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ECWP1: Electron Collision Working Party Report 1

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ECWP1: Electron Collision Working Party
Report 1

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Abstract: *TThe Electron Collision Working Party was an orginal objective of the ADAS-EU project, to be led by Dr. Allan Whiteford. The unexpected departure of Dr. Whiteford from the the Project caused a delay in establishing the working party. In Oct. 2010, Professor Nigel Badnell joined the project and it was possible to restart the Electron Collision Working Party in expert hands. This report summarises activities from Oct. 2010 to Dec 2011.*

Contents

Chapter 1

Introduction

The Electron Collision Working Party (ECWP) is a planned coordination activity under ADAS-EU to ensure effective communication of the evolving needs of electron impact collision data for fusion to colleagues in the atomic physics community. Whereas, original research activity in this area is outside the brief of the ADAS-EU support action, in practice the staff of the ADAS-EU project are drawn from this community and the part-time ADAS-EU staff, Professor Hugh Summers, Professor Nigel Badnell, Dr Martin O'Mullane and Dr. Alessandra Giunta, in their non-ADAS-EU time, do continue to participate in this community and conduct original research in the atomic collision area. The Strathclyde Atomic Physics group, led by Professor Summers and Professor Badnell, has trained many research students, engaged many post-doctoral scientists, and collaboratd with many external groups, of which a substantial number remain engaged in atomic calculations in various parts of the world. Their collective output is one of the largest sources of electron impact collision data in the world. The ECWP, under Profesor Badnell, is therefore uniquely placed to promote and enable key data of this form to flow into the ADAS databases in the interests of international fusion and the European contribution to it.

Particular attention is drawn to the following groups who work in close collaboration and co-ordination with each other and with the ADAS/ADAS-EU Projects: Professor Badnell and his postdoctoral co-worker, Dr. Guyan Liang (now at the National Institute for Astronomy, Beijing, China) who operate and advance the in-house capability at the University of Strathclyde; Professor Pindzola, Professor Loch, Dr Ballance at Auburn University, Alabama, USA who develop key codes and perform large scale production together with Professor Badnell, build new models for ionisation and excitation and extend the precision and scope of collisional radiative calculations, especially for light elements; Professor Griffin (formerly of Rollins College, Winterpark, Florida, USA) who develops and exploits key codes; Professor Gorczyca, University of Western Michigan, USA and co-workers who share in large-scale dielectronic calculations with Professor Badnell.

For many years, the above teams have prepared their data in the precise formats defined by the ADAS Project, so that the data can be used effectively immediately in fusion applications. In particular, they are very large scale suppliers of fundamental data in ADAS formats *adf04* (specific ion files), *adf09* (state selective dielectronic data) and *adf23* (ionisation cross-section data). These data are all made available freely under OPEN-ADAS and elsewhere. Collectively, they have provided many gigabytes of precision data, being probably the largest, freely available, such resource in the world. There is a substantial body of published papers in the literature. Reference is made to some of these in the following chpaters and section.

It was intended that the ECWP should commence its activities in 2009 under the leadership of Dr. Allan Whiteford, then on the ADAS-EU staff, based at the University of Strathclyde. The departure of Dr Whiteford to the private sector in Oct. 2009 created a gap of suitable personnel for this position through to Oct. 2010. At this point, Professor Badnell was freed-up from some of his university teachinga and astrophysical committments and was able to take up leadership of the ECWP. It is noted that, in early planning for ADAS-EU prior to its commencement in Jan. 2009, it was hoped Professor Badnell wouild lead the ECWP. So it was fortunate for ADAS-EU finally to obtain Professor Badnell's services. As a consequence of these events, the present report is the first by the ECWP.

Chapter 2

Review of progress 2011

2.1 Dielectronic recombination data

Badnell has over many years coordinated the production of stste selective dielectronic recombination data for plasma modelling purposes. The original ADAS data format (*adf09*) for such dielectronic data was prepared by Badnell and Summers. Badnell and co-workers have produced comprehensive dielectronic data to this format in both *ls* and *ic* coupling. Data for iso-electronic sequences up to Al-like have now been completed, with the Al-like case itself done in the 2011 period.

For ions with many electrons, in M and higher shells, dielectronic data sets to the *adf09* specification become very large and increasingly unsuited to heavy elements such as tungsten. So economies of method for dielectronic recombination are now required, without reverting to the over-simplicity (for finite density fusion applications) of the zero-density assumptions sometimes used in astrophysics. Griffin and Loch have implemented a dielectronic code, DRACULA, in the configuration average (*ca*) approximation. Also Badnell has in the last months implemented a *ca* variant within AUTOSTRUCTURE. On a finer level, Badnell and Summers have been considering the economies of using extrapolation of threshold energy partial wave collision strengths to evaluate state selective dielectronic rates more efficiently and to allow bundling methods (c.f. PUBL3) which are more finely targetted. The method is called the Burgess-Bethe-General-Program (BBGP) approach. Badnell has implemented a variant of his distorted wave approximation in AUTOSTRUCTURE to this end (sse section 2.2 below) while Summers has developed the BBGP approximation to work closely with AUTOSTRUCTURE *adf04* datasets. The primary development work has been completed in this 2011 period and testing is in progress. Comparisons have been taking place between these various approximations during 2011 and will be continued in 2012.

Special studies have targetted interesting heavy species ions which are an aid in deciciding how to proceed with yet more diificult cases. In the 2011, our publication "Dielectronic recombination of heavy species: the tin $4p^6 4d^q - 4p^6 4d^{(q-1)} 4f + 4p^5 4d^{(q+1)}$ transition arrays for $q = 1 - 10$" [1] is to be noted.

2.2 A new distorted wave code and its exploitation

Badnell has added a distorted wave electron impact cross-section capability to his AUTOSTRUCTURE computer code. Collision strengths for the electron-impact excitation of atomic ions are calculated using a Breit-Pauli distorted wave approach with the optional inclusion of two-body non-fine-structure and fine-structure interactions. Solution is based on a general multi-configuration Breit-Pauli atomic structure. It adopts a jK-coupling partial wave expansion of the collision problem and a Slater state angular algebra. Various model potentials, non-relativistic or kappa-averaged relativistic, can be used in the radial orbital solutions. The continuum distorted wave orbitals are not required to be orthogonal to the bound. (see "A Breit-Pauli distorted wave implementation for AUTOSTRUCTURE" [2]). The code prepares ADAS *adf04* datasets in both *ls* (LS-coupling) and *ic* (intermediate coupling) of type 5, that is with the transition cross-section data lines in terms of free-eelectron energy in th final state. A supplementary ADAS

Fortran program in the ADAS7#6 offline library, called *adf04_om2ups.for* (prepared orginally by Bryans and Summers, modified for general ADAS use by O'Mullane and corrected by Summers) converts the *type 5* data set to the familiar *type 3* form [1]. Badnell in further extensions to AUTOSTRUCTURE (to be released) enables a new *adf04 type 6* dataset to be produced in which the transition lines are partial collision strengths as a function of l at threshold. This is releveant to section 2.1 above.

Badnell in discussion with Summers has further tuned the AUTOSTRUCTURE distorted wave (DW) calculation for ADAS such that the final *adf04* datasets can be a direct substitution for the ADAS heavy species baseline data - with collisional data evaluated in the plane-wave Born (PWB) approximation. Summers has implemented PERL scripts in the ADAS7#6 offline library which allow semi-automatic preparation of driver datasets (ADAS *adf27* format) and then distributed AUTOSTRUCTURE processing on many machines simultaneously so that complete iso-electronic sequences can be executed in parallel. Such processing has been carried out for medium weight elements up to zinc in their H-like to Ar-like ionisation stages. This is a major new resource, which lifts the ADAS baseline for such systems to so-called *level 1 and level 2* precision. The data will be made available in OPEN-ADAS in a subsequent release. It is also an important step since, the spin-changing cross-sections, which are evaluated under DW, enable realistic modelling of the low-lying metastable populations in the generalised-collisional-radiative model. Full details of the various aspects, procedures and data will be included in ADAS-EU report PUBL3.

These new activities are substantial and important additions to ADAS-EU theme 1 which warrant the allocation of new work package numbers under theme 1 as in the table below.

Workpackage	**No.**	**Task**	**Task no.**	**Source**
AS/DW baseline lift to levels 1 & 2	27.	AS/DW implementation for adf04 production in *ls* and *ic*.	27-1	Strathclyde/ CCFE Culham/ EFDA-JET
		AS/DW mass production for medium-weight elements.	27-2	
GCR ionisation and recombination	28.	GCR ionisation fractionisation for level 1 & 2 *ls* and *ic*.	28-1	Strathclyde/ CCFE Culham/ EFDA-JET
		GCR BBGP dielectronic recomb. for level 1 & 2 *ls* and *ic*.	28-2	

2.3 Special studies of key tungsten ions

The objective, pursued in 2011, was to assess the feasibility of high grade calculation of ADAS *adf04*, *adf09* and *adf23* datasets for tungsten ions. There are three parts to this, namely obtaining a convincing atomic structure, simplifying this optimally to allow a valid R-matrix calculation of electron impact collisional rates and finally condensation/calculation of dielectronic pathways and excitation/autoionisation pathways guided by very limited experimental measurements (see ADAS-EU sub-contracts report SUBC1). The ions W^{+44}, W^{+20} and W^{+0} were chosen. W^{+44} is expected to be an emitter in the soft X-ray pass band of the refurbished KX1 spectrometer on JET. It is of medium complexity. W^{+20} is amongst the most difficult of the tunsgten ions because of it partially filled f-shell. W^{+0} has the extra complexity of being a neutral species, and therefore more prone to imprecision in theoretical studies. Yet such studies are essential to provide the "photon efficiency" estimates necessary for deducing its influx into a fusion plasma. Depending on the main power emitting transition arrays in W^{+44}, it may be possible to fit W^{+44} R-matrix calculations on a medium size ($\sim$ 50 processor) parallel computer system. On the other hand W^{+20} is likely to overwhelm even the largest supercomputers in the world. The following is a narrative on the studies and interchanges between Badnell and Ballance, with some contributions by Hibbert (see A.4).

For W^{+44}, both the R-matrix II (with Hibbert CIV3 structure/orbitals), Breit-Pauli R-matrix I (with AUTOSTRUCTURE structure/orbitals - non-relativistic or kappa-averaged) and DARC (with GRASP structure/orbitals) are in principle possible. A first question is whether the fully relativistic DARC/GRASP treatment is necessary. It is noted that quintet transitions must be included as they likely to be observed in JET/KX1. Badnell finds that including $3d^9 4s4p4d$ configuration increases the total number of levels wich must be handled to 326. This stabilizes the variability of the

[1] The *adf04_om2ups.for* procedure can also generate non-Maxwellian collisional rate data sets of format *adf04 type 4* but this is beyond the present purposes.

f-value for the two strong transitions of interest. That is there is little difference between the use of non-relativistic and kappa-averaged orbitals. There do remain other transitions which are still sensitive which could be due either to configuration interaction or be specifically induced by relativistic orbitals. Comparison with GRASP gives similar gf-values but the transition energies of the kappa average AUTOSTRUCTURE variant is very good compared with GRASP. The $^1P_1$is not much affected by $3d^94s4p4d$ configuration (15%) but the $^3D_1$ f-value changes by a factor of 3 without it. Behaviour of CIV3 needs to be compared and should be part of an ADAS-EU sub-contract with Queen's Belfast. On the other hand continuing on Breit-Pauli R-matrix I (with AUTOSTRUCTURE kappa-averaged orbitals) seems both feasible and desirable, but moves up into the supercomputer territory.

For W^{+20} our first concern is with the enormous dielectronic recombination (DR) cross-section enhancement, at threshold, measured by Müller and Schippers (see report SUBC1) and an assessment of the possible contributors to it. For W^{+20} with ground configuration $4d^{10}4f^8$, the $4f-4f$ fine structure target excitations would be usually expected to drive the low temperature DR. But it turns out that $4d^{10}4f^8 - 4d^94f^9$ dominates and that the *ic* results are up to a factor of 10 larger than the *ls*. Significant, but smaller (~20%) contributions arise from both $4d^{10}4f^8 - 4d^{10}4f^75l$ and $4d^{10}4f^8 - 4d^94f^85l$ core promotions. (For Au^{20} recombination, the $4d^{10}4f^{13} - 4d^94f^{12}5s, 5p, 5d$ appears to dominate and give acceptable agreement with Müller and Schippers but the $4f-4f$ route is constrained by the near closed shell.) For W^{+20}, *ls* calculations have been completed for the above indicated $\Delta n = 0$ and $\Delta n = 1$ promotions from the $4d$ and $4f$ subshells. *ic* calculations have been completed for all but the $4d-5l$ promotions — these should finish by the end of January. It seems likely, based-on the results obtained so far, that the theoretical results will still lie a factor 2–3 below experiment over 0–10eV. It should be noted that this is for the best case scenario of 100% population lying in the ground level. This seems unlikely to be the situation for the experiment. DR from progressively excited levels becomes progressively smaller due to the increasing number of alternative Auger channels that lie *below* the initial metastable. Even within levels of the ground term, DR from the highest level is a factor of two smaller than from the ground level!

It has taken some judicious insight and a fair amount of code development, over and above that for the half-open d-shell as exemplified by the tin problem, to tackle the $4d^{10}4f^8$ problem without an overwhelming requirement for resources: CPU RAM, disk space and processor time. However, this is about as bad as it gets. $4d^{10}4f^7$ only has a factor 8/7 more states and thus requires ~ $(8/7)^2$ more memory and ~ $(8/7)^3$ longer — a 30% increase in memory and a 50% increase in time is do-able. However, alternative, simpler, strategies need to be investigated to see if they can give an adequate baseline coverage across the 60 stages required for ITER. While configuration average fails badly at low energies, at temperatures of peak fractional abundance it agrees to within a factor of about two with the *ls* total DR results, although this appears to be due somewhat a fortuitous cancellation of under and over-estimates from different core excitation contributions. From the tin work, we find that BBGP can give more reliable agreement and should be pursued by Badnell and Summers speedily.

Bibliography

[1] N. R. Badnell, A. Foster, D. C. Griffin, D. Kilbane, M. O'Mullane and H. P. Summers. 'Dielectronic recombination of heavy species: the tin $4p^6 4d^q - -4p^6 4d^{(q-1))} 4f + 4p^5 4d^{(q+1)}$ transition arrays for $q = 1 - 10$'. J. Phys. B, **44** (2011) 135201. doi:10.1088/0953-4075/44/13/135201

[2] N. R. Badnell. 'A Breit-Pauli distorted wave implementation for AUTOSTRUCTURE'. Comput. Phys. Commun., **182**(7) (2011) 1528–1535. doi:10.1016/j.cpc.2011.03.023

Appendix A

ECWP documents

A.1 Electron impact data generation and exploitation for fusion and ITER: Proposal: 8 Sept 2010

Summary: With the ITER construction now underway and with the shutdown of EFDA-JET for its extended performance and ITER-like wall upgrade now halfway through, I suggest that it is an opportune time for like- minded electron collision computational theorists and fusion oriented atomic/plasma modellers to coordinate their actions. An action plan is proposed which links parties interested in R-matrix and its derivatives in the UK and USA with those supporting atomic physics exploitation in magnetic confinement fusion through the ADAS and ADAS-EU Projects.

Background: From its commencement at the European JET Joint Undertaking, ADAS has evolved as an international project, self-funded by its participants, to interface atomic physics to plasma diagnostic and models in magnetic confinement fusion. With the commencement of the international ITER program, the European commission , under FP7-Fusion, is funding the ADAS-EU project to support fusion laboratories in Europe and ITER in their use of atomic physics. ADAS, ADAS-EU and JET-ADAS (funded by CCFE Culham), managed through the University of Strathclyde, support around four full-time staff based at fusion laboratories in Europe to meet commitments. ADAS development takes place in Europe and in the USA at Auburn University. ADAS and ADAS-EU have a completed infrastructure, by which ADAS data and models enter all the leading plasma models in the world, all the principal fusion laboratories in the world are participants including ITER and all ITER partner countries are represented. With its baseline capability established, over the next years the ADAS and ADAS-EU Projects will be seeking to 'lift the baseline'. The projects are committed to the R-Matrix approach as their highest quality electron impact cross-section data inputs, building on a PWB/DW baseline. This proposal seeks to secure these inputs in the interests of the world fusion effort and in particular for Europe and USA contributions to it.

Interested parties: Within Europe and the USA, the groups at AMDPP, Department of Physics, University of Strathclyde; School of Mathematics and Physics, Queen2019s University Belfast; CSE Department, CCLRC Daresbury Laboratory, Warrington; Atomic Physics, Physics Department, Auburn University, Alabama are the key sites for the fundamental atomic calculations needed for ADAS and ADAS-EU. There is additional support from fusion Associated Laboratories in Lithuania and Romania.

The basic plan: The essence of the project is to lever up complex electron impact collision and the related atomic structure calculations for fusion through funding proposals to research support agencies and supercomputer facility providers. This should be progressive through pilot calculations leading to post-doctoral funding, leading hopefully finally to staff positions - noting that first plasma on ITER is probably ten years away. This should be a coordinated effort of the interested parties above. The ADAS and ADAS-EU Projects would seek to fund the pilot work and the preparation and selling of the principal proposals over a year or so. It is hoped that the profile of strong engagement of ADAS with ITER and the ADAS-EU project, along with the very high reputation of the fundamental producers above, would help to sell the proposals to our national research councils and universities. As more specific proposals, I would like to suggest (1) that Nigel Badnell be employed at 20% FTE by ADAS- EU until Dec. 2012 to oversee the implementation of an agreed plan; (2) that a person with atomic collision/supercomputer experience (Connor Ballance is one person who might be suitable) be seconded to us in the UK for a period , funded by the ADAS Project, to help to build the cases, trials and directions of supercomputer use; (3) the above person, possible based at the JET Facility, to act as a mobile link person between the interested parties - especially Queen's Belfast, Daresbury and Strathclyde; (4) that we go high European profile in supercomputer demands - HECTOR in the UK and JUGENE/ JUROPA / HPC-FF in Germany (5) ADAS-EU uses its ability to place small seed sub-contracts to help the work-up (6) ADAS-EU staff ensure very efficient paths for fundamental data into ADAS and on to fusion exploitation; (7) that assistance is used from smaller players such as Romania and Lithuania so that European cooperation and mutual support is maintained, eg. the atomic structure experts would assist in channelling the structure efforts from Lithuania into the collisional domain; (8) that Auburn looks after the USA needs for ADAS with central ADAS support; (9) that Auburn and the European laboratories operate to an agreed joint plan, with inclusion of names in proposals etc. (10) Hugh Summers, Martin O'Mullane and Stuart Loch determine with others the key species and ions for attention in response to the fusion programme.

A meeting: My original idea was to have a small meeting here at the EFDA-JET Facility in August to discuss the above ideas and possible variants. That opportunity has eluded us so now I thought a meeting one side or other of the ADAS Workshop while a lot of us are in Northern Ireland would be another chance - perhaps Wed 6 Oct. I have appended a set of persons to this document whom I would like to invite to participate. Please feel free to suggest others who might contribute while bearing in mind that what is proposed is a planning meeting and the objectives must remain focussed on fusion and R-matrix based atomic collisions. The ideal outcome should be an agreed plan for us to follow.

Beyond the electron collision and atoms-in-plasma theorist participants, I thought it might be helpful to try to draw in a person (probably Ruggiero Giannella) from the Commission (Euratom) in Brussels to advise and support us on access to the European supercomputers in Forschungszentrum Juelich. There is some background to this. Ruggiero Giannella, an old colleague formerly responsible for spectroscopic diagnostics at JET, is the Commission's member on the board for the Juelich supercomputers - and incidentally the Commission person responsible for monitoring the CCFE's fusion activities for Europe. Tim Hender, head of theory at CCFE, is also on the board and involved in allocations of time. CCFE has an account and Tim would allow us some access to that, without a proposal, for preliminary tests. The next main proposals should be submitted around Nov-Dec for action after May 2011.

Relevant persons: Phil Burke, Alan Hibbert, Penny Scott (or/and another representative from Queen's Belfast), Martin Plummer, Andy Sutherland (or/and another representative from Daresbury Laboratory), Nigel Badnell (Strathclyde), Mitch Pindzola, Connor Ballance, Stuart Loch (Auburn), Hugh Summers, Martin O'Mullane (Strathclyde/JET Facility), Ruggiero Giannella(EU Commission).

Please respond as soon as possible to this email if it catches your interest. If enough are interested, I shall follow up with a tentative agenda and definitive dates. The ADAS project will support travel/subsistence to the meeting to the limit of £120/person and up to two persons from each interested party, if not already at the ADAS Workshop.

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A.2 Planning Meeting: Queen's Belfast: 10.00am Wed 6 Oct. 2010

Tentative agenda

1. Views and perspectives of Queen's, Strathclyde, Daresbury, Auburn on a joint initiative and its scope (see initial concept document circulated by Hugh Summers).

2. Core scientific/computational objectives to include:
   (a) unifying underpinning atomic structure
   (b) two-stream parallel Rmatrix computations
   (c) European fusion associated lab/university engagement and unity.

3. Staffing needs and aspirations:
   (a) for preliminary studies and preparation of full funding proposal(s).
   (b) for proposal implementation and then long-term support.

4. Timescales and next steps.

HPS
29 Sep. 2010

A.3 Draft Working Document for 2nd ECWP meeting: EFDA-JET Facility: 12 April 2011

Abstract: This document is intended to form the basis for the 2nd meeting of the ECWP. It has been prepared by Nigel Badnell, Martin O'Mullane and Hugh Summers and so is a first cut from a one-sided perspective. It is hoped that at the 2nd meeting, discussion will lead to its evolution into a mutually acceptable document which will detail our forward plans for the next 2-3 years. The document should evolve with us from meeting to meeting, expanded with appendices and results as goals are reached, participants consolidate/appraise results and intentions are translated into realities.

Items:

1. Background
2. General goals and objectives
3. Computation scope and codes
4. 1st stage plan
   (a) Objectives
   (b) Personnel resources
   (c) Computational requirements/resources
   (d) Financial resources
   (e) Timeline and allocation
5. 2nd stage plan
   (a) Objectives
   (b) Personnel resources
   (c) Computational requirements/resources
   (d) Financial resources
   (e) Timeline and allocation
6. Appendices
   (a) Minutes of meetings
   (b) Results

2nd Meeting location/date: EFDA-JET Facility, Culham Laboratory - 1 Apr. 2011

1. Background: The Electron Impact Working Party is an activity of the ADAS-EU Project designed to raise the quality of electron impact fundamental data in the ADAS databases. Thus ADAS, which provides atomic modelling for the fusion regime in close association with plasma modelling and spectral analysis will be optimised in scope and quality for European fusion laboratories and ITER. The ADAS and ADAS-EU Projects are committed to the R-Matrix approach as their highest quality electron impact cross-section data inputs, building on a PWB/DW baseline. In this, there is a strong wish to maintain and exploit European and UK strength in this area, although the results will be of benefit to the world fusion effort and will be closely associated with the work of colleagues in the USA.

Following the ADAS workshop in Armagh in October 2010, a first ADAS-EU Electron Collision Working Party (ECWP) sponsored meeting was held at Queen's Univ. Belfast to discuss a possible coordinated effort. The initial proposal was to tackle the electron-impact excitation of tungsten ions for JET/ITER diagnostics. Those present included Alan Hibbert, Penny Scott, Cathy Ramsbottom (Queen's University Belfast), Martin Plummer, Andy Sutherland (Daresbury Laboratory), Nigel Badnell, Martin O Mullane, Hugh Summers (Strathclyde University), Connor Ballance (Auburn University) and Viorica Stancalie (NILPR, Bucharest). Apologies were received from Phil Burke.

It was agreed that there was sufficient interest in establishing a codebase from the various code suites available and to perform test calculations, which would lead to more realistic studies and to future funding opportunities. The details were to be worked-out at a follow-up meeting in early Dec at JET. Weather and other commitments meant a delay, until now, and so this meeting is now targetted for around the beginning of April.

2. General goals and objectives: The essence of the project is to lever up complex electron impact collision and the related atomic structure calculations for fusion through funding proposals to research support agencies and super-computer facility providers. This should be progressive through pilot calculations leading to post-doctoral funding, leading hopefully finally to staff positions - noting that first plasma on ITER is probably ten years away. This should be a coordinated effort of the interested parties above. The ADAS and ADAS-EU Projects would help to fund the pilot work and the preparation and selling of the principal proposals over a year or so. It is hoped that the profile of strong engagement of ADAS with ITER and the ADAS-EU project, along with the very high reputation of the fundamental producers above, would help to sell the proposals to our national research councils and universities.

A second objective is that Electron Impact Working Party along with ADAS should actively maintain links to the EFDA-JET programme through participation in its experimental campaigns and establish links to the UK forward fusion programme, in particular MAST Upgrade. JET resumes operation this year and will probably continue to 2015 and MAST upgrade and the SuperX divertor are scheduled for 2014. In this way, our Universities, through the Electron Impact Working Party and ADAS, may be initiators or participants in MAST facility enhancements, such as new large spectrometers, in due course.

At the upcoming JET meeting, it is hoped to agree initial methodologies/codes, calculation details, assignments and a schedule of initial collaborative study, called the 1st stage plan. A relatively simple ion (W^{+44}) [1] has been identified as a test-case which is relevant to JET core diagnostics. Its emission is expected in the wavelength range of the revamped KX1 X-ray spectrometer. The meeting should also look forward to the next phase, called the stage 2 plan. Future areas of interest are the JET EP2 divertor (ionisation stages $<\sim W^{+44}$) and emission near surfaces from inflowing heavy element ions (especially W and W^{+}). The meeting should include discussion of computer resources and use thereof and sight future funding opportunities, for staff, hardware and software.

3. Computational scope and codes: The relevant codes break down into two groups - those based on fully relativistic Dirac wavefunctions and the Breit-Pauli ones, which currently use non-relativistic wavefunctions. The former include GRASP and DARC while the latter cover CIV3/SS/AS on the structure side and ICFT/R-matrix-II FINE/traditional BP on the collisional side. It is likely that all will use the same outer region STGF suite, which simplifies deliverables (via ADASEXJ). However, radiation damping does require inner-region dipole matrices in standard/OP form.

4. 1st stage plan:

4.1. Scientific objectives: A key objective of the initial study is to identify whether the 'BP' models can be used for W^{+44} (and/or similar residual charge states) or whether this is the domain of GRASP/DARC. W^{+20} will be the starting point for use of BP within the current extended work programme. It is not clear whether there are any disadvantages (other than H diagonalization) of using DARC, apart from the necessity of using GRASP, hence the initial study. Certainly, at low-charge the expertise of Allan Hibbert and CIV3 is likely paramount. Within the BP suites it seems unlikely that a full BP calculation is necessary (re-coupling before H(N+1) diagonalization) and that "FINE" (recoupling the R-matrix, before outer-region solution) and/or ICFT (recoupling the K-matrix) should suffice and is beneficial for diagonalization. It is likely that SS/AS/CIV3 are interchangeable between the "BP" collision codes. AS is of use for its production of infinite energy PWB collision strengths. These, along with gf- values, can guide the likely validity of the Dirac vs BP approaches. Indeed, if GRASP is required to obtain a sufficiently accurate atomic structure for the W^{+44} diagnostic lines then the collision method debate is moot. The structure study will also guide the necessary CC and CI expansions. This is likely only an issue for the surface studies (near neutrals). Note also that radiation damping was found to be important [1] on effective collision strengths for certain transitions (e.g. 1-2) below T=1000eV in W^{+44} - so a final deliverable may be a hybrid adf04 file of Ballance & Griffin for the outer-shell and the present proposed inner-shell.

[1] Although a DARC calculation by Ballance & Griffin has been published [JPB40, 247(2007)], it did not include the states relevant to diagnostics which require opening-up the 3d10.

The Cowan structure code is used extensively in ADAS and by many groups in Europe. A second objective is to determine a mapping (if possible) between Cowan structure calculations parameters and those of CIV3/AS/GRASP, at least within some precision level. Such a link will allow ADAS/ADAS-EU to make best use of the work of other European collaborators in fusion, especially Mons-Hainaut and ITPA Vilnius - essentially extending their structure and wavelength research into the collisional domain. It is noted, but perhaps a bit beyond the immediate brief, that a number of Eastern European atomic physics university groups are seeking engagement with the ITER programme encouraged by the European Commission. The expertise of most of these groups is in structure and so the ECWP might see itself as a key enabling force/route for them which could be formally set up.

Should the ECWP seek to have a parasitic diagnostic experiment on EFDA-JET in to C28 and C29 campaigns? The call for proposals is imminent. As noted earlier, W^{+44} should give observable emission in the JET core - subject of course to sufficient tungsten penetrating to the core plasma from the divertor. A spectral observation from KX1 would be linked to ionisation state and transport. One would seek consistency with the SANCO modelling. In this context the ECWP should be aware of the ADAS-EU collaboration with Alfred Mueller and Stefan Schippers at Justus-Liebig, Giessen on ionisation/recombination cross-section benchmarks for tungsten. Should Justus-Liebig formally connect with the ECWP as this 1st stage?

4.2. Personnel resources: At the Strathclyde end, some staff time can be brought to bear. Nigel Badnell has 20% FTE on ADAS-EU with Electron Collision Working Party responsibility. Although part of Nigel's time is expected to be used to bring coherence and effective engagement (in the ADAS/ADAS-EU sense) to the broader European efforts on atomic physics for fusion, he is enthusiastic to assign time to bringing some of his shared development of RMPS/ DARC etc with the USA, carried on US supercomputers, back into hands-on use and feel in Europe. We see this as part of the setting up stage. About nine man-months out of two-years of Strathclyde post-doctoral activity can be expected to be available for this first stage. Subject to having the right post-doctoral person, this would be committed to supporting Nigel's build up of European supercomputer / apposite atomic model skill and to the interfacing to interfacing with ADAS and spectral analysis. On the latter, the support would be for Martin and his efforts to promulgate the work in JET/MAST/ITER forward predictive modelling and actual diagnostic experiments. Opportunities in this regard will come available first at JET in the C28 and C29 campaigns within our 1st stage time frame.

At the Belfast/Daresbury end, it is hoped some staff time can be committed from existing resources (with only very modest support via sub-contracting from ADAS-EU within the 2011/2012 time frame - see below). The 1st stage needs some Alan Hibbert time to guide structure optimisation for complex ion collision calculations, but also to help with the rationalising of mismatched approaches to structure. This latter time commitment would be helpful in 2011 as/if ADAS-EU seeks to link in other European groups productively. We would hope to have enough staff time found to push the R-matrix-II FINE on the tungsten trial cases on UK supercomputers. The provision of extra help through the Connor Ballance route now seems less likely, since Connor's focus is more on atomic physics activity growth in the USA rather than in Europe. The maximum extra post-doctoral help to Belfast/Daresbury we see at this 1st stage is $\sim$ 3 man-months (by full commitment of an ADAS-EU sub-contract entirely to this) plus 3 man-months allocated from the Strathclyde none-months explained in the previous paragraph. Also Nigel could be the mobile, visiting person who keeps things together, under separate (ADAS-EU) travel funds. We wonder if Viorica can assign some time, working within the remit of the Belfast part of the 1st stage plan.

4.3. Computational requirements/resources: We think the 1st stage plan must seek to establish the importance and legitimate claim to supercomputer time of atomic collision calculations for fusion. This point is probably adequately achieved in the UK through the Belfast/Daresbury use of the Edinburgh machines, although here it is the fusion, not astrophysics, angle which is to be pushed. The point is not yet made on the Juelich European supercomputers, although as pointed out at the first meeting, such a push would probably be sympathetically received. Proposals are already in the pipeline to Juelich for large scale close-coupling calculations for ion impact for fusion applications. Our suggestion, given the limited staff time for new development at this stage, is that Belfast/Daresbury stick with UK/Edinburgh for the 1st stage and Strathclyde tries to open the Juelich path. Tim Hender, head of theory at Culham Laboratory is prepared to assign some of the UKAEA's time allocation at Juelich to enable us to set up and get our proposals in. Tim will attend part of our JET meeting to elaborate and give guidance.

4.4. Financial resources: ADAS and ADAS-EU have ~15 months and ~9 months of post-doctoral funding resources available respectively of which the ADAS-EU part must be used by the December 2012. From the complete set of ADAS/ADAS-EU responsibilities which this resource needs to support ~9 months (6 ADAS and 3 ADAS-EU) can be assigned to the Electron Collision Working Party. It requires a single atomic/computation/plasma environment/theorist all rounder who can meet all aspects of the job specification. At this time, to Strathclyde knowledge, there is one (possibly two) completing post-docs who can fit the bill, but their availability is not certain. Are there others? ADAS-EU can place one £10,000 contract with Queen's within the sphere of this 1st stage plan. Subject to a clear specification and a satisfactory final report, this money's use is not prescribed in detail. It could be used therefore to support a post-doc for a modest period or enable travel to each other on the project for Belfast/Daresbury staff. This sub-contract really needs to be put in place as soon as possible and certainly within the next three months.

4.5. Timeline and allocations:

Group	Person	Apr./May	Jun./Jul.	August	September
Strathclyde	Hugh Martin	Procure Juelich SC alloc. Propose JET expt. Set-up Queen's/ ADAS-EU sub- contract	Action post-doc appoint. W^{+44}: CIV3 $\rightarrow$ Cowan,AS,GRASP	Assess ECWP-EU network potential post ADAS-EU	2nd stage proposal to EU Write paper & ADAS-EU report
	Nigel Alessandra/ a.n.other	W+44 local set-up & structure GRASP/DARC	W^{+44} set-up/1st runs: Juelich	Optimise/2nd runs Compare/contrast	2nd stage proposal: EPSRC joint Write paper
Daresbury	Martin & Andy	Procure Edinburgh SC alloc.	W^{+44} RMII set- up/1st runs: Edin	Optimise/2nd runs at Edin. SC	
Queen's	Alan	W+44 structure recommendation incl. 3d promotion	W^{+44} CIV3 $\rightarrow$ Cowan,AS,GRASP	W^{+20} structure recommendation	Write paper
	Cathy Penny	W+44 local set-up & structure for RMII	W^{+44} RMII set-up/ 1st runs: Edin.	Compare/contrast	2nd stage proposal: EPSRC joint Write paper & ADAS-EU report

5. 2nd stage plan: The full electron collision plan must recognize the importance of the low ionisation stages ¡= W+20, including for sure W+0 and W+1. The ions ¡ W+20 include those which generate a quasi-continuum (both in mass line emission and in DR modelling) as well as being the best prospects for identifiable individual lines from ions at shell boundaries. These span the ITER divertor ions and emission and the local tungsten sources and represent a substantial body of new work. The core ions of tungsten go up to at most W+60 with W+44 being a good representative one. The 1st stage work on W+44 should lead to fairly routine progress through these ions. It is noted that data are now nearly adequate for H-like to Ar-like at least as far as zinc, with some experience on to tin and xenon. These iso-electronic sequences, with the 1st stage decisions taken on Breit-Pauli versus full Dirac, can now be continued through to tungsten. Finally, although tungsten is the focus of attention, other 6th and 5th period element ions are of interest from time to time (eg. rhenium, tantalum, gold, xenon). Also confidence in theoretical collision data does come from checking adjacent iso-electronic systems, both from a purely theoretical perspective, but also from experimental benchmarks which usually include close iso-nuclear and iso-electronic ions (c.f. ion storage ring/merged beam studies).

Secondly, to ensure relevance and durability through to ITER, the 2nd phase plan must be sufficiently large and structured to suit both UK EPSRC requirements and European Commission framework purposes. For the European aspect to work, it must be inclusive in its aiming at ITER. ADAS-EU as a Support Action is allowing us to set up the infra-structure for ITER support. THE ECWP (perhaps called ECWP-EU) should build on that, in the sense of a European Network proposal, constructed on the ADAS-EU base and following on from it. ADAS will be the medium of delivery at the fusion plasma end, but there must be room for other European groups (Western and Eastern) to engage in the data generation and validation.

The current and near term fusion experiments must not be neglected. The 2nd stage data and results must translate to measurables and measurements on current machines and on to near/medium term developments such as MAST upgrade and the Super X divertor. All this will hold the project together and validate the work ready for ITER.

5.1. Objectives More detailed specification following on from above.

5.2 . Personnel resources Each of Strathclyde and Queen's want at least a post-doc and a research student from an EPSRC proposal. An EU network proposal would need at least two post-docs, probably one at the Culham/JET site and one at the ITER site. There would be others needed in Europe, perhaps two more postdocs and two more students, - such as another postdoc with Alfred Mueller and perhaps Vilnius with PhD students at other sites (Hungary, Poland, Romania).

5.3. Computational requirements/resources Division of major calculation demands between UK and Europe. Substantial demand of supercomputer time at Juelich.

5.4. Financial resources EPSRC proposal (Queen's and Strathclyde together for fusion). EU Network proposal , probably led jointly by Strathclyde/Queen's with splitting of responsibilities in integrating others. Strathclyde (Culham outstation) taking care of ADAS and communication through to fusion experiment . Strathclyde (Glasgow) and Queen's taking care of fundamental data (based on the two code routes and atomic structure issues/connections).

5.5. Timeline and allocation Three year EPSRC plan from mid 2012. Four year EU plan from start 2012. Expect to lever a permanent staff post at Strathclyde one or two years into the projects. Queen's should aim for the same.

6. Appendices:

6.1. Minutes of meetings

6.2. Results

NRB/HPS
28/03/11

A.4 ADAS-EU ECWP Meeting EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK. 25-26 May 2011.

location: EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK.
Date: 25-26 May 2011.
Present: Nigel Badnell, Martin Plummer, Andy Sunderland, Penny Scott, Cathy Ramsbottom, Alan Hibbert, Martin O'Mullane, Hugh Summers.
Purpose: Progress the electron collision working party activities for ADAS-EU.
Items:

1. Discussion, modification and agreement of plans and their documentation as drafted in document draft-discussion-document-qub-daresbury-strathclyde-23may.[2]

2. Review merit and opportunities for associated experiments at EFDA-JET .

3. Review merit and opportunities of access to Juelich HPC-FF supercomputer for calculations..

4. Decide basis and purpose of ADAS-EU sub-contract with QUB linked to ECWP activities. ADAS-EU ECWP running document and planning :

5. Nigel chaired the meeting using as a starting agenda, the document draft above prepared by Nigel and Hugh. Hugh explained that his hope was for a coherent forward plan for the ECWP, based on the document with suitable modifications. The document would evolve, operating as a running document which would include results, intentions, scheduled actions, meeting reports, as ECWP activities expand and change from talk to substance. Broadly the group went along with this and the meeting moved forward to specifics [3].

6. Some justification was given for the specific ions of tungsten proposed in the document. W+44 was accepted as a good starting point, seeming to provide a potential observable ion in JET, close to the limit of modest multi-processor computation. It has some R-matrix calculations (Connor Ballance) but which do not open the 3d shell to which the main predicted radiative loss transition occurs. It is also on the border of requirement between Breit-Pauli and full relativisitic calculation. W+20 and W+0 were the other two ions of special fusion merit which we wish to consider ultimately.

7. It was agreed that the group should split into two for a time. Alan and Nigel worked together on a first assessment of the structure of W+44 trying to decide on the number of states required for an R-matrix calculation meeting the needs of (6) above and also to contrast CIV3, AUTOSTRUCTURE and GRASP. Issues included the handling of the one- body non-fine structure relativisitic terms within a CIV3 slater-type orbital parametrisation contrasted with the use of kappa-averaged orbitals in AUTOSTRUCTURE. Nigel continued to work on the problem, following the meeting, and results will be appended to the running document [4]. The decision, which remains pending, is whether for ions as highly charged as W+44 is safe to follow a Breit-Pauli/RMATRX route or whether GRASP/DARC is the only way forward.

8. The second group focussed on the R-matrix side of the calculations, experience on HECTOR and on the latest code developments.

9. Martin Plummer indicated that there was a small-moderate amount of time on HECTOR available for tests via the ARC staff code development account, but extremely little staff time currently available from Daresbury for dedicated work (ie Martin and Andy in ˇ2018occasional spare momentsˇ2019). Cathy said that QUB had quite a big astrophysical cross- section allocation which might allow tests and that she is the most probable QUB person able to pursue the initial HECTOR/HPC-FF tests. It does appear though that experience is already strong on HECTOR and there is more a matter of deciding on which RMATRX codes sets to use and whether these are ready. Andy pointed out that the PRMAT package was due for finalising in April 2012.

[2]C:/Users./Hugh Summers/My Documents/Documents_work/adas_eu/planning/electron_working_party/
[3]Martin will set up an arrangement for us all to access and add to ECWP documents.
[4]c.f. footnote 2.

10. Hugh wanted to be clearer about the code sets available to us and their relative strengths. Andy drew attention to the appearance in April of Phil Burke's new book on the R-matrix method, which is up-to-date and spells out the computational tools and state-of-affairs. Hugh's understanding is that AUTOSTRUCTURE, parallel Breit-Pauli RMATRXI (cf Connor Ballance and Nigel) and PSTGF is the Strathclyde route, to be tried out on HPC- FF. CIV3, RMATRXII, PFARM is the QUB route, to be tried on HECTOR and HPC-FF. He remains unclear if there is inner region partitioning into Breit-Pauli and LSŎ3c0 parts required in either or both routes and if so how the frame transformation theory variants PFINE and ICFT are to be used and how all these parts fit into a massively parallel supercomputer!! Presumably this more of an issue for W+44 than for W+20 since W+20 and lower ions will be LSŎ3c0 in the inner region.

11. It was clear in the discussion that a new and very fusion relevant W^{+44} calculation is well within the supercomputer capabilities, but out-with local cluster capabilities. W+44 is therefore the ECWP first target out of which a joint paper is required (to prove our serious intention) by the end of 2011. By contrast, W^{+20} will naively overwhelm the supercomputers, but is the case of greatest teasing interest because of the open (half-filled) 4f shell and the need to get the number of target and coupled channels down to acceptable size. It seems that Cathy and Nigel will be the executors for the RMATRX calculations aided by Martin Plummer and Andy at HECTOR (and HPC-FF if new accounts are available) and by Martin O'Mullane at HPC-FF.

12. The working together of Alan and Nigel on the structure is a key issue. The relative merits and abilities of CIV3 and AUTOSTRUCTURE for generally safe structure in unknown systems around W^{+44} will be an important part of the paper. The orbital representations and their effectiveness within CIV3, when AUTOSTRUCTURE suggests kappa averaged orbitals needs to be established. Again presumably CIV3 comes into its own as we move down through W^{+20} and on to W^{+0} .

13. Discussion moved on to Hugh's wish to use an ADAS-EU sub-contract with QUB to oil the wheels and to put this into place as soon as possible. It was agreed that he would work this up with Penny speedily.

14. Hugh also aired his ambitions and suggestions for the ECWP to work up substantial EU and UK funding proposals for fusion support which would be a follow on from ADAS-EU supporting ITER. These would unite UK (QUB and Strathclyde) efforts, provide a valuable and probably dominating influence on electron collision inputs for ITER in Europe and be a centre of excellence in this area to which other European groups could attach.

    EFDA-JET experiments:

15. As outlined in the draft document, Hugh is of the view that, although ITER is the ultimate target for ECWP calculations on tungsten, that there is value in making connection of this theoretical work with current spectroscopic measurements. Such diagnostic studies, probably parasitic on the main plasma experiments, should be used to demonstrate firstly primary observability and so relevance of the reference ions and then hopefully quantitative checking of key cross-sections and effective rates.

16. Klaus-Dieter Zastrow, leader of Core Spectroscopy at EFDA-JET addressed the ECWP on the spectrometers, materials, design and programs of the JET restart, now just winding up following the extended performance (EP2) enhancements of JET. Klaus-Dieter led the ECWP on a guided tour of JET and used this as a vehicle for elaborating on and engaging in discussion of the machine characteristics and possibilities for contributions to the diagnostic analysis by the ECWP.

17. It is noted that the primary programme planning of JET 2011 campaigns C29 and C30 is now in place and so engagement with the experimental program means associating with scheduled experiments with ECWP key measurements made parasitically, possibly in late stages of a discharge, or in reserve or preparation time. Martin and Hugh noted the KX1 x- ray spectrometer revamp and the potential observability of W^{+44} by it. Jacek Rzadkiewicz is the responsible officer and some discussion has already been held with him on the atomic physics inputs to the diagnostic.

18. W^{+20} is a divertor species with UV, EUV spectrometry relevant (Andy Meigs) and W+0 an influx species observed in the visible (Mike Stamp, Costanza Maggi).

19. It is also noted that ADAS-EU has a close relationship with the German fusion programme, with the all tungsten wall ASDEX-U machine at IPP Garching of particular relevance. An ADAS-EU support research fellow (Luis Menchero) is based at Garching. Very experienced and supportive research leaders there include Ralph Dux,

Thomas Putterich and Rudi Neu. Clarification of effective ionisation and recombination rates of tungsten ions ~ W^{+15}- W^{+20} would be of special interest to Putterich.

Supercomputing issues:

20. The initial selection of ions requires supercomputer scale calculations. This includes W+44, based on the estimate by Nigel of the required number of states to open the 3d dipole promotions and include key consequential CI, made during this meeting.

21. Dr Tim Hender, Head of Theory at CCFE and chairman of the Juelich HPC-FF allocation committee, spoke to the ECWP on the possibilities of HPC-FF use. He pointed out that the machine was for EURATOM fusion use exclusively. It has 1104 nodes each of 8 cores, allowing 100 teraflops and 300,000 cpu hours/year. Access is channeled via CCFE Culham for the UK. This HECTOR size machine has an easier calculation proposal system. There will be a small Sept 2011 submission and allocation possibility, completing the year total and then next main submission in April 2012. CCFE Culham has a default allocation, and Tim can countenance some use of this for first try-outs prior to proper proposals. Tim noted that he would speak to Peter Knight at CCFE to obtain precise details for setting up user accounts through this mechanism - done!

22. There was a general view that the hoops to jump through to gain time on the EPSRC/HECTOR supercomputer system are now very irksome and repelling. By contrast the HPC-FF path seemed more reasonable. There was therefore enthusiasm to try it out as soon as possible, via the CCFE quota. It was felt that most of the ECWP participants would wish an account. Penny was keen to get a first true proposal in for September. Hugh, after the meeting, followed up the access mechanism, and received instructions from Peter Knight about on-line registration. Peter wished a single person from each ECWP site to handle their access. Martin has tried the on-line set up process successfully. It ties access to a the user's local machine, which means one user per ECWP site.

23.) There is little or no transferable time to test ECWP calculations from existing HECTOR allocations to QUB and Daresbury.

QUB sub-contract: It was agreed that Hugh would draft as ADAS-EU sub-contract for QUB, based on the expected initial calculations and ions stemming from this meeting and the running document. It is envisaged that the sub-contract would be used facilitate and prepare the way for a substantive European level proposal which would be the follow-on from ADAS- EU in 2013. It was suggested that ADAS-EU sub-contract funds would be used, inter alia, to support QUB/Daresbury staff travel on ECWP business.

HPS
30 June 2011