The history of the ADAS Project

ADAS had its origin at the JET Joint Undertaking in 1984, when a decision was made to underpin the evolving plasma interpretation and its associated plasma modelling, diagnostic measurements and spectral analysis with an in-house comprehensive theoretical atomic physics capability. It was also recognized that the usual practice of embedding atomic physics development and atomic data in a theoretical plasma physics division was unsound. The relatively crude modelled quantities such as total radiative power generated in typical plasma transport modelling are not adequate for validation of atomic physics data. It is analytic spectroscopy which provides the critical testing and validation and primary need for high grade atomic physics. The JET decision to base theoretical atomic physics in the experimental spectroscopy division and to centralise atomic data for modelling and analysis there was far sighted. Atomic data was exported to the theoretical plasma division from the experimental spectroscopy.

First placement of theoretical atomic physics personnel at JET was in 1984 and the centralised atomic data handling and coding in Experimental Division II commenced in 1985. Programming assistance was provided from 1987 to consolidate codes and data in a robust maintained system to professional standards and the first integrated release of interactive ADAS was in 1989. This was on the (then) large on-site IBM mainframe under the MVS/ISPF environment. JET was a European venture and recognized its responsibilities to its EURATOM partners. European scientists from JET returning to their home laboratories sought to have the same ADAS facilities there. Also scientists in the UK and Germany preparing for the new SOHO satellite inquired if ADAS could be provided as ground segment support software. Rutherford Appleton Laboratory funded a preparatory study in 1993 to assess feasibility of conversion of ADAS to UNIX from MVS/ISPF. The conversion programme called the ADAS Project was set up as a self-funded activity by five laboratories and JET, managed by Strathclyde University and overseen by a steering committee. The conversion was completed in 1995. The first ADAS workshop was held in 1995 and the Project was perpetuated as an on-going ADAS maintenance and development project. Membership has grown strongly with now both full voting large laboratory members and non-voting smaller university members. At the end of 2009 there are around twenty-five active Project members from all over the world and include most of the main fusion laboratories (see table).

Targets of ADAS

In the modern fusion plasma device, a number of different regions are recognized, especially the bulk or core plasma, the edge and divertor plasma and finally the beam penetrated plasma. The high temperature core plasma was the original target of atomic modelling for fusion. Impurity species, especially heavier species which are not fully ionised in the core plasma, are efficient radiators and may prevent achievement of the fusion break-even or ignition criteria. Also they affect the plasma resistivity and hence the distribution of toroidal current flow in tokamak devices. Transport modifies the radial distribution of the ionisation stages of impurity species. Spectral observations are used to infer these transport parameters an important issue in modern high performance scenarios such as H-mode and ITBs (internal transport barriers). The divertor plasma is markedly different. The plasma is in contact or close to material strike zones which are in turn the principal source of impurities. The divertor must accept the enormous power flow down the scrape-off-layer from the bulk plasma, seek to minimise the release of impurities from the strike zones and retain released impurities in the divertor. The plasma is dynamic and cool. Choice of materials is critical and active control of divertor radiating

Site	Country	Contact Person
Armagh Observatory	UK	Gerry Doyle
Birla Institute of Technology	India	Ram Prakash
Centre de Recherches en Physique des Plasmas	Switzerland	Basil Duval
Commissariat à l'énergie atomique Caderache	France	Rémy Guirlet
Consorzio RFX	Italy	Marco Valisa
FOM — Instituut voor Plasmafysica Rijnhuizen	Netherlands	Gerard van Rooij
Forschungszentrum Jülich	Germany	Phillipe Mertens
General Atomics	USA	Todd Evans
INAF — Osservatorio Astrofisico di Catania	Italy	Alessandro Lanzafame
Institute for Plasma Research	India	Parameswaran Vasu
ITER	-	Richard Pitts
Japan Atomic Energy Agency	Japan	Tomohide Nakano
JET	EU	Martin O'Mullane
Kungliga Tekniska Högskolan	Sweden	Elisabeth Rachlew
Max-Planck-Institut für Plasmaphysik	Germany	Thomas Pütterich
National Fusion Research Institute	Korea	Mi-Young Song
National Institute for Fusion Science	Japan	Takako Kato
Nat. Inst. for Laser, Plasma & Radiation Physics	Romania	Viorica Stancalie
Oak Ridge National Laboratory	USA	Dave Schultz
Princeton Plasma Physics Laboratory	USA	Doug McCune
RRC Kurchatov (ITER Domestic Agency)	Russian Federation	Sergei Tugarinov
Southwestern Institute of Physics	China	Xuru Duan
STFC Rutherford Appleton Laboratory	UK	Andrzej Fludra
CCFE	UK	Martin O'Mullane
University of Auburn	USA	Mitch Pindzola
University of Strathclyde	UK	Hugh Summers
University of Toronto	Canada	Peter Stangeby
University of Wisconsin	USA	Daniel Den Hartog

conditions, by gas injection, is practised. Neutral beams of hydrogen and sometimes helium isotopes provide a main heating procedure for the plasma. The high energy neutrals penetrate the confining magnetic field, ionise through collisions in the core plasma and then thermalise. The beam/plasma zone leads to charge exchange emission and beam emission, both driven primarily by ion collisions. The resulting spectra observations, so called CXS and BES, are key diagnostic indicators. All these scenarios require substantial atomic modelling and data and are addressed in detail by ADAS.

The ADAS Project has an equivalent involvement in the observation and analysis of astrophysical plasma emission. This is closely linked to spacecraft observatories, especially SOHO, CHANDRA and XMM. Targets of current interest are spectral emission from the solar atmosphere, X-ray emission from cometary and planetary atmospheres and finally VUV, XUV and X-ray line emission from gas clouds and other hot cosmic sources. The ADAS Project has benefited strongly from the mutual interest and shared activity of its members between fusion and astrophysics. Many of the techniques and types of derived data need are similar. However the lack of independent, non-spectroscopic, electron temperature and density diagnostic measurements in astrophysics does require some special methods, such as DEM (differential emission measure analysis), and associated data such as GTEs (contribution functions) which are not used in fusion. The solar astrophysics members have been critical in specifying and orienting the spectral fitting tools of ADAS. Also recent astrophysical observations has stimulated the development of ADAS along new pathways. Some of these are briefly summarised in the following paragraphs.

A number of connections between the fusion and astrophysical plasma scenes are of note and connected with the new and more subtle developments of ADAS. The light element ions such as the carbon ions, seen radiating in the quiet sun spectrum, are similar radiators in the divertors of fusion plasmas, albeit at higher electron densities and with strong influence of wall and recycling sources. Moving away from the divertor strike zones towards the confined plasma, we progress through higher ionisation stages up to the bare nuclei. Moving upward in the solar atmosphere, we see the same progression with the bare nuclei of carbon, nitrogen, oxygen, along with protons and electrons, escaping in the solar wind and within which they are spectroscopically invisible. However, the solar wind does impinge on planetary atmospheres and on ebullient cometary atmospheres. CHANDRA soft x-ray spectral observations of comets show emission from such species (particular K-shell lines). The emission though is complex, with a bremsstrahlung contribution along with spectrum lines which appears to be non-thermal. The proposed mechanism is that the streaming solar wind plasma, encountering the weakly ionised comet atmosphere, provokes a modified two-stream instability which in turn energises the electron distribution. Such a phenomenon is probably quite widely occurring in astrophysics (planetary atmospheres, supernovae remnants etc.) but in different energy regimes. Non-thermal electron distributions but with depleted high energy tails (Druyvesteyn distributions) occur in low pressure discharges and non-thermal distributions with both enhanced and reduced high energy Maxwellian tails are certainly expected in various parts of the fusion plasma. The extension of ADAS to non-Maxwellians is a current focus.

In high temperature plasmas such as flares and core fusion plasma as well as in cosmic sources, we note that species such as argon, calcium, iron and nickel show well-known and distinctive features in the soft x-ray — the so-called 'satellite line' spectra. Analysis considers the set of lines collectively and their differential dependence on electron temperature, electron density, transient ionisation state, ion temperature and impulsive flow velocity. This is the prototype for 'special features' which we return to later in the course.

The advance towards a working fusion reactor and the appraisal of plasma facing materials for it means that the avoidance of heavy species in the past, because of their deleterious radiating efficiency in the plasma core has had to be re-appraised. Experiments with thermally resistant materials such as tungsten do indicate encouragingly low penetration into the core plasma. Heavy species in the first and second long periods will not be fully ionised even in ITER core plasmas and so are suitable as markers, detectable spectroscopically. The survey spectrum of a heavy species such as hafnium, ablated into a fusion plasma, in the VUV and XUV is a complex envelope of transition arrays in which the individual lines are largely unresolved. Atomic data and modelling for such species are certainly now necessary, yet the complexity does mean that somewhat different approaches from that used for light elements are required. These matters are currently being addressed by the ADAS Project.

Objectives of integrated modelling

ADAS seeks to provide integrating modelling. This is based on a number of strategic objectives which have become points of principle. These are to separate local atomic tasks from non-local issues, to provide derived atomic data close-linked to experimental spectroscopic data reduction, to provide consistent source function inputs to theoretical plasma modelling and to provide central management of atomic data. In the remainder of the course, it will be shown how ADAS seeks to satisfy these principles.

General principles

The broad mechanism for radiation emission from a hot tenuous plasma is simple. Thermal kinetic energy of electrons in the plasma is transferred by collisions to the internal energy of impurity ions. This energy is then radiated as spectrum line photons which escape from the plasma volume. Similarly ions increase or decrease their charge state by collisions with electrons. In this case the escaping photon may be a continuum one. The picture is often loosely referred to as the ‘coronal model’. A detailed quantitative description is complicated because of the need to evaluate individually the many controlling collisional and radiative processes, a task which is compounded by the variety of atoms and ions which participate. The coronal model has been the basis for the description of impurities in fusion plasmas for many years. However in fusion, the progress towards ignition and to higher density plasmas, the use of neutral heating and diagnostic beams and the importance of divertors for impurity control requires a description beyond the coronal approximation. ADAS is centred on generalised collisional-radiative theory. The theory recognises relaxation time-scales of atomic processes and how these relate to plasma relaxation times, metastable states, secondary collisions etc. Attention to these aspects - rigorously specified in generalised collisional-radiative theory - allow an atomic description suitable for modelling the newer areas above (McWhirter & Summers, 1984).

Concerning time constants, the lifetimes of the various states of atoms, ions and electrons in a plasma to radiative or collisional processes vary enormously. Of particular concern for spectroscopic studies are those of translational states of free electrons, atoms and ions and internal excited states (including states of ionisation) of atoms and ions. These lifetimes determine the relaxation times of the various populations, the rank order of which, together with their values relative to observation times and plasma development times determines the modelling approach. The key lifetimes divide into two groups, namely, the intrinsic atomic group comprising metastable radiative decay, τ_m, ordinary excited state radiative decay τ_o and auto-ionising state decay τ_a, and the extrinsic collisional group comprising free electron thermalisation τ_{ee}, positive ion thermalisation τ_{ii}, ion-electron equilibration τ_{ie} and ionisation τ_{ion}. Evidently, the first group are purely atomic parameters while the latter depend on plasma conditions. The intrinsic group are ordered as

$$\tau_a \ll \tau_o \ll \tau_m \tag{1}$$

Typical values for them, in seconds, are given by

$$\tau_m \sim 10/z^8 \qquad \tau_o \sim 10^{-8}/z^4. \tag{2}$$

The extrinsic group are ordered as

$$\tau_{ion} \gg \tau_{ie} \gg \tau_{ee} \tag{3}$$

in general. The intrinsic and extrinsic groups are to be compared with each other and with times for plasma ion diffusion across temperature or density scale lengths, τ_{diff}, the relaxation times of transient plasma phenomena under study, τ_{phen} and instrumental observation sampling times τ_{obs}. For fusion plasmas, usually

$$\tau_{diff} \sim \tau_{ion} \sim \tau_m \gg \tau_o \gg \tau_{ee}. \tag{4}$$

From these time-scales, it may be assumed in most circumstances that the free electrons have a Maxwellian distribution and that the dominant populations of impurities in the plasma are those of the ground and metastable states of the various ions. The dominant populations evolve on time-scales of the order of plasma diffusion time-scales and so should be modelled dynamically, that is in the particle number continuity equations, along with the momentum and energy equations of plasma transport theory. The excited populations of impurities on the other hand may be assumed relaxed with respect to the instantaneous dominant populations, that is they are in a quasi-equilibrium. The quasi-equilibrium is determined by local conditions of electron temperature and electron density. So, the atomic modelling may be partially de-coupled from the impurity transport problem into local calculations which provide quasi-equilibrium excited ion populations and emissivities and then effective source coefficients (collisional-radiative coefficients) for dominant populations which must be entered into the transport equations. The solution of the transport equations establishes the spatial and temporal behaviour of the dominant populations which may then be re-associated with the local emissivity calculations, for matching to and analysis of observations.

To make effective use of an atomic modelling system of the above kind, it is helpful to consider the relationship of calculated spectral features to observed features. The starting point is the emission associated with a particular impurity excited level. It is is called a *feature primitive*. It is the set of transition energies and transition probabilities originating from the level. These purely atomic quantities determine positions and relative emissivities of spectrum lines driven by the level population. The level and its population may be a bundled one. All the component lines associated with the bundle constitute the feature primitive in this case, statistical weights alone determining their relative emissivities. No knowledge of the excited state population structure is required to prepare feature primitives. A local quasi-equilibrium population calculation establishes the dependence of the populations of excited levels on each metastable state. In turn this allows combination of feature primitives to form a *feature*. A feature is the set of line positions and local emissivities associated with a metastable and is determined by a local population calculation. A *superfeature* is a set of line of sight integrals of spectral emission. It is obtained by combining features with the line of sight distribution of metastable populations derived from an impurity transport calculation. A superfeature includes line broadening and distortions due to the dynamics of the plasma along the line of sight. It is at the superfeature level that the confrontation of experiment and theory takes place. ADAS may be viewed as providing the tools for

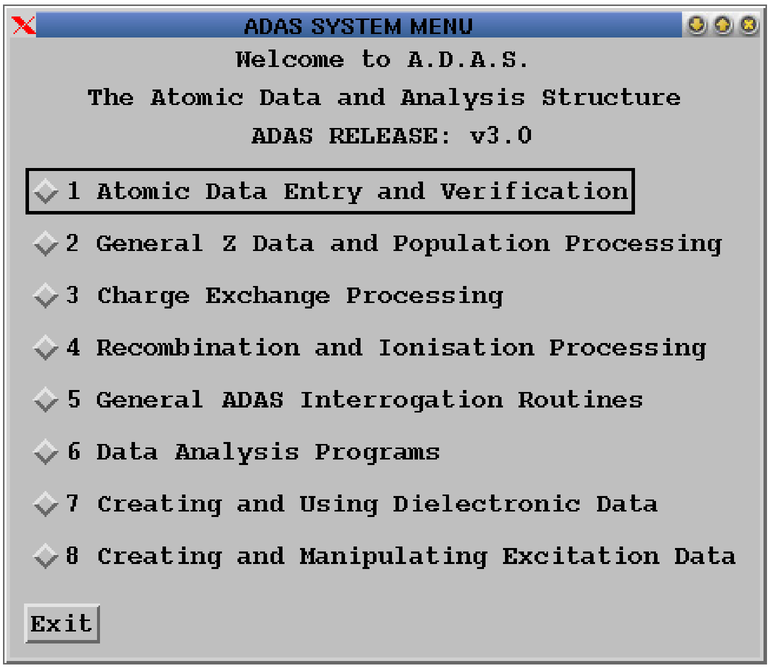
feature primitive → *feature* → *superfeature* spectral synthesis. Practical implementation and exploitation of these ideas follow in the remainder of the lecture course.

General organisation of ADAS

The Atomic Data and Analysis Structure (ADAS) is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas and for assisting in the analysis and interpretation of spectral measurements. The four components of the package are an interactive system, a library of key subroutines, codes and scripts for large scale off-line calculation and a very large database of fundamental and derived atomic data. The interactive part provides immediate display of important fundamental and derived quantities used in analysis together with a substantial capability for preparation of derived data. It also allows exploration of parameter dependencies and diagnostic prediction of atomic population and plasma models. The second part is non-interactive but provides a set of subroutines which can be accessed from the user's own codes to draw in necessary data from the derived ADAS database. The large scale off-line part of ADAS is a new and growing development. ADAS interactive codes are used to define and prepare drivers for the off-line calculations. The latter are normally implemented on and are tuned for massively parallel systems. The database spans most types of data required for fusion and astrophysical application

Interactive ADAS

The various ADAS routines are essentially of three types, namely those which execute atomic modelling calculations, those which are interrogative on the ADAS database (both fundamental and derived parts) and those which produce driver data sets for other large scale codes. The first group may relay substantial quantities of data for further processing or for addition to the derived database.



In the interrogative codes, the principle objective has been to allow graphical display of any part of the database. All codes satisfy this quick look and check facility. In ADAS interrogation codes, cubic spline interpolation is performed on the source data from the database. These interpolated values are given as convenient printer tabulations. Atomic modelling codes generally create output data sets as well as normal tabular output. These files are structured according to the requirement of the ADAS data base or for further ADAS programs. It is anticipated that the user will edit these files into standard ADAS named files when establishing a personal database after being satisfied of their correctness.