ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Nigel Badnell, Martin O'Mullane, Francisco Guzmán, Luis Menchero and Alessandra Giunta

ADAS-EU setup report 3

8 February 2012

Workpackages : 22-1-3, 22-2-3, 23-1-3, 23-2-3, 24-1, 25-1-3, 25-2-3, 26-3-3, S1, S5, S7
Category : DRAFT

ADAS-EU setup report 3

Hugh Summers, Nigel Badnell, Martin O'Mullane, Francisco Guzmán, Luis Menchero and Alessandra Giunta

Department of Physics, University of Strathclyde, Glasgow, UK

Abstract: *The report reviews setup task completion for project months 19-36*

Contents

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Chapter 1

Overview

The milestone STP3 has been respecified to include the decision to appoint a third postdoctoral research associate (PDRA3) and modified handling of the cross-support of PDRAs on external placment. The present report and milestone span the period from months 18 through to month 36. The main events and activities are given in the following paragraphs, with details in the later work package sections.

In the light of the residue of seven months of total ADAS-EU PDRA time (due to the unavoidable delay in completing the appointments of PDRA1 and PDRA2), a third appointment, PDR3, was made with divided time between ADAS-EU and ADAS. Appointment process details are in section 1.1 below. The scheduled initiation training of PDRA2 and appropriate training of PDRA3 were completed as planned (see section 1.2 below). Annual recall and review of PDRA1 and PDRA2 in 2010 and 2011 took place as scheduled, as did the planned relocation of PDRA1 to CEA Cadarache in Jan 2011(see section 1.3 below). Annual visits of senior ADAS-EU staff visits to PDRA staff on-site did not, in all cases, take place to the extent and duration intended. It was a consequence of the departure of Dr. Whiteford and the extensive demands on the time of Dr. O'Mullane at ITER. The gap in on-site PDRA support was felt and was an anxiety. A mechanism of monthly ADAS-EU group video-conferences was put in place which has helped this situation (see section 1.4 below).

The expected placement of the final sub-contracts S1 and S7 in this period have not yet taken place and the intentions for these residual sub-contracts have changed (see section 1.5 below).

In summary STP3 has been almost fully met and the part of milestone STP3 within this eighteen month timeframe.

1.1 Work package 25-1-3

The unassigned ADAS-EU postdoctoral support staff time, following the appointments of PDRA1 and PDRA2 and including the short period appointment of Dr. Adam Foster in 2009, was 7 months. In early 2011, in the light of this and funds available from the ADAS Project, it was decided to seek to appoint a third postdoctoral research associate, PDRA3. The appointment would be for two years, based at CCFE Culham Laboratory/EFDA-JET and STFC Rutherford Appleton Laboratory UK, commencing 1 Aug 2011, shared between ADAS-EU and ADAS in the ratio 37.5% to 62.5% - the ADAS-EU part then amounting to 7 months FTE.

The position description was completed and issued for advertisement on 25 May 2011. The advertisement was placed with Physics World (web - online) in addition to the circulation lists and mechanisms used on the previous occasions. The post descriptor is attached in Appendix A [1] along with the advertisement in Appendix A [2]. The detailed scheduling of shortlisting and interviews is given in Appendix A [3]. Candidates were short listed by Professor Hugh Summers and Dr. Martin O'Mullane. There were nine applicants for the position. Four candidates were short listed and references taken up.

The interview board comprised Professor Hugh Summers (Chair) ADAS-EU Director, Physics, University of Strathclyde; Dr. William Morris, Head of Experiments, UKAEA Culham Laboratory, Professor Nigel Badnell, Physics,

Strathclyde and Dr. Martin O'Mullane, Physics, University of Strathclyde. Dr. Morris is a member of the ADAS-EU Governance Committee. Interviews took place on 7 Jul 2011 at CCFE Culham Laboratory/EFDA-JET. It was possible to interview two candidates in person. Two candidates, located in mainland Europe, were interviewed by video-link. The candidature was very strong. Two candidates were deemed appointable.

Position PDRA3 (CCFE Culham Laboratory/EFDA-JET and STFC Rutherford Appleton Laboratory, UK) was offered to Dr.Alessandra Giunta and was accepted. The agreed starting date was 1 Aug. 2011.

Interview assesment forms, supplementary interview assessment forms and interview decision forms are archived at Human Resources, University of Strathclyde.

1.2 Work package 23-2-3 and 22-1-3

As indicated in SETUP2, the scheduled training of Dr. Menchero (PDRA2) completed with attendance at the UKAEA Culham Laboratory Summer School 12-23 Jul. 2010 and with his attendance, as a participant, at the ADAS-EU course 11-15 Oct. 2010.

Concerning Dr. Giunta, it is notd that she had in a previous year, as a research student, attended the UKAEA Culham Laboratory Summers School in Plasma Physics. Also in a previous year, she attended the ADAS-EU training course. As an experienced worker in the ADAS framework of collisional-radiative modelling of plasmas and as an expert in implementing measurements and analysing spectroscopic data (from spacecraft), no special training was necessary. In-so-far as Dr Giunta is on-site with Professor Summers and Dr. O'Mullane, the ADAS-EU managers, she has daily contact with them on atomic/plasma issues. Dr Giunta, as part of her engagement with the fusion programme at CCFE Culham Laboratory, is examining the spectroscopic issues of the planned SuperX divertor configuration for the MAST spheromac upgrade. Details are in report SCIENCE6 and the periodic reports of the SuperX/ADAS-EU atomic physics working party are available. An ADAS-enabled laptop has been purchased for the use of Dr. Giunta.

1.3 Work package 22-2-3, 23-1-3 and 23-2-3

The work package tasks concern annual update training for the PDRAs at UKAEA Culham Laboratory/JET and an on-site visit at point of placement annually by the ADAS-EU mentor. Follow-up annual recall of Dr. Menchero in 2011 took place from 4-6 Jul. 2011. The report is given in Appendix B [1]. The annual recall of Dr. Guzmán in 2011 took place on 13-14 Jun. 2011 with the report in Appendix B [2], the 2010 recall having taken place in Mar. 2010 (see SETUP2). Detailed specification of local objectives took place with Dr. Guirlet when Dr. Guzmán relocated to CEA Cadarache. The frequent visits of Dr. O'Mullane to CEA Cadarache/ITER has allowed close monitoring and adjustment of priorities. For Dr. Giunta, there has been continuous interaction, monitoring of objectives and task completions and meetings. Professor Summers and Dr. Fishbone at CCFE Culham Laboratory have overseen this. Reports are in Appendix B [3,4,5]. For Dr. Menchero, the on-site suppport has not come up to the same level. We are intending to correct this, but note section 1.4 below.

1.4 Work package 23-2, 24-1 and 24.2

A view espressed by the ADAS-EU staff on external placement is that they would benefit from a greater degree of technical dialogue and interaction with Professors Summers and Badnell and with Dr. O'Mullane. The original ADAS-EU perceived need for this area was intended to be met by periodic visits by the senior staff. The pressure of other visits associated with support to ITER, other places and to sub-contracting institutions, combined with allowable working time has made this unachievable. In a connected context, frequent ADAS-EU travel was planned between ADAS-EU staff at the University of Strathclyde (Dr. Whiteford) and staff at CCFE Culham Laboratory/EFDA-JET (Professor Summers and Dr. O'Mullane) to align the technical/computational developments of ADAS/ADAS-EU. The latter has been replaced by the technical/computation alignment with Professor Badnell at the University of Strathclyde in the framework particularly of the Electron Collision Working Party (ECWP) and the computer hardware infrastructure at

Strathclyde. It was agreed in July 2011, following the annual reviews, to hold video-link meetings between the ADAS-EU staff at approximately monthly intervals to attempt to deal with the above problems. The video-link capabilities at the participant laboratories under EFDA are very good, so this plan would be both very economical in travel costs and in avoidance of waste of staff time while travelling. In practice, the freqency of video-link meetings have been about two-monthly. These have been held on 28 Jul. 2011, 22 Sep. 2011, 18 Nov. 2011 and 12 Jan. 2012. They have focussed in turn on the work of one (or two) members along with other general business and minutes of the meetings have been prepared. Short viewgraph presentations also formed part of these video-link meetings. Summary pages of these documents are given in Appendix C. The consensus view is that they have been helpful in filling the mutual support gap. Although code content, updates and validation are discussed at these meetings, the primary ADAS archive update and validations are done by Dr. O'Mullane with some support from Professor Summers.

1.5 Work package 25-2-3, S1, S5 and S7: Sub-contract technical specification

Sub-contracts S1 and S7 have not yet been placed. Also, sub-contract S5, with University of Groningen has been terminated in a one quarter completed state, with the agreement of both parties, due to a shift of research focus at KVI, Groningen. There are therefore 2.75 sub-contract monies remaining.

Sub-contract S1 was intended to be placed with Queen's University Belfast, for special R-matrix II calculations in which they have unique expertise. The delay in getting the ADAS-EU Electron Collision Working Party into play was the main cause of the delay. Studies by Badnell and Hibbert (see report ECWP1) indicate that an acceptable structure for the tungsten ion W^{+44} can be obtained both under CIV3 and AUTOSTRUCTURE (AS) with interesting insights into the use of semi-relativistic and relativistic orbitals. This clarifies that an R-matrix collisional calculation with 326 levels seems necessary - a supercomputer task. We intend to move forward in parallel with Badnell/O'Mullane using the Breit-Pauli parallel R-matrix I approach on the Juelich machine and Queen's Belfast using Rmatrix II on the HECTOR machine in Edinburgh. A sub-contract will be placed with Queen's University as soon as possible.

Sub-contract S7 was intended for a line-broadening special feature development. The departure of Allan Whiteford and the completion by Christopher Nicholas of his PhD and work for ADAS/ADAS-EU makes this development less appropriate. On the other hand, the completion of sub-contract S2 by University of Mons-Hainaut both provided key data for W^{0}, W^{+1} and W^{+2} and enabled a computer-link path of refined structure data between Mons-Hainaut databases and ADAS databases. We wish to exercise this capability further for a range of neutral and near neutral systems and shall re-assign sub-contract S7 monies to Mons-Hainaut to this end.

The unused S5 residual money is sufficient for an extension step to the completed ITPA University of Vilnius sub-contract S3. The opportunity for a very fruitful extension lies in the efforts of Bogdanovich at ITPA and Badnell for ADAS-EU to take the very large Yutsis configuration interaction approach to structure into the Born collision cross-section regime. From the ADAS/ADA-EU perspective this yields ADAS adf04 format specific ion files for a range of low charge states of tungsten ions. Subject to confirmation of a usable orthogonal orbital basis from the Bogdanovitch method, we shall place the residual S3 monies in a further sub-contract with ITPA University of Vilnius.

These sub-contracts, if they can be implemented by around the end of February 2012, will deliver results towards the end of 2012 in time for full inclusion in the ADAS-EU final scientific delivery.

1.6 Work package 26-3-3

The work package task comprises the preparation of this report.

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Appendix A

ADAS-EU appointment PDRA3

[1] adas-EU/adas_pdra3_post_specification_details
[2] adas-EU/adas_pdra3_post_advert
[3] adas-EU/adas_pdra3_recruitmemt_schedule

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Ref: JA/R31/2011

University of Strathclyde Glasgow

Principal: Professor Jim McDonald

RESEARCH FELLOW
(Fixed term period until 31 July 2013)
(Salary range £29,099 - £31,798 per annum)

DEPARTMENT OF PHYSICS

1. NATURE OF APPOINTMENT

You will participate in the ADAS Project on atomic data and analysis of astrophysical and fusion plamsas and in its associated Euratom Framework 7 Support Action on atomic physics for magnetic confinement fusion research in Europe, called ADAS-EU. You will bring to bear special expertise in atomic data, atomic models, spectroscopic diagnostic methods and the plasma environment in support of the European and world fusion programme. You will also apply such expertise to electron-excited and photo-excited plasmas in astrophysics.

You will join a team of experts, linked to the ADAS Project, who have for many years engaged in furthering world fusion research and in sustaining forefront atomic physics inputs to it.

This 24 month position will be based at the Culham Centre for Fusion Research and at the Space Science Department of the Rutherford Appleton Laboratory. These are nearby laboratories close to Oxford in the UK. This is an exciting and challenging position for an ambitious and dedicated candidate committed to international collaboration and long-term fusion and astrophysical objectives.

More information about ADAS-EU and ADAS may be found at http://www.adas-fusion.eu/ and at http://www.adas.ac.uk .

2. APPLICATION PROCEDURE

- A letter of application telling us why you have the energy, skills, knowledge and understanding of Higher Education or other 'Not for profit' sectors to make a real and strategic difference in the post described.
- A completed application form to which a full curriculum vitae should be attached. The names and addresses of three referees should be given on the application form. The referees may be contacted by the University without further permission from the candidate unless you indicate to the contrary.

Applications should be lodged with Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow, G1 1XQ by Friday 24 June 2011**.**

Applicants who wish an acknowledgement of their paper application should address and stamp the enclosed postcard. Online applications will be acknowledged electronically.

Informal enquiries regarding the post can be directed to Professor Hugh Summers via email summers@phys.strath.ac.uk

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3. DUTIES OF THE POST

You will play a key role in delivering the primary scientific objectives of ADAS and ADAS-EU, that is, the provision of analysis tools and necessary atomic and molecular data for atomic and molecular spectroscopy and broadband radiation detection at all wavelengths and in all plasma regions and for plasma models. All these aspects to be in the context of world-wide unified/shared methodologies, databases and maintenance. You will also share in exploiting these analysis tools in fusion and astrophysics.

There are five main themes, three relating principally to fundamental atomic physics and two to exploitation: (1) Extension of generalised collisional-radiative models to medium weight species; (2) Modelling of emission from dynamic plasmas; (3) Effective coefficient modelling for photo-ionised plasmas; (4) Prediction and interpretation of transient spectral emission from the planned MAST Super-X divertor upgrade; (5) Differential emission measure and related diagnostic analysis of solar and stellar atmospheres. You will acquire the ability to support all these areas. You will share leadership in the development of themes 1, 2 and 5. You will be concerned with the application of the themes to fusion at the EFDA-JET/CCFE-MAST facilities and to astrophysics at RAL.

4. PERSON SPECIFICATION

The following criteria are considered essential:-

- PhD in physics or theoretical physics in one of the areas - radiating properties of plasmas, plasma modelling, diagnostic spectroscopic analysis of plasmas, calculation of atomic structure and electron-collisions.
- Experience of working and collaborating in a large experimental environment - magnetic or inertial confinement devices, astrophysical spacecraft or similar.
- Experience of the computational and data flow infrastructure of large scale experiments.
- Experience in atomic population structure and ionisation state modeling.
- Ability to organise, plan and use time efficiently.
- Ability to analyse and then think creatively.
- Excellent written and verbal communication skills.
- Strong interpersonal skills, friendly and responsive.
- Willingness to keep learning and adapting.
- Team orientated.
- Willingness to travel.
- Ability to work in an IDL/Fortran computational environment.
- Required to publish scientific papers and present at conferences.

The following criteria are considered desirable:-

- Relating to the full scope of a problem - fundamental to applied, theoretical to experimental.
- Ability to engage with theorists and experimentalists.

5. THE DEPARTMENT OF PHYSICS

The Department of Physics is part of the Faculty of Science.

For further information on the Department, see http://www.phys.strath.ac.uk/.

6. THE UNIVERSITY OF STRATHCLYDE

The University of Strathclyde, in the heart of Glasgow, is a vibrant, international, academic community of 16,000 full-time students from 100 countries, and over 3,000 full-time equivalent staff. With a turnover of £220m, we are the third-largest University in Scotland. While still honouring the 200 year old founding vision of Professor John Anderson to be a "place of useful learning", today's Strathclyde is a modern, outward-looking, research-led University with a distinctive reputation for innovation and enterprise. Known for our high entry standards, the quality of our student learning experience, our impressive record on graduate employability and business spin outs, we have led the UK trend by continuing to increase our undergraduate numbers in Science and Engineering.

Within the past two years we have embarked on an ambitious change programme - the Agenda for Excellence - further enhancing the quality of our Research, Education and Knowledge Exchange. This commitment to excellence is supported by major investment in high calibre staff and an ambitious £350M sustainable estate development programme. Already this strategic focus is bearing fruit http://www.strath.ac.uk/about/strategy/. Last year we achieved consistent improvement in overall institutional rankings in all major league tables of up to 10 places. According to Research Fortnight, Strathclyde is the only University in the UK top 20 grant earners showing increases in awards in 2006/2007 from all 6 research councils. The Financial Times ranked our Business School's MBA 30th best in the world and first anywhere for value for money.

Presently the University is located on two campuses, the John Anderson (Glasgow City Centre) and Jordanhill (Glasgow West). We are also organised into five main budget areas; our four Faculties (Science, Engineering, Business and Humanities and Social Sciences) and Professional Services.

7. THE FACULTY OF SCIENCE

For further information on the Faculty of Science, please visit http://www.strath.ac.uk/science/

8. THE CITY OF GLASGOW

Glasgow is the industrial and commercial capital of Scotland and the various groups that have contributed to its population over the centuries have given it a cosmopolitan feel. It has a lively cultural life as home of the national orchestra, opera and ballet and several theatre companies and it possesses a number of fine art galleries; it is the headquarters of the national press and broadcasting media. Its numerous higher and further education establishments have made it a major educational centre.

The Scottish countryside and its splendid recreation and sporting facilities are easily reached from Glasgow.

9. SALARY, CONDITIONS OF SERVICE AND BENEFITS

The appointment will be made at an appropriate point on Grade 7 Salary Scale (currently £29,099 - £31,798 per annum) (Appendix 1), depending on the qualifications and experience of the successful candidate. The conditions of service applicable to the post are attached (Appendix 2). Please note that although the successful candidate will be subject to University terms and conditions of employment, annual leave entitlement and specific local rules will be determined by Rutherford Appleton Laboratory. This post is available for a fixed-term for a period until 31 July 2013.

We also offer staff a range of other outstanding benefits, including:

- Training and Development opportunities underpinned by a 10 year commitment to the Investors in People Standard.
- Reduced or remitted fees for vocational and non-vocational study.
- Particularly relevant to Research staff is the PG Cert Advanced Academic Studies (Researcher Development) which is offered by the University's Centre for Academic Practice and Learning Enhancement.
- Sports, Recreation and Wellbeing facilities, including Ross Priory, a stunning 17th century house situated in 200 acres of land on the south shore of Loch Lomond, just 40 minutes drive from Glasgow.
- Childcare facilities and voucher scheme.

10. POSITIVE ABOUT DISABLED PEOPLE

The University is accredited as a "Positive about Disabled People" employer and operates a guaranteed interview scheme for disabled candidates who meet all of the essential criteria for the post that they are applying for. On the appropriate section of the application form please indicate if you consider yourself to have a disability **and** wish to be considered under the scheme.

The Equality Act (2010) defines disability as "a physical or mental impairment which has a substantial and long term adverse effect on a person's ability to carry out normal day to day activities".

Please note that if you indicate that you have a disability then you may be asked to provide information on this at interview. The University needs this information to consider the likely impact of your disability on the duties of the position you are applying for and what reasonable adjustments can be made to the position. This allows the University to comply with the Equality Act (2010)

11. REMOVAL AND RESETTLEMENT

Any removal expenses, which are incurred on taking up this appointment, will be reimbursed to a maximum of £200 against receipts.

We value diversity and welcome applications from all sections of the community.

SALARY SCALES FOR RESEARCH STAFF

University of Strathclyde Glasgow

Grade	1 August 2010
Grade 6	£25,101
	£25,854
	£26,629
	£27,428
	£28,251
	£29,099*
	£29,972*
	£30,870*
Grade 7	£29,099
	£29,972
	£30,870
	£31,798
	£32,751
	£33,734
	£34,745
	£35,788
	£36,862*
	£37,990*
	£39,107*
Grade 8	£36,862
	£37,990
	£39,107
	£40,280
	£41,489
	£42,733
	£44,016
	£45,336
	£46,696*
	£48,096*
	£49,539*
Grade 9	£46,696
	£48,096
	£49,539
	£51,025
	£52,556
	£54,133*
	£55,758*

Note: * Contribution Points

February 2011
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Appendix 2

CONDITIONS OF EMPLOYMENT
RESEARCH STAFF

University of Strathclyde Glasgow

1. GENERAL CONDITIONS

Members of staff are subject to the Charter and Statutes and the Ordinances and Regulations of the University, published in the Calendar, and to any amendments or additions thereto approved by the University Court and, in the case of the Charter and Statutes, Privy Council.

The University Court recognises the Strathclyde University and Colleges Union (SUCU) as the sole body with which it will negotiate and consult on all collective issues concerned with the terms and conditions of employment of Research staff. Such terms and conditions may be varied by the University Court after negotiation and consultation with SUCU.

Further information on the terms and conditions specified in this document is contained in the Staff Handbook, which also includes further details of such conditions as provision for sick/injury leave and pay, leave of absence, holidays and holiday pay, individual grievance procedures, review and disciplinary procedures and collective agreements. Should you not receive a copy of the handbook on appointment a reference copy is accessible by visiting Human Resources.

2. CONTINUOUS SERVICE

In the case of new appointments, unless otherwise stated in the letter of appointment, the date of continuous employment for the purposes of statutory employment rights will be taken to be the date of appointment contained therein. In the case of promotions, regradings or transfers, previous service is continuous.

3. ALLOCATION OF POST

The post to which each member of staff is appointed is allocated to the department or other area named in member's letter of appointment and any accompanying papers. Should the University Court deem it necessary, in the furtherance of the objectives of the University specified in its Charter, it shall, having consulted with the parties concerned and having received the advice of the Senate, re-allocate the post and/or the duties pertaining partially or wholly to it to another department or area. Any such re-allocation will be without prejudice to the other conditions of employment of the holder.

If the need arises during the course of employment for members of staff to work outside the U.K. for a period (or periods) of more than one month then such arrangements will be subject to mutual agreement. Members of staff would then be provided with a statement in advance setting out the terms covering such periods of employment.

4. RESPONSIBILITY AND SERVICE

Each member of staff is responsible for the proper performance of allocated duties to the person or persons specified in the member's letter and any accompanying papers. Unless otherwise indicated members of staff are appointed for full time service. Members of staff may not accept outside paid employment, including personal consultancies without the permission of Court, which will not be unreasonably withheld.

5. WORKING TIME

Working time is that required to fulfil the duties of the post. The University Court recognises that research Staff carry out these duties in a variety of ways appropriate to the nature of the research activity, but expects regular contact to take place between the research staff employee and the supervisor/grantholder (where these positions are occupied by different individuals) during normal working hours on week days. There are exceptions to this pattern which may involve contact at other locations or in the evenings, or at weekends, but these arrangements will be made with the agreement of the member of staff concerned.

Duties may, by arrangement with Head of Department, include some teaching associated with the post (up to a maximum of 40 hours per semester) for which no additional payment will be made.

Additional work which does not fall within the scope of that described above may by arrangement attract payment which must be authorised and processed through the payroll.

6. HOLIDAYS

Research staff have an entitlement to accrue days of paid annual holiday at the rate of 2.5 days per calendar month; this equates, for staff employed throughout the leave year, to an annual leave entitlement of thirty one days per year. The University leave year begins on 1st October. Research staff will normally be expected to take holidays accrued within the leave year. In exceptional circumstances, accrued leave days may be carried forward into the next leave year. Holidays accrued must be taken by arrangement with the Head of Department within the contract period. There are eleven days of public holiday to which research staff are also entitled if these days fall within the contract period. In addition to the eleven public days of holiday the University presently closes on four additional days over the Christmas and New Year period. **These four days count against the accrued annual holiday entitlement.**

7. SICK LEAVE

During any period of absence through illness or injury provided the appropriate medical certificates are received the University will pay a member of staff (having taken account of the aggregate of all periods of absence due to illness during the twelve months immediately preceding the first day of the current absence) as follows:

Period of Continuous Employment at commencement of absence from work	**Full Pay**	**Half Pay**
Less than 1 year	1 month	1 month
1 year but less than 2 years	2 months	2 months
2 years but less than 3 years	4 months	4 months
3 years but less than 5 years	5 months	5 months
5 years or more	6 months	6 months

In order to manage the University's sick pay scheme the University requires to maintain sickness absence records on individual members of staff. When making payments after the expiry of statutory sick pay the University will deduct an amount equivalent to any benefit normally payable by the Department of Health and Social Security. For this and other details see staff handbook.

8. SALARY AND SUPERANNUATION

Appointments are made within an appropriate grade of the University's grading structure for Research staff, which is linked to that for academic staff; any nationally awarded enhancements of the grade will be paid. Placing on grade is according to qualifications and experience, and where the post derives from externally provided financial support, to the nature of support. Salaries are payable monthly by means of a credit transfer to a specified bank account.

New members of staff, under age 60, will be admitted to membership of the Universities' Superannuation Scheme on taking up appointment unless they notify the University in advance that they do not wish to be admitted to membership of USS. USS requires a contribution from the member (currently 6.35 per cent of salary), to which a contribution of salary is added by the University as required by USS. New members of staff over age 60 are not admitted automatically as special terms, and a higher contribution rate (7.35 per cent), apply. Such staff should contact the Pensions Section if they wish to join the scheme.

New members of staff may opt out of USS within three months of taking up appointment when they will be treated as if they had never been members. After three months members of Staff who wish to withdraw from USS during their employment will be required to give a minimum of 28 days' notice in writing to the University. Any member of staff who wishes to opt out should contact the Pensions Section in the first instance.

Full details of the Scheme are available for reference purposes at the Pensions Section of Finance Office, John Anderson Campus and from Human Resources, Jordanhill Campus.

9. PLACE OF RESIDENCE

The University does not normally place specific restrictions upon the place of residence of members of staff. They are, however, expected to reside in a location which is compatible with the satisfactory fulfilment of all the duties associated with their appointment and with membership of the academic community.

10. PERIOD OF EMPLOYMENT

Members of staff are employed on the conditions indicated in individual letters of appointment and any accompanying papers. The University is not obliged to give notice of termination or continue any employment beyond the end of that period. Where the period of the contract of employment is for one year or less it may be terminated short of the fixed term period by 1 month's notice on either side. Where the period of the contract of employment is for more than one year, or where there have been a further contract or series of contracts immediately consecutive, the employment may be terminated short of the fixed term period by 3 months' notice on either side.

If the appointment is for a fixed term it will expire at the end of the period without the necessity for notice.

Revised November 2006

Appendix 3

University of Strathclyde Glasgow

Service Commitment to
Applicants for Employment

Our commitment to you as the applicant is:

- Your application will be acknowledged *unless stated otherwise in the advertisement* within five working days of receipt. To enable us to meet this, acknowledgement postcards, where enclosed with further particulars, should be completed and returned with your application. Unless otherwise stated in the advertisement, you will also be informed of the outcome of your application as soon as possible.

- If called for interview you will be advised promptly and clearly of the interview arrangements. Your interview will be conducted in a businesslike and friendly manner and will comply with recognised good employment practice. To assist us in meeting our standards we ask that you promptly confirm your attendance (or otherwise) at interview and advise us of any change in your address or Curriculum Vitae.

- You will also be advised of any major delays in the appointment procedure. We will only approach referees nominated by you.

- You will be informed of the outcome of interview as soon as possible. If you are being offered a post you will be written to within 2 working days of the decision being taken. The offer will normally include a duplicate copy which you are required to sign and return to conclude the contract. **Payment of an appropriate salary is dependent on this.**

- We are committed to achieving the standards we have set and to receiving and acting upon constructive feedback from our clients.

- If you are not satisfied with the service you have received, please raise the matter in the first instance with the person with whom you have been dealing. This person will either deal with the complaint to your satisfaction or else advise you how to proceed next. If you feel that dealing with the matter in this way is inappropriate, then write to me at Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow G1 1XQ, and I will respond.

Sandra Heidinger
Director

Human Resources
University of Strathclyde
John Anderson Campus
McCance Building
Glasgow G1 1XQ

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University of Strathclyde

Research Fellow
Department of Physics

(Fixed term to 31 July 2013)
£29,099- £31,798 per annum

You will participate in the ADAS Project on atomic data and analysis of astrophysical and fusion plamsas and in its associated Euratom Framework 7 Support Action on atomic physics for magnetic confinement fusion research in Europe, called ADAS-EU. You will bring to bear special expertise in atomic data, atomic models, spectroscopic diagnostic methods and the plasma environment. You will also apply such expertise to electron-excited and photo-excited plasmas in fusion and astrophysics.

You will join a team of experts, linked to the ADAS Project, who have for many years engaged in furthering world fusion research and in sustaining forefront atomic physics inputs to it.

This is an exciting and challenging position for an ambitious and dedicated candidate committed to international collaboration and long-term fusion and astrophysical objectives.

You will be based at the Culham Centre for Fusion Research and at the Space Science Department of the Rutherford Appleton Laboratory, UK. The scientific focus will be on modelling atomic population structure and ionisation state of dynamic plasmas and photo-ionised plasmas and application of these models to transient emission observed from EFDA-JET/CCFE-MAST facilities in fusion and to diagnostic analysis of solar and stellar data from space borne instrumentation.

More information about ADAS-EU and ADAS may be found at http://www.adas-fusion.eu/ and at http://www.adas.ac.uk.

For an application pack visit **http://vacancies.strath.ac.uk** or contact Human Resources, University of Strathclyde, Glasgow G1 1XQ. Tel. 0141 553 4133, quoting ref: JA/R31/2011

Applications closing date: 24 June 2011.

We value diversity and welcome applications from all sections of the community.

Recruitment Schedule

For completion by recruiting department:

ATA reference number	**ATA Number: 2783**
Lead departmental contact	*Prof Hugh Summers*
Methods of advertising	*Strathclyde website, Jobcentre Plus and www.jobs.ac.uk*
Advertising dates	*Advertise on 27.05.11 for 4 weeks to ensure that requirements are met in the event of appointing a non EU national*
Hours:	*37.5 working week. Holidays follow the practice of placement laboratories*
Closing date	*24 June 2011*
Preferred shortlisting date(s), times and location	*30 June 2011 CCFE Culham Laboratory*
Shortlisting panel members	*Prof Hugh Summers* *Dr. Martin O'Mullane*
Preferred interview date(s) and times	*7 July 2011*
Interview location	*CCFE Culham Laboratory, Abingdon, Oxon., UK*
Additional selection tools	*None*
Interview panel members	*Dr William Morris (CCFE Culham Laboratory)* *Prof Hugh Summers* *Prof Nigel Badnell* *Dr Martin O'Mullane*
Additional interview requirements	*Non-UK shortlisted applicants will be interviewed by videolink*

Please note that our normal practice is to schedule the interview date and shortlisting date before an advert is published. The interview date will be published in the FPs.

For completion by HR:

Date schedule agreed by HR and recruiting dept	
Main HR contacts for this post	
Approved by (HR Manager/Adviser)	
Advertising reference number	***JA/xxx/2011***

Appendix B

Annual review reports and on-site planning reports

[1] Annual review 2011 Menchero
[2] Annual review 2011 Guzman

[3] Planning report for CEA Guzmán
[4] Planning report for ITER Guzmán
[5] Planning report for MAST Giunta

ADAS-EU Recall Travel Report

Location: EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK.
Date: 4-6 July 2011.
ADAS-EU staff: Martin O'Mullane, Hugh Summers, Luis Menchero
Purpose: L. Menchero periodic recall, work review and forward planning

Items:

(1) Summary of activities and primary work targets.
(2) Discussion of code development and critical physics issues impacting model.
(3) Planning and scheduling of periodic video-conference and recall meetings for improved coordination and guidance.
(4) ADAS-EU document and science completion responsibilities.

Primary work targets:

(5) Luis indicated that he was settled in at IPP, with Ralph Dux as main contact point, with some interaction with Thomas Puetterich. Kurt Behringer was now a less frequent visitor. Although it is early days for a strong engagement yet with IPP and their experiments, it does appear that Luis is experiencing some degree of isolation. Hugh noted that, unfortunately, Allan, before his departure, was expected to be the frequent visitor at IPP Garching. It is apparent that Luis' background is quite theoretical. The strategy should perhaps be for Luis to work quite intensively on theoretical development and that senior ADAS-EU staff should visit to assist in engagement when possible. Martin noted an intention to visit IPP Garching in the near future.
(6) Since Fran is already quite involved in the state selective charge exchange aspects of ion-atom collision data for ADAS, it was intended that Luis should focus on the beam atom aspects. This is certainly relevant to IPP interests and measurements. Also incomplete work of Hugh Summers and Stuart Henderson on beam atom population modelling and emission is a starting point. IT would be good to push strongly on this.

Critical physics and code development:

(7) Luis gave a presentation of project progress (see /../adas-eu/ presentations/ menchero_project_progress_jul11.pdf). Luis, based on earlier start-up discussions, had worked on the disturbance of the trajectory and so collisions of ion/atom encounters due to the near atom partially screened potentials. Luis considered path deviations arising from this and presented viewgraphs of this.
(8) Hugh was concerned that this was a very detailed specific point, off the main stream of the needs for examination of directional effects in beam atom collisions with plasma ions. The issues there concern the orientation effects of the motional Stark and magnetic fields on the beam atomic structure and the cone of attack for a plasma ion encountering a fast moving beam atom. Luis had begun to extend his work into this area.
(9) Hugh was keen that a composite picture of the electric and magnetic effects on the beam atom should be followed, including the issues of field ionisation and unbounded wave functions and the ambiguity of good quantum numbers, especially *m* in the mixed field case. On field ionisation, Hugh felt that a full solution for the eigenstates would be necessary to cover the Stark field energy range of the neutral beams. Existing studies of field ionisation which gave parametric fits to energy ranges and n-shells appeared, from the examination of Henderson to be inadequate. Hugh drew Luis attention to methods such as the complex domain approach to eigenfunction solution.
(10) Fran in his extension of ADAS into the molecular domain has set up a new code development area called MADAS under CVS on ferro. It was suggested that Luis mike to do something similar, called perhaps BADAS, for the beam development and that Fran could show him how to do the set up.

Periodic video-conference and recall meetings:

(11) It was noted that in the recall meeting for Fran, that he felt a lack of sufficient interaction and guidance from Hugh and Martin. He suggested that more frequent visits by him to JET, perhaps three monthly, would help. Also it would be a good idea to have quite frequent

video-link meetings of the group, perhaps monthly, to keep in touch better. All were enthusiastic for this. It seemed clear that this would help Luis, as he is probably the most isolated of the group. Such a system could bring in Nigel Badnell as well from Scotland. It was also suggested that these video-link meetings could in turn be focussed on one person primarily and that they could, if wished, make a viewgraph presentation. It was agreed to activate such a system. Fran will start it off.

ADAS-EU documentation::

(12) Hugh drew attention to the large integrated documents, called PUBl - PUBL6 in the ADAS-EU document repository under SVN. PUBL4 is assigned to beam population modelling and contains at the moment the write-up of the development done by Stuart and Hugh. Hugh stressed that Luis should take this over and modify it as he thought fit. As it stands, it is incomplete work, probably with errors, which could do with working over by a true collision theorist.

(13) Hugh suggested that, in an effort to maintain steady progress on the beam work and to help to get a better of engagement of Hugh and Martin with it, a brief progress-tracing document (for example publ_4_progress_tracking.tex) might be kept in the PUBL1 file space. This would be like a diary with more broken-down, short term targets, completions etc. could be noted for everyone to see. If these were maintained for all of the PUBL1-PUBL6 documents, it might encourage us to get on with completion in the late stages of the ADAS-EU project. Hugh suggested that these 'diaries of progress' could be 'checked-off' by a PUBL monitor (as distinct from author) and the set of them emailed out automatically periodically to keep us all up the mark.

HPS
7 July 2011

ADAS-EU Recall Travel Report

Location: EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK.
Date: 13-14 June 2011.
ADAS-EU staff: Martin O'Mullane, Hugh Summers, Francisco Guzman (A. Giunta - part)
Purpose: F. Guzman periodic recall, work review and forward planning

Items:

(1) Discussion of progress in the ADAS-EU molecular data and collisional-radiative modelling theme.
(2) Discussion of critical physics issues impacting model and data advance (2nd session).
(3) Planning and scheduling of periodic video-conference and recall meetings for improved coordination and guidance (4th session).
(4) Update on state selective charge exchange data extension for medium/heavy species (3rd session).

ADAS-EU molecular data (1st session):

(5) Fran opening the meeting sessions with a viewgraph presentation updating the principal aspects of his development of the theme. The presentation is appended to this report.
(6) A molecular ADAS development environment, called MADAS, organised in a manner paralleling ADAS itself has been set up by Fran. This is available for exploration of the development by team members. Codes in development at this stage are in Fortran language and are numbered as ADAS901, ADAS902 etc. The development will eventually be incorporated in ADAS as series 9.
(7) Data formats for molecular data have been allocated 'mdf' numbers, again in analogy with 'adf' numbers. It is planned that the 'mdf' formats will exist as such in the ADAS databases.
(8) Molecular data formats in use are:
    a. mdf00: reference data in sub-directories spanning A-values, isotopic vibrational energy level structure and Franck-Condon factors arranged by diatomic system
    b. mdf02: electron and ion impact collisional cross-section data between electronic states.
    c. mdf33 and mdf34 : Maxwell averaged rate coefficients between electronic states, derived from mdf02 for electron collisions and ion collisions respectively.
    d. mdf04: accumulated energy level, A-values and collisional rate coefficients in vibronic resolution.
(9) ADAS902 is the collision cross-section to Maxwell averaged rate coefficient convertor which handles both electron (single Maxwellian) and ion (double Maxwellian) collisions. At the moment, input driver data are assembled in the madas/pass directory for testing. ADAS902 is designed to process a set set of electron collision data from mdf02 to (1-d temperature vector set - T_e) mdf33 and a set of ion collision data from mdf02 to (2-d temperature array set - T_i / T_{mol}) mdf34.
(10) An initial look at the Fortran coding of ADAS902 was made by Martin and Hugh to assess compliance with ADAS layout, particularly of header comments etc. Broadly this is good, but needs to be done in a more complete way for all of series 9 and also for all the new 'mdf' formats for final matching into ADAS. It is proposed to start these detailed adjustments now and record matters in a running document to accompany the planning and meeting evolution of the molecular theme following item (3) - see later comments.
(11) ADAS90,1, the mdf04 display and exploration code, is in progress but was not presented at the meeting.
(12) Fran outlined his proposed timeline for development, which progressed through data expansion and handling using ADAS901 and ADAS902 over the next few months, onto the molecular collisional-radiative model for H_2 towards the end of the year. Hugh expressed anxiety with this schedule, since he felt that the collisional-radiative model was of central importance for the theme delivery and that in his experience, an early model, even with imperfect data, is an important guide in the working up of the fundamental data. See item 16 for the new mutually agreeable plan.

Model and data issues:

(13) Fran felt that more guidance from Hugh and Martin would be helpful in the theme development. Hugh, explained about the gap in supervisory capability because of Allan's departure, Martin's engagement with ITER and his own obligation to the completing PhD students. With the very successful delivery of Chris Nicholas and Alessandra Giunta's theses, Hugh expressed the view that the light/medium weight element GCR theme and the special feature themes of ADAS-EU were now in a stable and secure state for final write-up and he felt confident that better systematic supervisory attention could now be given to the molecular and charge exchange themes.

(14) Hugh was strongly of the opinion that the work-up of the molecular collisional-radiative model should not be delayed. He outlined a first set of steps towards bringing the model into realisation. These included evaluation of H_2 , H_2^+ , H and H^+ ground state on-diagonal relaxation time constants resolved by type of process, Extension to excited electronic states and then to ground vibrational states of H_2 and H_2^+. He felt that plots of these values as contours in temperature/density plane would clarify the primary partitioning of the whole collisional-radiative matrix. The next step would be evaluation of the coupling matrix partitions linking the H_2 and H_2^+ systems to the excited states of H. It was agreed that Fran would try to follow these indicative directions in the next weeks. The details and progress will be recorded in the running document as mentioned in (10) above.

(15) Fran indicated a need to fill in a range of data between excited vibronic states for which primary sources were not available. Gryzinski's approximations along with IPRATE from ADAS had been used for such transitions by Fantz and Wunderlich. Fran considered whether ECIP and or EIQIP from ADAS might be suitable. Hugh outlined the basis of both ECIP and EIQIP. In particular he pointed out the dipole only character of EIQIP and some of its special features for handling the strong coupling regime, its use of hyperbolic orbits for collisions with targets of positive charge and its application to positive ion colliders as well as electrons. Hugh also elaborated on ECIP including its connecting of a classical binary encounter exchange model for close collisions with a semi-classical impact parameter treatment for distant collisions. He also explained the use of threshold and equivalent electron manipulation of ECIP to handle auto-ionisation. Hugh felt this had relevance to pre-dissociation. Martin has been working on tiding EIQIP and it seems therefore appropriate to include EIQIP and ECIP exploration in the molecular theme.

Improved Coordination and support

(16) It was agreed by all that the molecular theme now needs to be pushed fairly quickly to completion, since it has implications for the next visit by Ratko Janev and for a possible ADAS-EU sub-contract for specific high grade electron impact molecular cross-section data. A number of procedures were discussed and it was agreed to implement the following:

   a. An approximately monthly tele-conference between Martin, Hugh, Fran and Luis to examine progress and completions over the month.
   b. A recall of Fran to JET for detailed work and analysis at three month intervals through to the completion of ADAS-EU.
   c. The activation of a running working document recording decisions, intentions and completions of agreed items for execution. This document will include selected results, figures, charts etc. as necessary to allow all to keep up to speed and measure progress.
   d. The primary ADAS-EU molecular theme publication/manual PUBL-6 should be started immediately so that completed items such as molecular data format specifications, code descriptors, exploratory figures and theoretical developments can be assembled in a timely manner.

(17) It was agreed that Fran would circulate dates for the first tele-conference and that Hugh would write-up the meeting minutes and prepare the running document and PUBL-6 structures and first entries.

State selective charge exchange data:

(18) Fran drew attention to the improved CTMC for krpton, Kr^{+36} for which Clara has now produced an ADAS adf01 dataset. Fran commented that the density of energy points was a little low in the key 40-80keV/amu region, but that he had asked Clara to expand in that regime. It was noted that the data extended to very high n-shell.

(19) Martin was keen to complete this to the derived adf12 data and to make comparisons with the universal CX parametric form and data developed by Adam and Hugh. Also the universal form parameters should be re-assessed and updated.

(20) Martin and Fran drew attention to the additional light element state selective CX data in adf01 format from Katherina Igenbergs for N^{+7} and Fran's work on B^{+5} and his update on Be^{+4} Some of these are already validated and included in ADAS. This work needs to be completed, combined with the universal parametric form adjustment and passed through to adf12. The Universal form parameter optimisation code, which updates adf49 needs to be brought into the ADAS series 3 code framework.

(21) Hugh again stressed the importance of the write-up and publications from this work. He suggested that there was the material for an publication, probably in PPCF with Clara, Katherina, Adam, Martin and Fran as authors. He wished to see the material also incorporated coherently in the PUBL_1 as soon as possible. There was general recognition of these necessities.

(22) It seemed appropriate to incorporate these items, their scheduling and progress in the working/running document referred to earlier in (17).

Actions and other issues

(23) Hugh, while recognising the range of interesting queries coming from the different ITER divisions and also our wish to get involved, was concerned that ADAS/ADAS-EU should present a single consistent accurate interface to ITER. It appeared that somewhat similar questions could come to Martin and Fran, without cross-awareness, possibly leading to different replies and even inconsistency with best ADAS practice. . Also, some suggested routes for engagement of Fran with ITER transport were felt by Hugh not to play to ADAS-EU group strengths, and would probably remain very peripheral. These issues can be resolved by working the ADAS-EU line management correctly. All ITER queries and suggestions must be discussed between Fran and Martin, with Hugh also brought in if necessary, so that a properly based management decision to proceed or not can be made.

(24) Fran will check up and notify about the date for the first video-link meeting.

(25) Hugh will set up the working document and prepare an initial list of actions and timescales for their execution, to be agreed or modified in discussion with participants.

HPS
17 June 2011

ADAS-EU Report

Location:	CEA – Cadarache, Saint-Paul-lez-Durance, France.
Date:	January 2011.
ADAS-EU staff:	Francisco Guzmán (FG).
Persons met:	Rémy Guirlet (RG), Yannick Marandet (YM), Olivier Meyer (OM), Rémi Dachicourt (RD).
Motivation:	CEA and ADAS-EU collaborations during stay of F. Guzmán in Cadarache.

A series of meeting were taken during the weeks following the arrival of F. Guzmán to Cadarache where he will be working as an ADAS-EU fellow the next two years (until the end of 2012). The possible topics of collaboration between F. Guzmán and CEA staff were discussed looking at the interest of the lab and the background knowledge and skills of F. Guzmán. The summary of them and conclusions and agreements follows:

1. F. Guzmán gave a talk (attached) including his background, the work already done for ADAS, the work that is under progress, the collaborations with FZJ-IPP and other European labs and a proposal to develop at CEA. RG expressed his concern that it was already too much to do for a single person and that the work should be rationalized. It was agreed to divide the work of FG in three parts corresponding to the ADAS-EU molecular collisional radiative models, the collaboration with CEA and the collaboration with ITER.

2. In the CEA collaboration part it was agreed to have a job that can be done in a short period of time in order to get results fast and publications as soon as possible and other more midterm jobs. The short-term part was agreed to be the proposal of FG of using CHEAP (for which the previous experience of FG with CHEAP is a good added value) with various atomic data to analyze Ar CXRS data in order to obtain different Ar ionic abundances and compare them with the soft X-ray diagnostics. This will allow to compare the different and very discrepant sets of CX data that are actually in ADAS and that come from different CTMC calculations using a different set of initial conditions [1-3].

3. OM is working in the plasma edge spectroscopy. It is possible that a contribution of CX is affecting C passive spectroscopy. This contribution should come from excited donors to be comparable to the electron impact excitation. FG could work in that as the midterm project. It was agreed that first is needed a preliminary study of the relative values of the CX and electron impact rates to see if the CX contribution can be taken in account. To do so plasma parameters such as neutral densities are needed. It is also necessary to get the excited level populations together with the electron density and temperature profiles and impurity temperature profile. Previous experimental work about that has been done in [4].

4. YM collaborates with Detlev Reiter (FZJ-Jülich). YM is interested in having an interface between HYDKIN and EIRENE codes but both FG and Detlev Reiter said that this is out of the topics of ADAS-EU project. YM is also interested in the energy of the dissociation fragments which is wrong in EIRENE. FG does not have in the priorities of his molecular CR model to get this energy as this is a little off-topic of a CR code but could be a derived quantity to test the code and to provide experimental quantities once the code has a working version.

5. Another test arising from the molecular CR model is the contribution to the Dα line of the dissociation fragments when there are ion plus atom.

6. Some support was required from RD who works with transport models of C in plasma edge and uses ADAS to get ionization and recombination data in order to perform a time dependent ionization balance model to use in his model. He would like to learn about which data are good for his purposes and where they come from. A meeting will be arranged with him.

In conclusion there are two main topics to work in the collaboration with CEA, namely i) Ar CXRS experiments to discriminate between the different sets of data from calculations and ii) CX contribution to passive spectroscopy in the plasma edge. The rest of the topics are linked to the successful building of a molecular CR model and a link with EIRENE.

F. Guzmán
26/01/2011

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[1] ADAS database. www.adas.ac.uk.

[2] Whyte et al. Phys. of Plasmas **5**, 3694 (1998).

[3] L. F. Errea et al. J. Phys B **31**, L91-L97 (2006).

[4] W. R. Hess et al. Nucl. Inst. and Meth. in Phys. R. B **98**, 95 (1995).

ADAS-EU Report

Location:	CEA – Cadarache, Saint-Paul-lez-Durance, France.
Date:	25 January 2011.
ADAS-EU staff:	Francisco Guzmán (FG).
Persons met:	CEA: Rémy Guirlet (RG), Yannick Marandet (YM) . ITER: Richard Pitts (RP), Robin Barnsley (RB), Steve Lisgo (SL), Andrei Kukuschkin (AK).
Motivation:	ITER and ADAS-EU collaborations during stay of F. Guzmán in Cadarache.

A meeting was held about possible collaborations between F. Guzmán and ITER in the frame of the ADAS-EU project. That was done looking at the interests of the ITER organization and the background knowledge and skills of F. Guzmán. The summary of discussions, conclusions and agreements follows:

1. F. Guzmán gave a talk (attached) including his background, the work already done for ADAS, the work that is under progress, the collaborations with FZJ-IPP and other European labs and a proposal to develop in CEA. RP expressed his concern that it was already too much to do for a single person and that the task corresponding to the construction of a molecular collisional radiative model is enough to absorb a person for ten years. FG answered that this task is intended as to have a first version of a CR model with basic performance, with the further possibility to let it grow, but it is not intended to have a final and comprehensive version of it in the ADAS-EU time following FG interpretation of it. RP was also informed of the agreement taken to divide the work of FG in three parts corresponding to the ADAS-EU molecular collisional radiative models, the collaboration with CEA and the collaboration with ITER. That was accepted by the ITER persons.

2. Answering questions of SL about details of molecular CR models objectives and data precedency, FG explained that the main objective is to obtain a molecular collisional radiative model that can serve for different molecules and that can provide the tools to do molecular studies in the plasma edge. This model is being made now for H_2 as this is the most extensively studied molecule and whose data are widely accessible. This will serve also as a benchmark as the results can be compared with the ones from other CR models already developed as YACORA model [1]. The data for H_2 come from R. Janev who is partly employed by the ADAS-EU. FG expressed his agreement with RP that he has no time to assure the quality of the data and that this work is made by R. Janev in his part-time collaboration, so the focus of FG is to develop the physics of the CR model and program the corresponding ADAS routines.

3. SL asked about the program timeline for the molecular CR model too. FG explained that, after some delay related with sick leave in november and the moving affairs to Cadarache, it could be possible to have a first version in summer and with a high probability before the end of this year.

4. RP is interested also in molecular CR data, but in this case related with the N_2 molecule as Nitrogen has become a better candidate as a seeding impurity than Ne and Ar (it has better radiative properties in ITER conditions). Once a working version of the molecular ADAS is available a mdf02 file can be made with the N_2 data and the molecular CR quantities will be obtained running the routines.

5. AK said that the CR data coming from STRAHL code for C are different from the ADAS ones. A cross checking is needed to see where are the differences as STRAHL has been used for many ITER design studies. FG said that if the differences come from different sets of data coming from different calculations the only thing to do is to document the calculation method and try to state what is the most “desirable” set. This proposal of checking the origin of the difference between STRAHL and ADAS data was agreed as one of the tasks of the collaboration. RP is also interested in checking if there are differences concerning Nitrogen data so that was added to the task.

6. RB has various possible topics (in spectroscopy) that are suitable for working together. However, RB prefers to wait for the next visit of Martin O'Mullane (in a couple of weeks) to discuss the topics already covered by Martin and the topics that FG can contribute. FG asked RB to send him a list of them so he can select the ones that suit better to his preferences and skills.

In conclusion, atomic physics support is needed by ITER in many topics. FG can contribute some of them. The collaboration will be based in the following main lines:

- Look for the origin of the differences in C data between STRAHL and ADAS and try to state which are the most recommendable data.
- Support of RB in an atomic physic topic to be determined in a next meeting during the visit of M. O'Mullane.
- Use the molecular CR model to support ITER studies of H_2 and N_2 in plasma edge. This a long term task as a working version of these models is necessary.

F. Guzmán
26/01/2011

REFERENCES

[1] D. Wünderlich et al. J. of Quant. Spec. & Rad. Trans. 110, 62 (2009).

ADAS-EU Report

Location:	CCFE Culham Laboratory.
Date:	11 March 2011, 20 May 2011.
ADAS/ADAS-EU staff:	Hugh Summers, Martin O'Mullane
Univ. of Strathclyde:	Stuart Henderson, Alessandra Giunta
Persons met:	Geoff Fishpool, James Harrison
Motivation:	ADAS-EU support of the MAST-Upgrade Spectroscopic Divertor Diagnostics Project

Initiating meetings for a long term collaboration and support by ADAS-EU/ADAS took place on 11 March 2011 and 20 May 2011. It is intended that Alessandra Giunta or another will carry the project for ADAS-EU. Minutes of the two meetings are on the following pages.

Meeting 11th March, 2011

Attendees: Geoff Fishpool (GF), Hugh Summers (HS), Martin O'Mullane (MOM), Alessandra Giunta (AG), James Harrison (JH)

The meeting was intended to follow on from the previous meeting in November, to establish continued interest in the project and to determine how the current proposed divertor diagnostic set can be improved.

- It was agreed that discussion of atomic and molecular processes would benefit from having results of plasma fluid simulations to provide estimates for electron temperature and density within the Super-X divertor (SXD).

- Diagnostic impurity puffing was discussed:
  - Spectroscopic imaging of extrinsic impurities is best performed if the diagnostic can look across the plume, i.e. for a gas jet at the top of the SXD chamber, the sightlines should be as close to horizontal as possible.
  - Imaging helium emission lines may indicate the presence of non-Maxwellian electrons.

- Imaging of BI lines could be used to measure the rate of erosion of boron coatings after boronization.

- The development of a divertor spectroscopy framework for MAST-Upgrade, with significant input from external collaborators, would be strongly encouraged.

- Investigation of how to characterise relaxation phenomena, principally ELMs (notionally 100Hz), was discussed. It was agreed that further work would be required to have a more informed discussion concerning spectroscopic lines of interest, relevant timescales and measurement techniques.

- Gold foil bolometers are the currently preferred option for radiated power measurements, as they can better withstand operating on 320^0C surfaces in the MAST-Upgrade divertor. Currently 32 channels have been budgeted for.

Actions:

- GF to provide data from B2-SOLPS simulations of n_e, T_e and, if possible, neutral atomic and molecular densities.
- JH to continue finalising diagnostic sightlines using numerical models of diagnostic sightlines.
- HS, MOM to look into making measurements of plasmas undergoing periodic relaxation processes.

It was agreed the next meeting will be held on Friday 13th May.

Meeting 20th May, 2011

Attendees: Geoff Fishpool (GF), Hugh Summers (HS), Alessandra Giunta (AG), Stuart Henderson (SH), James Harrison (JH)

The meeting was called to discuss the results of work carried out by AG to estimate the distribution of impurity (He, C, O) charge states, and to discuss how to proceed further, both in terms of this study and possible future collaborations.

AG presented equilibrium ionisation balances of He, C, O, based on the results of a B2-SOLPS simulation of a super-X diverted plasma in a state of detachment, and ADAS data. AG outlined how she will build upon this work by calculating line integrals through the simulation domain. This will allow "mass production" of synthetic line-of-sight integral measurements, to assist in the optimisation of diagnostic placement.

- The consensus was that the results are encouraging and show the development of a basis for future work

During the discussion of AG's calculations for oxygen, the possibility for measuring these lines in MAST was discussed, and in particular recent ideas for looking at impurity evolution from the target tiles. HS suggested that this work might benefit from referring to earlier work carried out by Behringer (J. Nucl. Mater., 145-147 (1987) 145-153).

HS explained how he saw the work developing, based on two of the topics identified in the first meeting

- Diagnosis of a dedicated He puff in the Super-X chamber
- Time evolution of atomic states (and spectra) during plasma-induced transients, particularly during ELMs.

He suggested that this work be developed so that it might form the basis for a joint grant proposal.

- The meeting agreed that this was very much the direction in which it was hoped that the work would proceed.

Possible bottlenecks in data production and analysis were discussed.

- HS, AG agreed that the data from the B2-SOLPS simulation was sufficient for the present study and grid resolution was adequate.
- Provision of data from other, including future, simulations was discussed. It was agreed that care and co-ordination between all interested parties is required in order to prevent duplication of effort.

Actions:

- JH to provide information regarding the MAST-Upgrade structural geometry, to assist in developing diagnostic sightlines.
- AG to build on the work presented, as described above.

A date for the next meeting is to be decided. It was agreed that it would be held in approximately 6 weeks.

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Appendix C

Group videolink meeting reports

C.1 Minutes

[1] Minutes group videoconference 28 Jul. 2011
[2] Minutes group videoconference 22 Sep. 2011
[3] Minutes group videoconference 18 Nov. 2011
[4] Minutes group videoconference 12 Jan. 2012

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ADAS-EU Teleconference Meeting Report

Location: Teleconference ADAS-EU hosted from CEA-Cadarache, France.
Date: 28 July 2011.
ADAS-EU staff: Martin O'Mullane (CEA, France), Hugh Summers(EFDA-JET, UK), Francisco Guzmán (CEA, France), Luis Fernández Menchero (Garching, Germany), A. Giunta (EFDA-JET, UK)
Purpose: F. Guzman periodic work review and forward planning. Other ADAS-EU issues.

Items:

(1) Discussion of progress in the ADAS-EU molecular data and collisional-radiative modeling theme.
(2) Discussion of critical physics issues impacting model and data advance.
(3) Discussion of Charge Exchange advances and planning a paper with universal formula.
(4) Other issues: Introduction of A. Giunta as new ADAS-EU staff, recall of APIP conference (Belfast).

ADAS-EU molecular data:

(5) Francisco Guzmán presented a talk where the last advances in the molecular data and collisional radiative model where shown according to the plannings on the last recall meeting in June.
(6) In the talk time constant for the different process were presented and compared. FG arrived to the conclusion that electron impact excitation are the most contributing processes while CX are the only ones to contribute in ion impact. In dissociation, dissociative excitation and excitation to triplet *b* state are competing and contributing in a similar quantity in the interesting region.
(7) FG has developed a new code called *gettaus.for* that is situated in ADAS901 (that will correspond to interrogative routines) at the moment. This work has been useful to obtain a clear idea of which processes are the most important and representative.
(8) FG has outlined his future work that involves to obtain potential curves for H_2 and H_2^+ and finish programming ADAS903 as well as document formally ADAS902 and contribute to Publication 6 ADAS-EU report. As an approximate date beginning to middle of October is given.

Charge exchange universal formula paper:

(9) A discussion was made on coordination to make a paper on universal formula which will fit the charge exchange data on ADAS and will allow to obtain results for heavy species collisions that have not been yet calculated. This formula will be updated using the new results of Ne and possibly Ar (from K. Igenbergs, TUW) and Kr (from Clara Illescas, UAM). FG thinks that the article could be oriented as a checking of the formula using heavy species and Martin thinks that, as the formula already works well and has been thoroughly checked, main orientation should be in the new fitting of the formula using new results. Hugh thinks that both objectives can be maintained in it. FG and Hugh will create an outline and work in the article while Martin will engage in the work with the new data.

APIP:

(10) Hugh assisted and presented a paper in APIP conference (now under revision). In that conference K. Igenbergs (TUW) that is contributor to ADAS presented new charge exchange data in fully stripped Ar using AOCC new improved method developed in Vienna. This calculations agree with ORNL calculations in capture to low n shells and with UAM group in high n shells. That seems to support the theory that microcanonical distribution in CTMC are adequate to capture to low n while improved hydrogenic initial distributions are more adequate to high n as they model better the tail of the initial quantum distribution in the target. These data could be the necessary data to solve the high discrepancies in Ar charge exchange data (one order of magnitude) between the different CTMC calculation that are currently in ADAS. Martin will visit Vienna on 6 of September and committed to speak with Katharina Igenbergs about it. FG wanted to contact her by email as well.

(11) In APIP conference a poster was presented by Palmieri (Mons University, Belgium) about the new results on neutral W. These results are committed to ADAS data base.

Other issues:

(12) Alessandra Giunta was presented to the ADAS staff as new ADAS-EU fellow after the selection process taken in July.

(13) Luis Fernandez Menchero will held a teleconference about the new software of ADAS305 that deals with the cross sections under motional stark effect in plasmas. This teleconference will be under the frame of coordination and management teleconferences to be held in a monthly basis.

Francisco Guzmán
18 August 2011

ADAS-EU Teleconference Meeting Report

Location: Teleconference ADAS-EU hosted from IPP-Garching, Germany.
Date: September 22nd, 2011.
ADAS-EU staff: Luis Fernández Menchero (Garching, Germany), Martin O'Mullane (CEA, France), Francisco Guzmán (CEA, France), Hugh Summers (EFDA-JET, UK), Alexadra Giunta (EFDA-JET, UK).
Purpose: Exposition of L. Fernández-Menchero periodic work and forward planning. Other ADAS-EU issues.

Items:

(1) Discussion of the software package ADAS305a, atomic part of the Motion Stark Effect (MSE) package ADAS305.
(2) Discussion about the physic models employed to calculate the atomic wave functions of a Hydrogen atom under simultaneous non parallel electric and magnetic fields and the numerical methods used to calculate the quantitative results.
(3) Show the limitation of perturbation theory to obtain good quality results in the case of MSE in the conditions relevant in fusion.
(4) Brief exposition of the objectives of ADAS305b, the dynamical part of ADAS305.
(5) Other issues: the other assistants in the meeting made a brief exposition of their work until the date and plans in a short period.

ADAS305a:

(6) Luis Fernández Menchero (LFM) presented a talk, which explained the steps of the program package ADAS305a, the physical models used and the numerical methods.
(7) LFM showed in the talk preliminary results of energies and wave functions of hydrogen under the MSE. These preliminary results showed that perturbation theory is not applicable to an atom under a constant electric field, so an alternative method should be used to obtain the zero-order functions in the perturbation serie. Complex coordinate integration was proposed as a viable alternative.
(8) LFM gave his idea about the working of the next step ADAS305b and in general of the ADAS305 package.

Other issues:

(9) Francisco Guzmán (FG) is preparing to assist to the meeting of the EPS in Cyprus in October.
(10) Martin O'Mullane (MOM) and Alexandra Giunta (AG) are preparing to assist to the ADAS Workshop 2011 in Auburn (USA).
(11) AG will held the next teleconference meeting in the ADAS-EU group in a date to determine in October. She will show her progress in the expansion of ADAS to data and routines of astrophysical interest.

Luis Fernández Menchero
September 22nd, 2011

ADAS-EU Video-Conference Report

Location: Video-conference between JET-Culham, CEA-Cadarache and IPP-Garching sites.
Date: 18 November 2011.
ADAS-EU staff: Francisco Guzman (CEA), Luis Fernandez(IPP) , Hugh P. Summers (JET), Martin O'Mullane (JET) and Alessandra Giunta (JET)
Purpose: A. Giunta and H. P. Summers current work and forward planning

Items:

(1) Presentation by Alessandra Giunta
(2) Presentation by Hugh Summers
(3) Presentation byFrancisco Guzman

OIV emission in the sun and GCR modelling

(4) Alessandra presented the status of her work on the self-consistency of OIV emission in the lower corona/chromosphere boundary. In contrast with Muglach, using accurate GCR data and her latest observations, there is good consistency with equilibrium ionisation state and emission ratios. The publication has been accepted for publication in Astron. and Astrophys.
(5) Alessandra is extending the generalised-collisional-radiative work of her thesis from silicon up to argon at the moment, with the wish to carry on later through the iron period. The fractionation of ionisation between metastables is her current task. She is developing a code to do the complete job, which was previously done by hand on spreadsheets. The code is nearly complete. Details of these items are in the veiwgraphs presented at the meeting

ADAS: Lifting the baseline data

(6) Hugh gave a presentation of the latest steps in lifting the ADAS baseline for heavy elements to leve;ls 1 and 2. He is doing this from the starting point of AUTOSTRUCTURE (AS) as the underlying structure code. He described the latest details and new variants of the adf04 format to include type 6. Also he described exploiting the new distorted wave capability of AS put in place by Nigel.
(7) The mass production of adf04 data for medium weight elements is handled by PERL scripts for distributed processing on JAC computers. adf27 drivers are created automatically for iso-electronic sequences from templates, currently covering elements up to zinc. This processing is working well and nearing completion.
(8) Hugh described briefly adf04 type 6 and its purpose for BBGP calculation of dielectronic recombination of complex systems. For Nigel and Hugh this, in asosciation with AS is the way forward.

ADAS: Lifting the baseline data

(9) Fran gave an update on the molecular CR modelling. The presentation is attached. Fran raised issues about the size and storage needs for the calculation. Hugh felt that economic methods, perhaps along the lines of the atomic bundle-n and bundle-nl approaches, would help. Hugh and Martin will advise Fran on details.

Other business

(10) Hugh expressed concern that ADAS-EU formal talks on the state and capabilities of ADAS should be kept up-to-date. In particular he was worried that Fran's talk at IPP Garching did not touch the latest work. Also that Martin had recently given a fully up-to-date talk and it was therefore wasteful and inconsistent for each person to do their own thing. He proposed that a single up-to-date ADAS overview talk should be prepared and revised in a timely manner so that each of us could use it and so all 'sing from the same song sheet'.
(11) Hugh drew attention to the up-coming 18 month review of ADAS-EU and the need to get all documentation in place. He exhorted all to make sure their travel reports, timesheets etc were up-to-date. Also he requested that the science in the primary documents PUBL1-6,

ADAS-EU Video-Conference meeting Report

Location: Video-conference between JET-Culham, CEA-Cadarache and IPP-Garching sites.
Date: 12 January 2012.
ADAS-EU staff: Francisco Guzman (CEA), Luis Fernandez(IPP) , Hugh P. Summers (JET), Martin O'Mullane (JET) and Alessandra Giunta (JET)
Other staff: Remy Guirlet (IRFM-CEA) (only the first hour)
Purpose: 2012 planning

Attached: planning_2012.doc, 2011_AR_CX_CROSS_SECTION_guzman1.pdf
Items:

(1) A meeting have been held to clarify issues corresponding to the 2012 year planning as a proposal from FG. A document was elaborated with a number of point to discuss or clarify (attached).
(2) ADAS-EU training course will be held in Padua between 26-30 March. It will be based in CX and lectures and structure is already clear and worked. HPS asked from FG,LF and AG to establish contact with known laboratories to promote and give visibility to the course.
(3) FG expressed the need of a week in close work contact in JET. At this respect Martin will be at ITER between 30 of January – 11 February and he will be able to dedicate some hours to work with FG. After that, is fixed that FG will visit JET the week 13-17 February. HPS wanted it to be specific work issues rather than general discussions. FG answered that what he had necessity is to solve specific issues. LF will do another visit at beginning of March.
(4) HPS stressed the need of having advances in publication report number 6 form FG. FG alleged that he wanted to advance in the finalization of the molecular CR modeling before to stop to write and that writing would suppose a delay in his advances in programming. HPS said that writing the report will improve the interactivity of the work with the others ADAS-EU members and that this would be the basis of the reports needed by Brussels about the work progress.
(5) HPS will take over the paper of universal formula and publication report 3. He is very happy with the work done by the ADAS-EU contractors in the universities of Vienna and Madrid as this completes the ADAS atomic database together with the universal formula. The paper will be written by HPS together with the publication report. HPS foresees a 2 month to finish this work.
(6) It is encouraged the experiment of Ar-CX in ASDEX (the proposal is attached). HPS suggest the participation of Luis Fernandez being in place and Costanza Maggi as the original work where this experiment was foreseen was a collaboration between her and FG.
(7) About the ADAS Workshop 2012 and the ADAS-EU training course 2012, it was agreed that RG (not present at this moment) and FG make an Outline of the agenda to be ready by beginning of March. Advertising must be done at summer.
(8) FG explained that Jaime Suarez (UAM) suggested him to perform calculations on CX data and asked about the necessities. FG wanted him to perform W^{60+} + H as it will be on the core. HPS and MOM said that necessity of this kind of data was not urgent anymore and what was needed data of capture to low levels of light elements (eg. Be) in cool divertor (energies of a few eV). FG and LF said that the specialty of J. Suarez in calculations is intermediate high energy method and that for this kind of calculations the person to contact is Luis Mendez.
(9) FG informed about the paper he has in progress with Madrid UAM group about the recommended ion-impact excitation cross sections which are already in ADAS as a result of his work extracting these cross sections and joining the different methods. These cross sections have not been published and now a paper is being performed departing from the internal report he wrote for ADAS.
(10) HPS asked the ADAS-EU members to participate in the report-writing and wanted to assign to each ADAS-EU member a different scientific report. FG will do the report SCIENCE_4 for 2nd semester 2010, LF will do SCIENCE_5 (1st semester 2011) and AG will do SCIENCE_6 (2nd semester 2011).
(11) No more points where to be discussed. A new meeting will be held in a month time.

F. Guzmán
16 January 2012

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C.2 viewgraphs

[1] Viewgraphs Guzman videoconference 28 Jul. 2011 (first three pages)
[2] Viewgraphs Menchero videoconference 22 Sep. 2011 (first three pages)
[3] Viewgraphs Giunta videoconference 18 Nov. 2011 (first three pages)
[4] Viewgraphs Summers videoconference 18 Nov. 2011 (first three pages)
[5] Viewgraphs Guzman videoconference 18 Nov. 2011 (first three pages)

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ADAS-EU: Progress Report.

Francisco Guzmán

ADAS-EU
University of Strathclyde

July 28, 2011

Outline

1. Codes
   - Up to now
   - Time constants
   - Electron impact
   - ion impact
2. Going forward
3. Other topics

Outline

ADAS305a. The H atom under a simultaneous electric and magnetic fields.

L. Fernández-Menchero

ADAS, University of Strathclyde. United Kingdom.

September 22, 2011

Contents

Contents

Main points

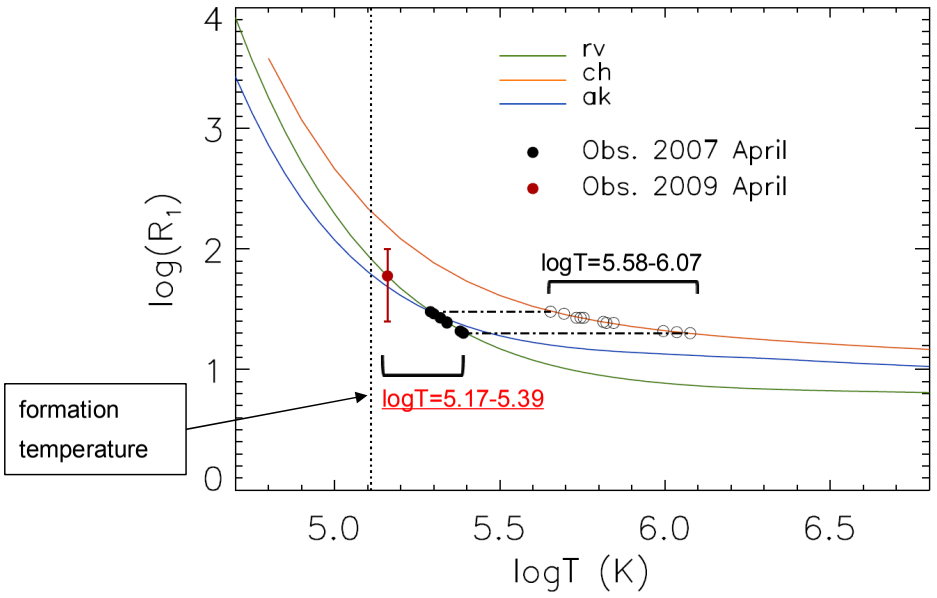
- Work on O IV line ratio as observed in the solar spectrum.

- Extension of Generalised Collisional-Radiative (GCR) model up to Argon and possibly beyond.

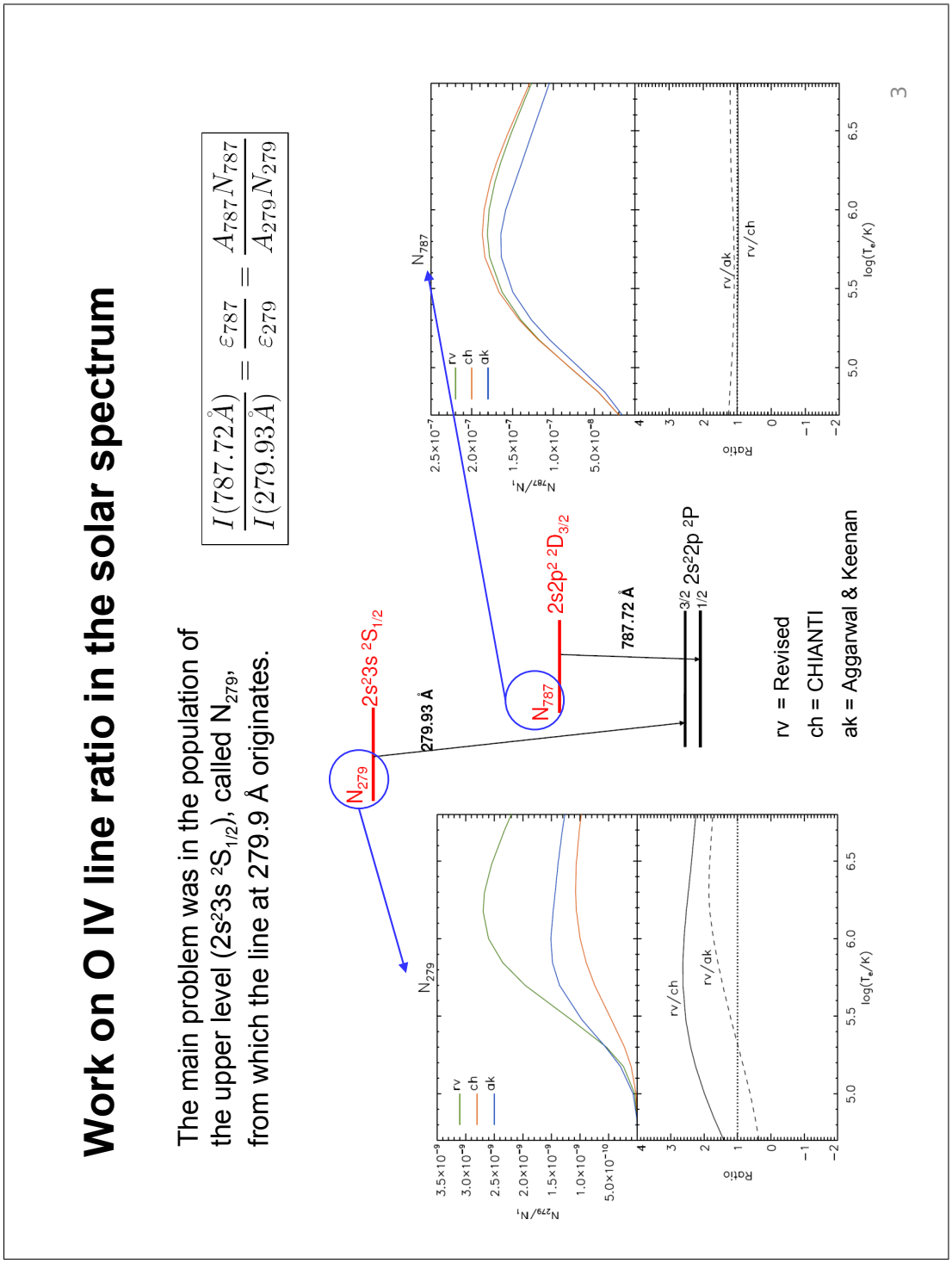
Work on O IV line ratio in the solar spectrum

- The discrepancy of a factor 2-5 between the measured and theoretical R_1=O IV I(787.7 Å)/I(279.9 Å) line ratio, found by Muglach et al. (2010), has been solved.

- The paper on O IV ratios has been submitted.



rv = Revised
ch = CHIANTI
ak = Aggarwal & Keenan


Work on O IV line ratio in the solar spectrum
The main problem was in the population of the upper level (2s²3s ²S1/2), called N279, from which the line at 279.9 Å originates.
$\frac{I(787.72\mathring{A})}{I(279.93\mathring{A})} = \frac{\varepsilon_{787}}{\varepsilon_{279}} = \frac{A_{787}N_{787}}{A_{279}N_{279}}$
N279
2s²3s ²S1/2
279.93 Å
N787
2s2p² ²D3/2
787.72 Å
3/2
1/2
2s²2p ²P
rv = Revised
ch = CHIANTI
ak = Aggarwal & Keenan
N279
N787
rv
ch
ak
rv/ch
rv/ak
Ratio
log(Te/K)
3

ADAS: lifting the baseline data

Hugh Summers

18 Nov. 2011
JET Facility

ADAS data formats

The ADAS data formats associated with the ionisation state and excited population structure of ions in an electron excited plasma are

- *adf04*: resolved specific ion data collections
- *adf11*: iso-nuclear master files
- *adf15*: photon emissivity coefficients

Alessandra here and in her thesis has taken you through how these and related datasets are put together for the highest precision GCR ADAS work and how she is moving GCR on to medium-weight elements.

Baseline data

You are all also familiar with the baseline data in ADAS created originally by Martin exploiting the Cowan atomic structure code and the plane-wave Born approximation

- adf04 data collections such as *copmm#18*
- adf11 data collections such as *acd89*

Adam carried this approach and level of approximation forward to all heavy elements – albeit with the complexity of automation, promotion rules , ca, ls and ic resolution levels and superstages.

ADAS-EU: Progress Report.

Francisco Guzmán

ADAS-EU
University of Strathclyde

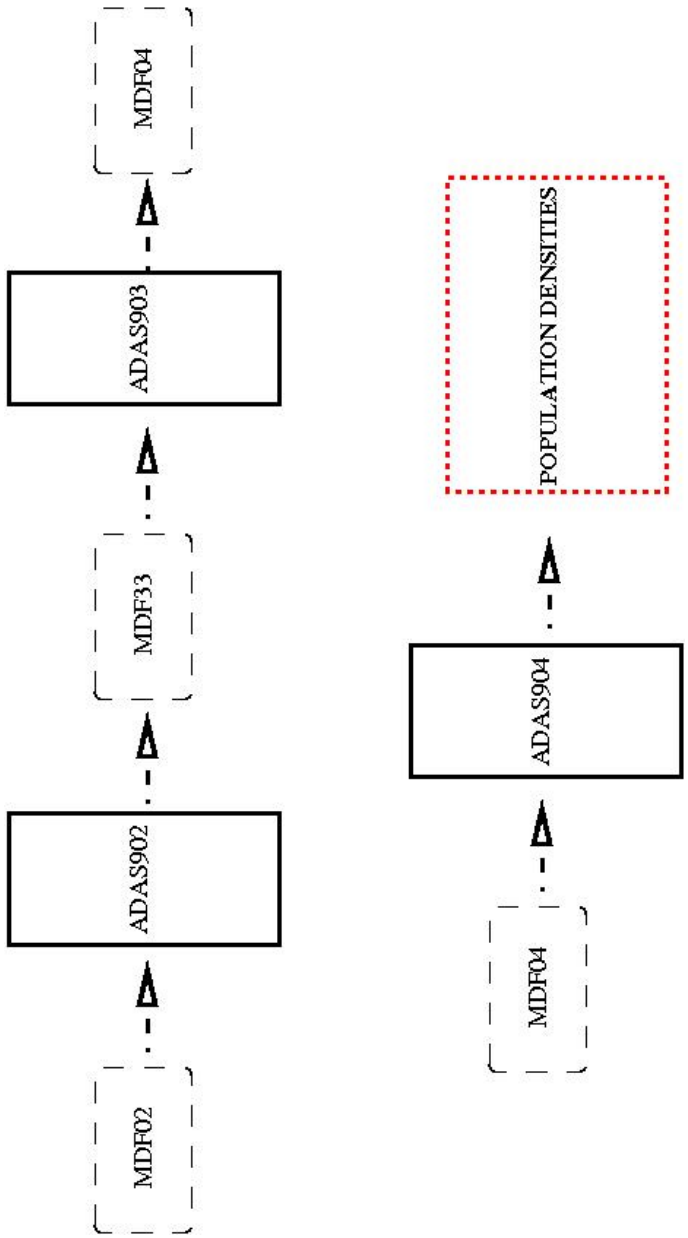
November 18, 2012

Outline

Codes

Up to now

General Scheme



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