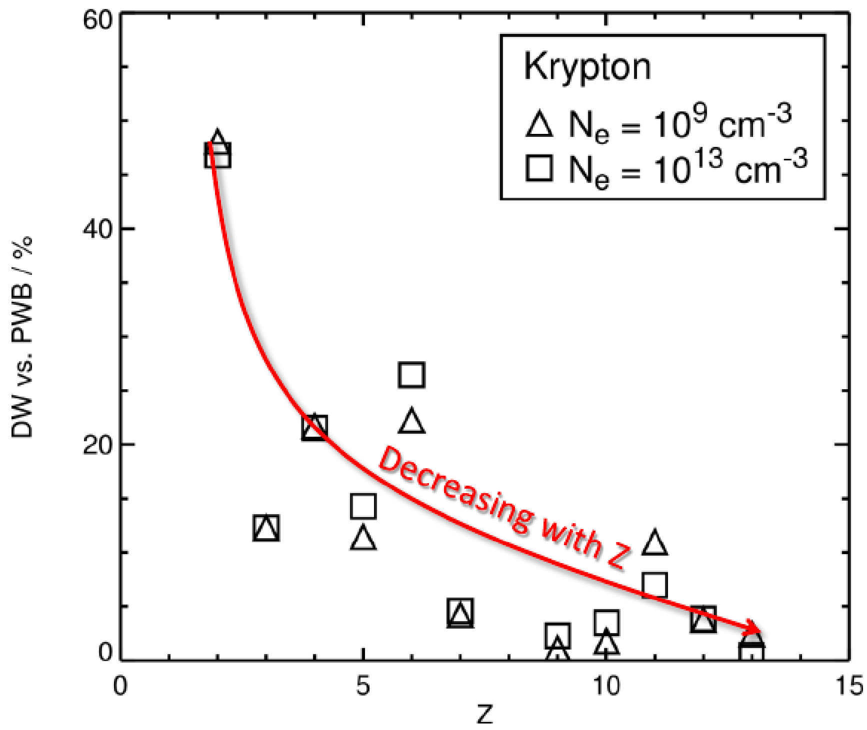


CADW ionisation, average ion recombination and ADAS PWB radiated power. T Pütterich

New approach – optimizing the radiated power

- Develop rule-based methods to optimize the total radiated power.
- Structure and method differences give a measure of the confidence/uncertainty of the radiated power coefficient.
- Complementary to the one-method, self-consistent, approach.



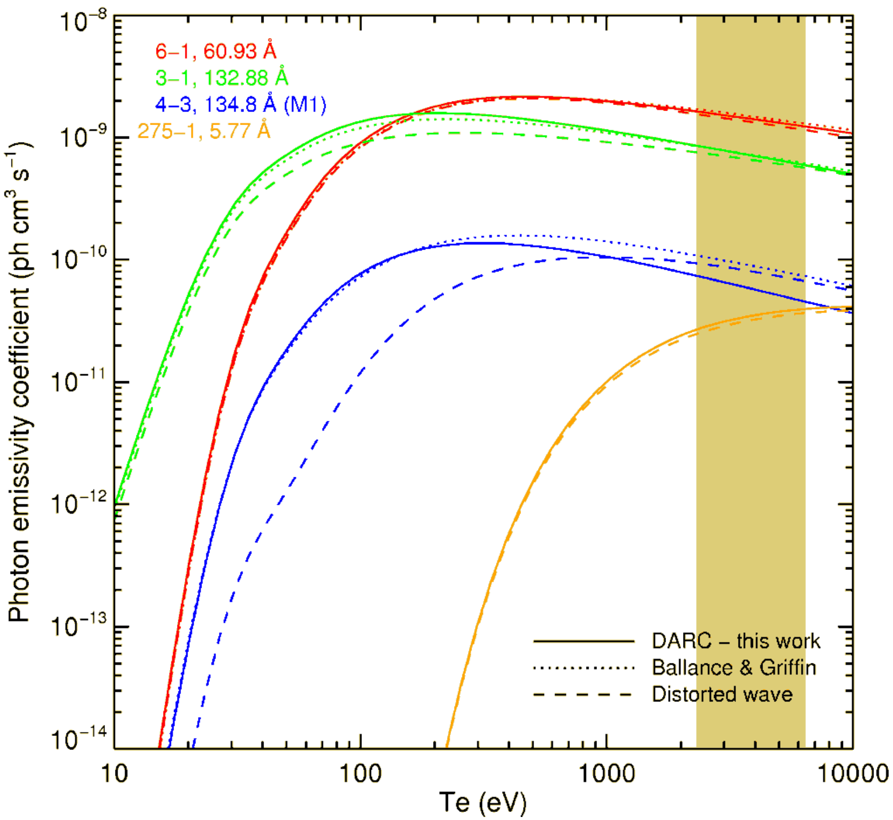


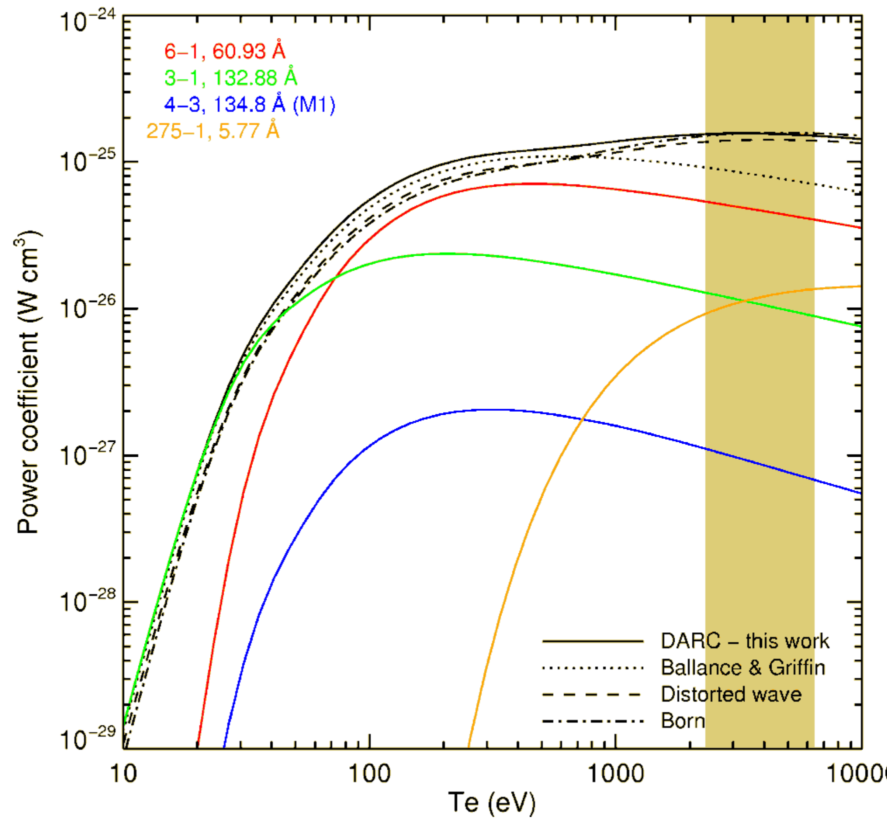
- 'Missing' configurations are significant
- Methods converge with increasing Z

New data – individual ions

- For diagnostically important ions we want the best data possible.
- R-matrix iron data for Fe^{2+}, Fe^{8+} and Fe^{12+} and W^{44+}

Consider W^{44+} ($3d^{10}$ $4s^2$) a new calculation, yielding a range of values and showing the effect of omitting a configuration ($3d^9$ $4s^2$ $4f$).

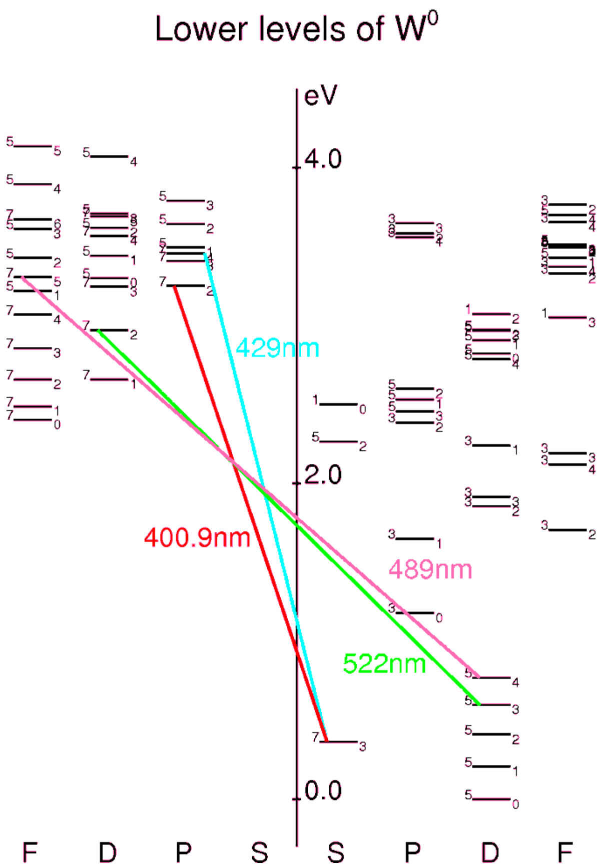


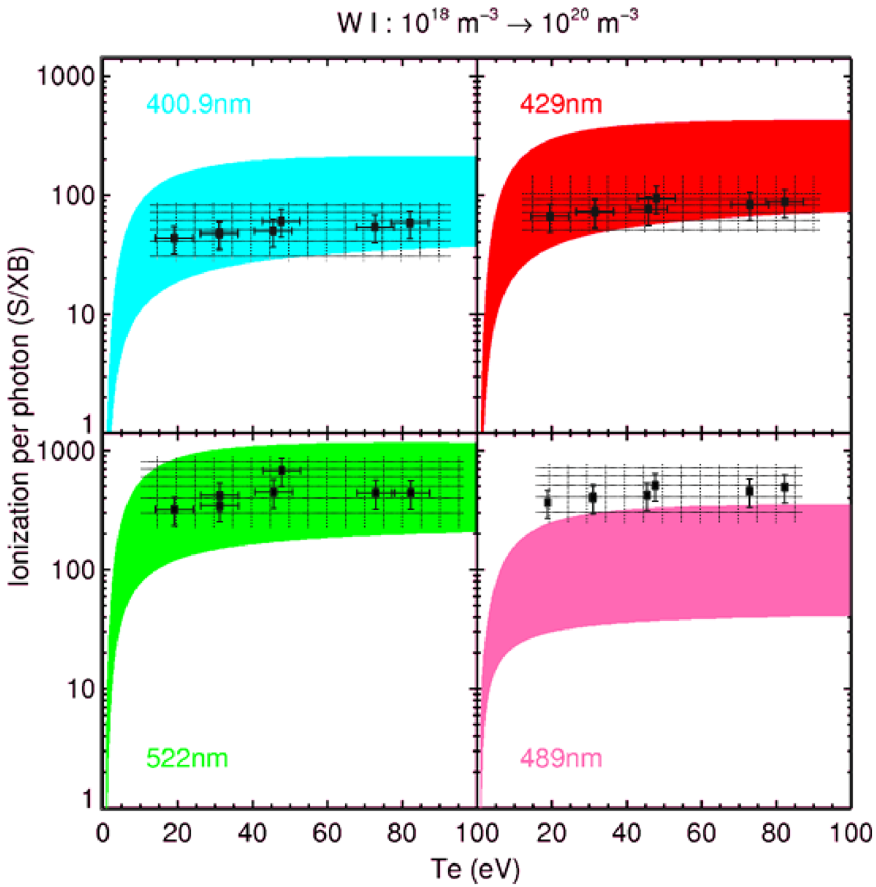


M Bluteau et al, J. Phys. B, **48**, 195701 (2015)

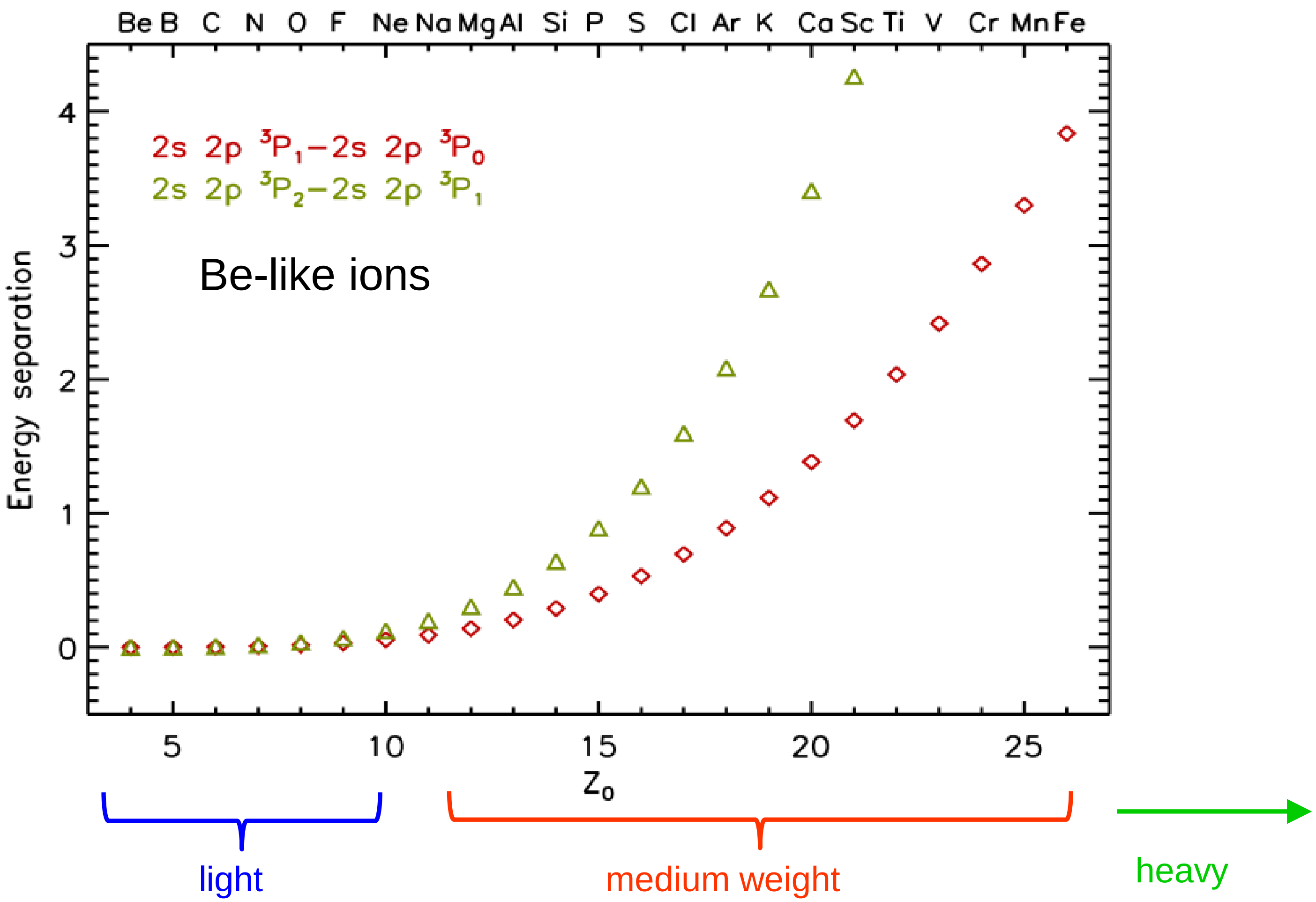
Code update – improvement in atomic structure

- Calculating the structure of neutral tungsten is a challenge.
- Large CI with core-polarization gets close. P Quinet el al, J Phys. B, 44, 145005 (2011)
- Modify adas8#1 (Cowan code) to include these effects for structure while keeping the number of excited levels manageable.





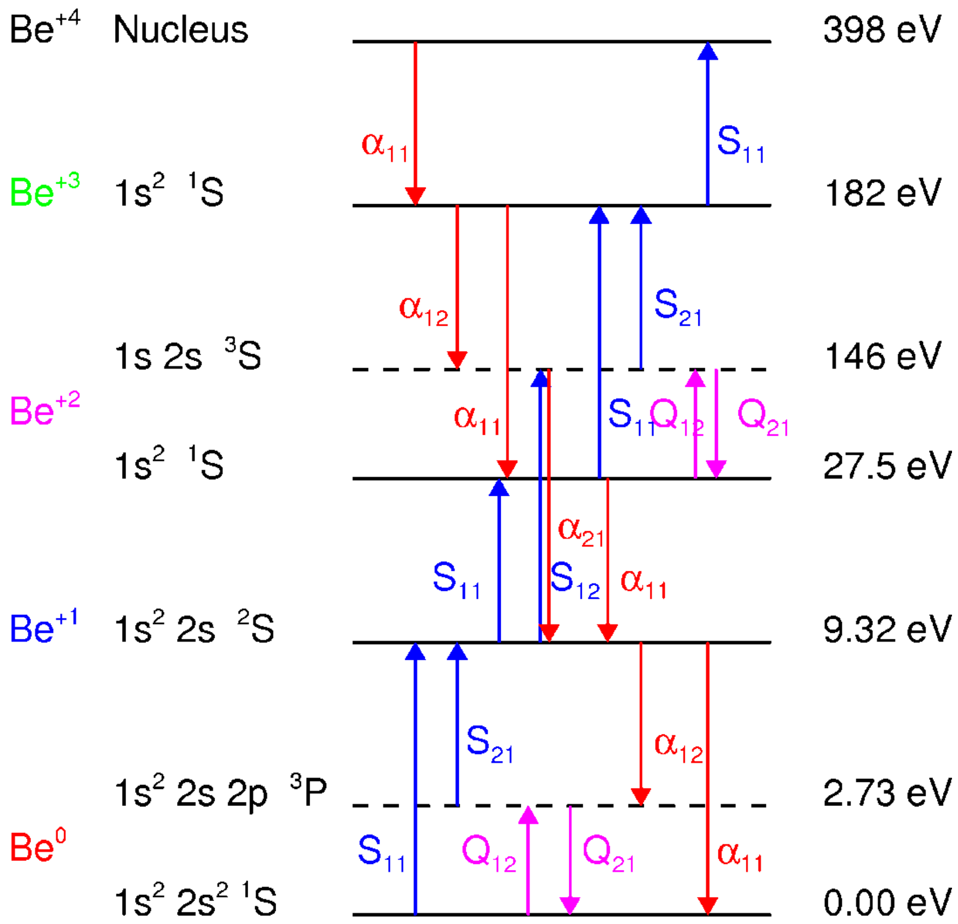
New code – intermediate coupling and fine structure



Cannot ignore the divergence for Z>10 so ion impact must be explicitly accounted for.

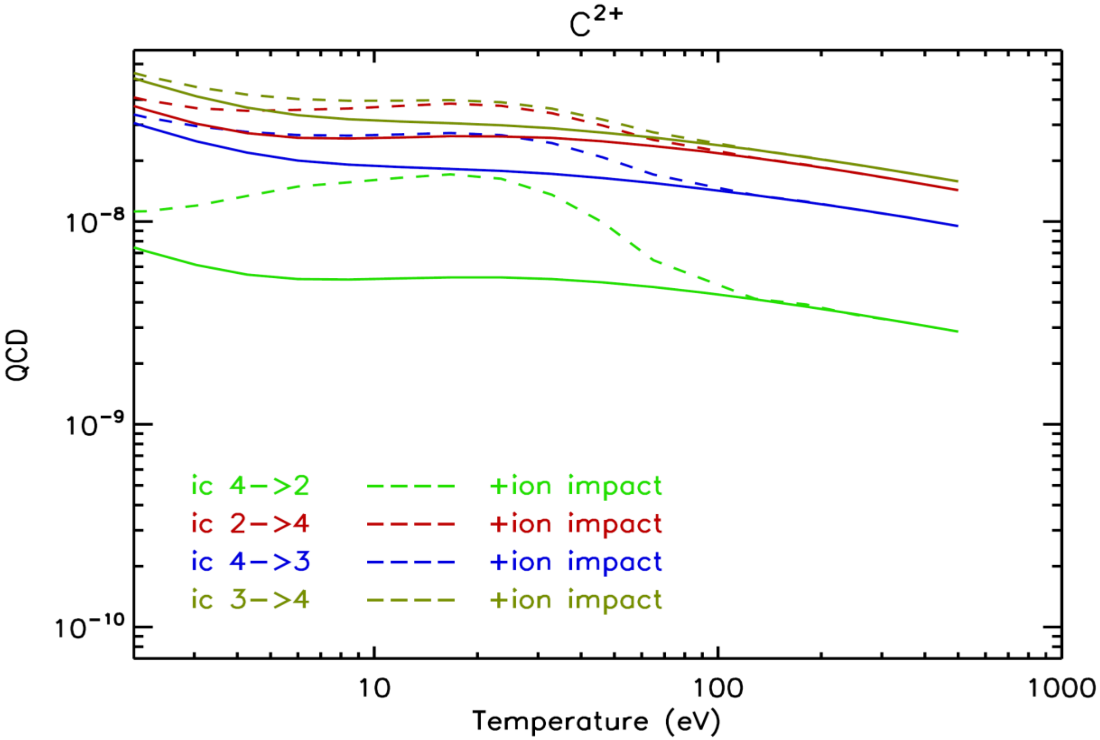
Ionization balance and GCR coefficients

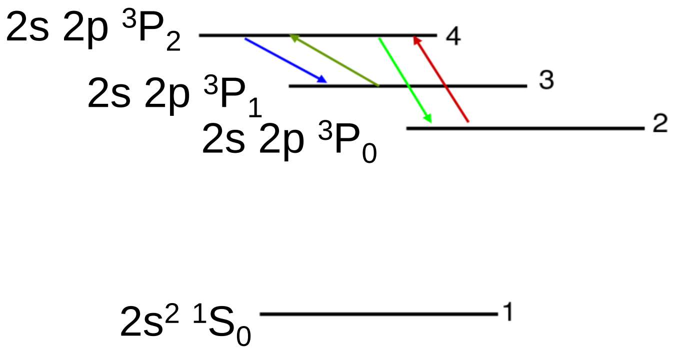
$$\frac{dN_{\rho}^{+z}}{dt} = -(N_e \boxed{S_{CD,\sigma\to\nu}} N_{\sigma}^{+z} + N_e \boxed{\alpha_{CD,\nu'\to\rho}} N_{\nu'}^{+z+1} + N_e \boxed{Q_{CD,\sigma\to\rho}} N_{\sigma}^{+z}) + \ldots$$



Q_{CD} – metastable cross-coupling

Only levels within the fine structure are affected significantly by ion impact.





$$Q^{total}_{CD,\sigma\rightarrow\rho} \simeq Q^{(e)}_{CD,\sigma\rightarrow\rho} + \left(\sum_{ion} N_{ion} q^{ion}_{\sigma\rightarrow\rho} \right) / N_e$$

Develop code (Bely-Faucher or Burgess-Tully) for ion impact and store in *adf06* datasets

Code improvements – fitting spectral features

We have generally considered ADAS to be a reaction database.

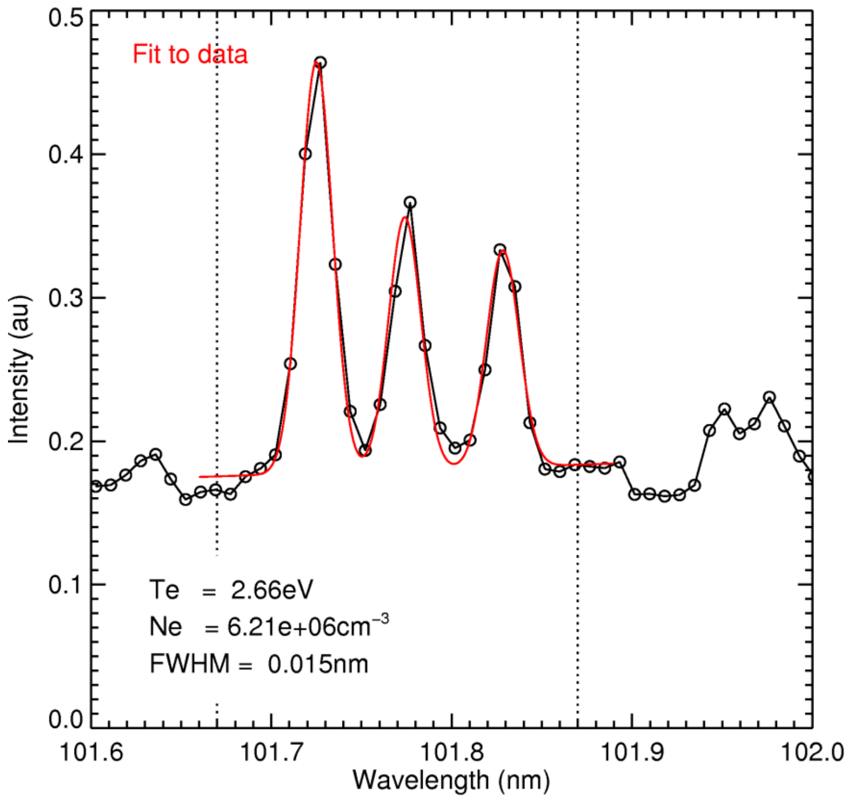
- Collection of data for modelling transport and diagnosing emission.
- We ‘know’ which element and which transitions are under study.
- adf11 PLT, adf15 PECs, adf12 CX emissivities, or Zeeman features are catalogued and compared to *identified* energy-integrated or spectroscopic measurements.
- High precision wavelengths are not required for population modelling.
- Spectral synthesis was not a priority for ADAS.
- Effort was directed to improving *y-axis* accuracy.

Reasons to question/re-assess this stance:

- The experimental measurements we want to confront are complex features.
- Remove a degree of freedom in fitting models of spectral lines.
- Variations in the underlying structure are now noticeable in the derived emissivity and power coefficients.
- Part of concerted approach to quantifying uncertainty.

Note that this does not mean that ADAS will try to replace/compete with NIST (ASD).

Example: fitting a solar Fe^{2+} multiplet



$3d^6\ ^3H - 3d^5(4G)4p\ ^3H$

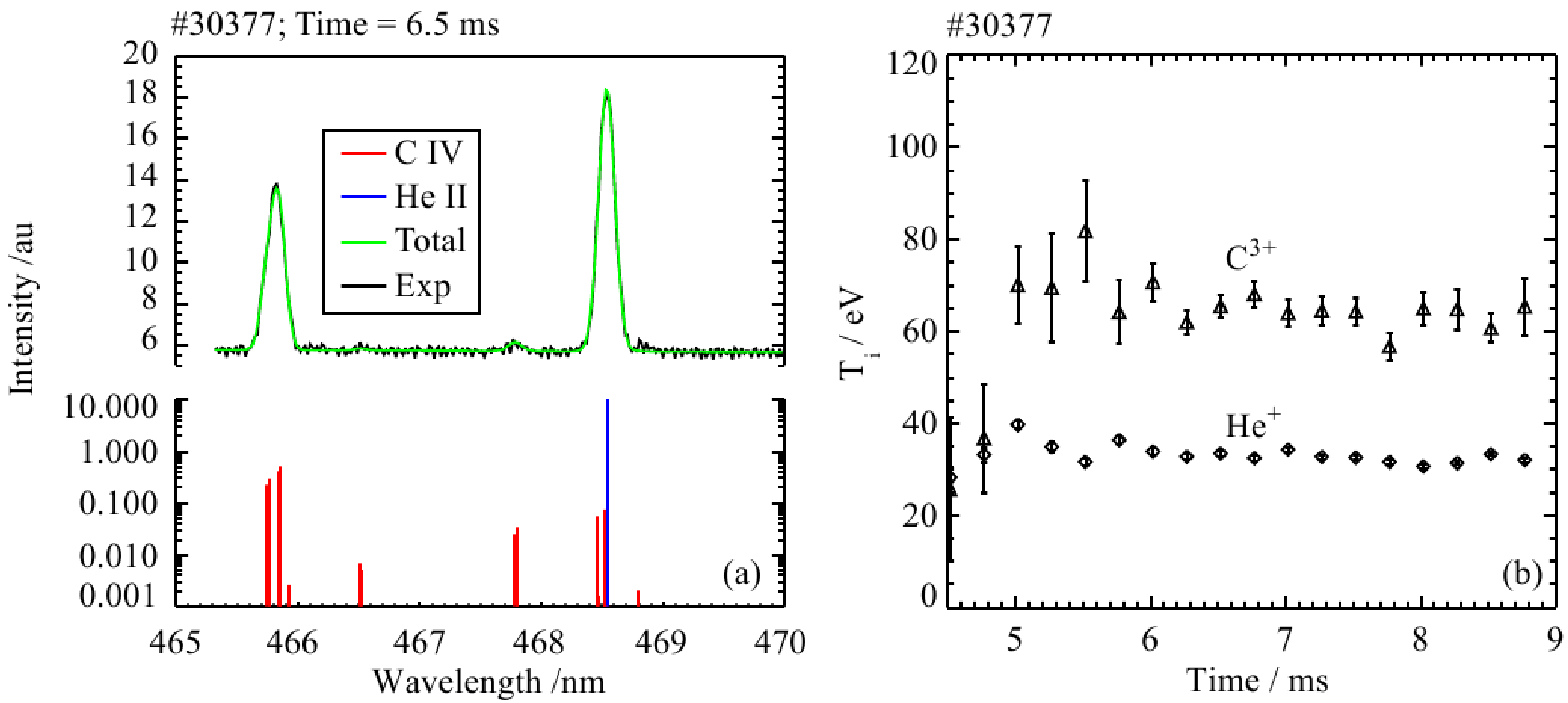
	Edlén	R-matrix (optimized)
3H_6	20050.3	23018.5179
3H_5	20300.0	23235.0067
3H_4	20481.1	23451.3811

and

3H_6	118354.21	127294.3864
3H_5	118556.45	127673.1821
3H_4	118685.45	127878.7733

- R-matrix collision data: Badnell, Ap. J, **785**, 99, (2014)
- NIST energy levels: Edlén, Ap. J, **95**, 532, (1942)
- Match energy levels with *adas7#5*
  – adf04/nist#26/ic#fe2.dat and adf04/crlike/crlike_nrb13#fe2.dat
- Fit with ADAS ffs/afg framework.

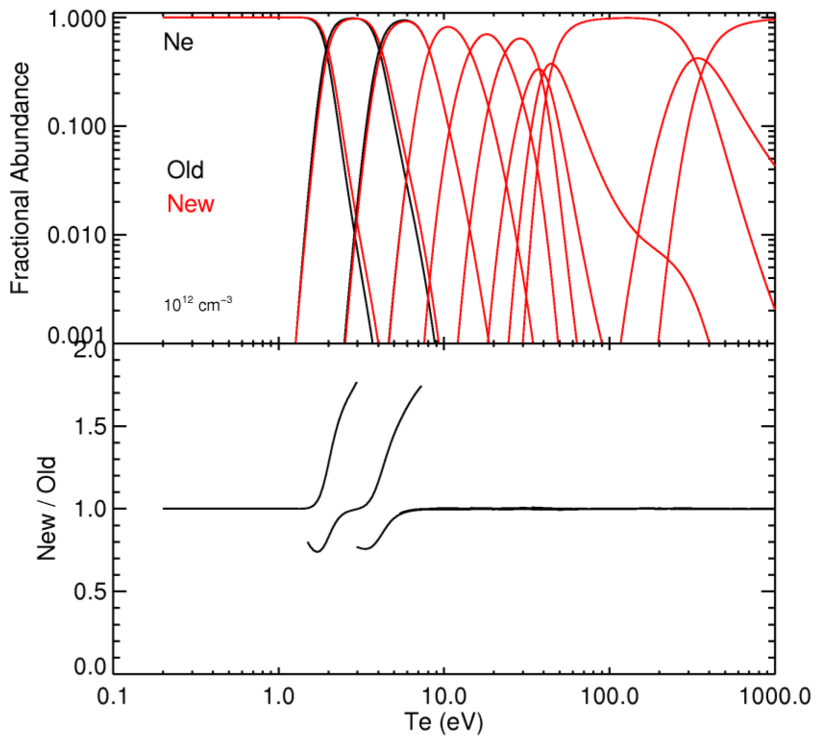
Example: fitting a beam driven CX feature

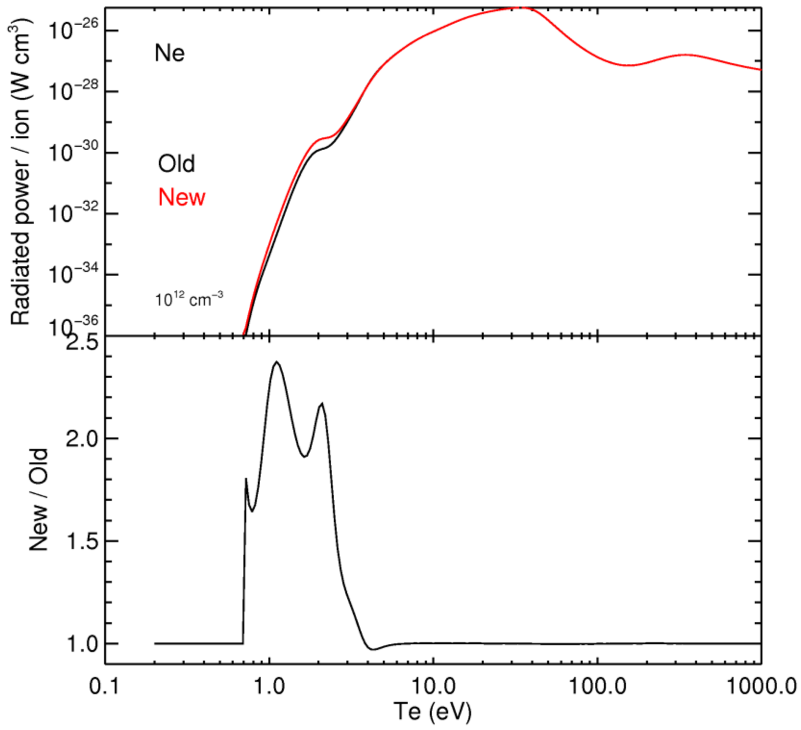


- MAST plasma with added helium and intrinsic carbon.
- The spectrum is an overlapping core C CX feature and edge (thermal) He line.
- The plasma physics model wants to know the ion temperature profile.

Fixing mistakes in existing data

- ADAS policy is not to replace existing data with ‘better’ or more sophisticated data
- A new dataset is produced with the old ones remaining.
- But mistakes happen and occasionally data need to be updated and replaced.





The consequence of a mis-indexing the 4th (2p^3 3s ^{5}S) metastable

Atomic, Molecular, Nuclear & Surface Data in IMAS

- IMAS – integrated modelling system for ITER
- Systematic recording of atomic data used in IMAS simulations in IMAS database
  - No hard-coded atomic data in codes, no untraceable direct access to external database for atomic data
  - Provenance traceability (recording source of atomic data tables)

- AMNS package provides methods to:
  - Import atomic data tables from other databases (e.g. ADAS) into a local storage (includes recording data provenance)
  - Read atomic data tables from that storage and calculate the requested information (e.g. interpolation of tabular data)

Simon Pinches, ITER IO

Traceability of atomic data

Funding agencies – definitely in UK and EU – and probably elsewhere insist on:

- A data management plan for research outcomes
- Store sufficient data to independently re-run simulations

From a data point of view these requirements can be summarized as:

1. Decide the terms under which data can be made available, taking in consideration commercial/confidentiality constraints and third party claims.
2. Publications must state where data can be found and it must be citable.
3. Data must be preserved long term (10 years or more) and must be shareable with other researchers.
4. Data should be clearly described with appropriate metadata.

eg At JET *all* experimental data is stored and tagged in a central data store and all analysis must be performed on this centralized repository. Referencing this is therefore straightforward and there is an appointed RO in the operational unit .

eg ADAS data in OPEN-ADAS can be referred to via its URL.

What about atomic and molecular data?

Many organizations, including universities have setup information and publication repositories to fulfil these requirements. *eg* PURE platform for UK universities.

- Data is assigned a stable, unique and non-changeable reference using a digital object identifier (DOI) – see http://dx.doi.org/
- Longevity is assured by being formally hosted by the university.
- But alternative archives based around subject, national, international or academic journals may also be more suitable repositories for data.

At the moment there does not appear to be any great desire on behalf of the funding bodies, or the universities and research institutes, to specify where and what data is stored, just that it is preserved and can be found.

- Pragmatic decision based on collaboration and multi-institutional sources.
- ADAS, and other DCN databases, are 'suitable' repositories.

Can we make these (slightly onerous) requirements work for us?

- The minimal approach is a repository (with DOIs) but is just a dump of files.
- ADAS is in discussion with our university to issue DOIs for each dataset.
- Then we need to build tools to enable traceability of ADAS data through modelling and analysis codes.
- ADAS data in EU and ITER integrated modelling systems will have the DOI tag.