Computational Atomic and Molecular Physics for Transport Modeling of Fusion Plasmas

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ITER relevant modelling efforts

Numerous issues are now pertinent in the run up to ITER operation. A collaboration has been brought together to implement state-of-the-art atomic and molecular collision codes on the next generation of terascale computing facilities, to assist in answering questions such as

- The final choice for plasma-facing materials, in particular the possible use of
  - Be, C, and W components for the first wall
- Relevance of innovations on operational regimes
- Study of ELM transient in standard ITER operation

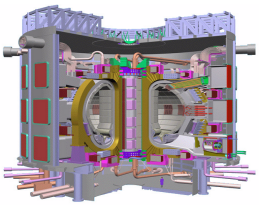

Figure 1. Schematic of ITER.

Plasma transport codes (such as SOLPS, SANCO) provide an insight into the transport of plasma impurities, the radiated power loss from various plasma impurity mixtures, and the behaviour of ELM and transport barriers. These codes require good atomic and molecular data for

- effective ionization and recombinations rate coefficients to track the ionization balance, and hence the plasma transport of impurity species
- emissivity coefficients to predict radiated power losses, and to compare with spectral observations.

Collisional-Radiative Modeling using ADAS

A modeling suite of codes called ADAS (Atomic Data and Analysis Structure) processes fundamental atomic data into a form useful for such transport codes, which are then used at facilities such as JET, ASDEX-Upgrade, DIII-D, JT-60, Tore-Supra and Alcator C-Mod.

- Solution to collisional-radiative equations to get the emitting populations requires:
  - Atomic structure for energies
  - Radiative rate coefficients
  - Collisional electron excitation, ionization and recombination rate coefficients
  - Collisional charge transfer recombination with neutral beam species

Various coefficients are produced from the ADAS codes, which can be transparently used in transport codes, namely:

- Generalised collisional-radiative coefficients
- Radiated power loss coefficients
- Photon emissivity coefficients

We have completed state of the art calculations for the following systems

- He, Li and Be

The accuracy of the coefficients which are passed to the transport codes is directly related to the atomic data which is used to generate them. Thus, much work has been done on generating highly accurate atomic data for key fusion species. These calculations are pushing the limits of current large scale computational resources, and are opening up new frontiers in atomic collision theory. We present some of these calculations in the following sections.

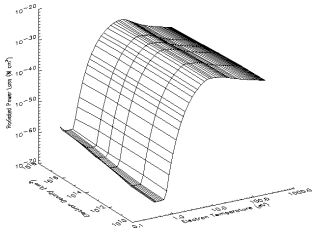

Figure 1. Radiated power loss from Li^+ as a function of electron temperature and density. The results were calculated using the recent lithium data, and the corresponding generalised collisional-radiative coefficients.

R-Matrix with Pseudo-State Codes

- Developed in the UK by P.G. Burke and co-workers, the method can be used to generate electron collisional excitation, ionization and recombination cross sections.
- All eigenvalues and eigenvectors of 50,000 x 50,000 matrices are required. Thousands of energies are needed to map out the Feshbach resonances sections. This can only be achieved on modern massively parallel computers.

R-Matrix with pseudo-states calculations are completed for

- He, He^+, Li, Li^+, Li^{2+}
- Be, Be^+, Be^{2+}, Be^{3+}
- B^+, B^{4+}, C^{2+}, C^{3+}, C^{5+}, O^{5+}

Standard *R*-Matrix calculations are completed for

- Ne^+, Ne^{4+}, Ne^{5+}, Fe^{20+}, Fe^{21+}, Fe^{23+}, Fe^{24+} and Fe^{25+}

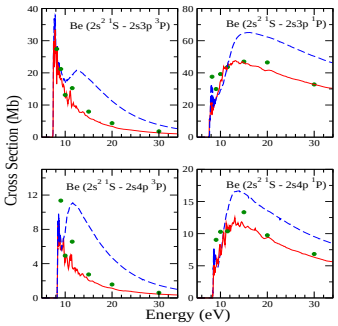

Figure 4. Electron excitation collision strengths for Be, from the recent RMPS calculations. The red curves show the pseudo state calculations, the blue curves the results with non-pseudo states, and the circles show CCC results. The effects of including pseudo states can be clearly seen.

Time-Dependent Close-Coupling Codes

- Treats the three body Coulomb breakup exactly for atoms
- Close coupled set of 2D lattice equations
- Calculations are completed for
  - H, He, He^+, Li, Li+, Li^{2+}
  - Be, Be^+, Be^{2+}, Be^{3+}
  - B^{2+}, C^{3+}, Mg^+, Al^{2+}, Si^{3+}
- Treats the four body Coulomb breakup exactly for atoms and molecules
  - Close-coupled 3D and 4D lattice equations
  - Calculations are complete for He and H_2^+.

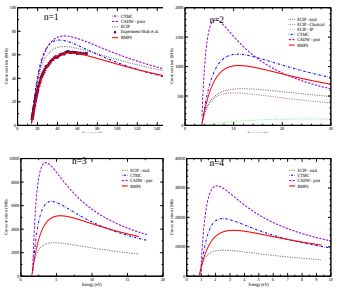

Figure 6. Excited state ionization cross sections for hydrogen.

Time-Dependent Semi-Classical Codes

- Especially useful for charge transfer cross sections, of relevance for fusion studies
- Applications such as p+H, p+Li, α + H, Be^{4+} +H, p+H_2^+

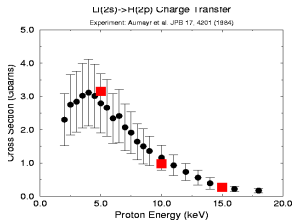

Figure 8. State-selective charge transfer cross section of protons on ground state lithium.

Distorted-wave and Classical Trajectory Codes

The distorted-wave techniques use perturbation theory

- They are accurate for radiative and autoionization rates, and for electron collisions with highly charged ions.
- There are various levels of calculation
  - Intermediate coupled distorted-wave (ICDW)
  - LS coupled distorted-wave (LSDW)
  - Configuration-average distorted-wave (CADW)
  - Classical Trajectory Monte Carlo (CTMC)

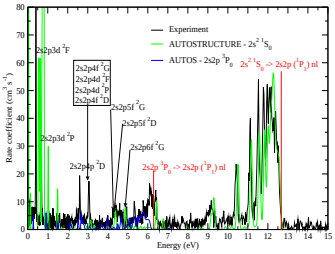

Figure 9. Dielectronic recombination resonance plot for C^{3+}, compared with recent measurements at the CRYRING, in Sweden.

Computational facilities

The large computational demands of the codes described previously means that they have to be run on large scale massively parallel machines. Thus, the following computers were used in the calculations presented here.

- NERSC - IBM-SP
- ORNL - IBM-SP, CRAY
- MANCHESTER - IBM-SP
- SAN DIEGO - IBM-SP
- LANL Q MACHINE

Figure 10. Images of the IBP-SP at NERSC (left) and the CRAY at ORNL (right) computers which were used in the calculations presented in this poster.

Applications of our data

Data we have generated is in use at various fusion institutes.

- ASDEX-Upgrade : Tungsten ionization data is to be used in heavy species studies
- EFDA-JET : Helium excitation data we generated is in use in He beam studies
- RFX : Krypton ionization data we made is in use in impurity transport studies
- DIII-D : Lithium effective ionization and recombination data is being used for impurity transport studies, and C^{3+}, B^{2+} data is being used to calculate the background emission in a proposed charge exchange spectroscopy diagnostic.

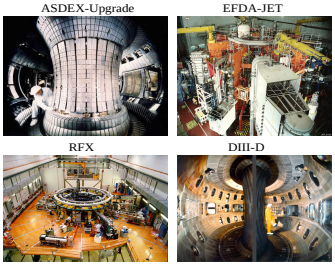

Figure 10. Images of various tokamaks where our data is being used.

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Fig. 2.—

Fig. 3.—

Fig. 4.—

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Fig. 9.—