Apr18-04 ADAS Bulletin

At this release, we were originally planning to issue two new/adjusted groups of codes. These deal with non-Maxwellian modelling and the partitioning of ionisation stages for heavy elements. However, we have also been planning a change from SCCS to CVS for version control and archive maintenance of ADAS and its data as well as the issue of the first group of access routines from MATLAB. Altogether, that is too much for one release. Therefore we have decided to put out the current set of corrections, more modest code adjustments and new data into a 'bug fix' release first - taking us to version 2.7.1. Then in about two months, we shall make the big jump to version 2.8.

Version 2.7.1 does none-the-less include quite substantial tidying up and improvements as well as significant new data. Heavy species have again pointed up a number of flaws. You will see that Martin has continued to tighten ADAS801 and ADAS8#1 as well at the codes which exploit the baseline heavy species *adf04* files – ADAS407, ADAS408, ADAS810, ADAS209. Beam stopping has come in for some attention. Also, we have continued to add to the '*run_*' procedures. The dielectronic database continues to expand. Also stopping data for fast beams (from negative ion sources) has been added. Transport modelling prompted some additions for tritium and molybdenum.

Incidentally, this is the first release being handled by Allan Whiteford, who has taken over from Ricky Martin.

1. Corrections and additions to codes (ADAS v2.7 to ADAS v2.7.1)

C.1 Addition to the set of IDL run time versions of the interactive codes continues. The latest is *run_adas408.pro*.

C.2 A left-over debug print statement in ADAS502 (*cw_adas502_proc.pro*) has been removed.

C.3 There were inconsistent lengths of character variables between ADAS310 subroutines and the routine used to access the *adf07* data. Some routines also relied on variables being saved between calls. As these were not explicitly saved, compiled binaries under *g77* failed.

C.4 Some changes have been made to ADAS801

- There was an incorrectly placed initialisation of a index variable when checking the untied levels in the postprocessor stage.
- Also, too few transitions were defined for the postprocessor stage. This has now been increased to 120000 which is sufficient for Xe^{+10}.
- There was an error in counting the number of forbidden transitions in *ifg*.
- In complex ions not all levels have a unique <configuration>LSJ label. ADAS801 assigns the unused basis labels to the less dominant levels. Until now this was done within a configuration. However for some Xe ions the configuration must also change.
- All the routines in *adas801/ifg* and *adas801/ifgpp* have been lightly altered to regularise and update comments.
- The number of significant digits in the orbital energies has been increased by introducing a varying format. It is not necessary to recompile *xxdata_04.for* to read the new format.
- The *ifgpp* post-processor did not scale well. Beyond 200,000 transitions memory swapping to disk caused dramatic slowdowns in processing speed (the response of the machine was also affected which is not good in a multi-user environment). The algorithm was re-worked to use direct access files which moves the burden from memory to I/O but is far more scalable and does not adversely affect machine performance.
- The maximum L-value is now l=U (15) for $4d^q\ 4f^r$ configurations.
- The L field in the level list can now accommodate l larger than 10. *xxdata_04* can read the new variable size lines.
- *rcn* now reports if the self-consistent field (SCF) calculation does not converge.
- *rcn2* now gives details at the 'STOP 140' message.
- For very highly ionised species, eg W^{+66}, the admissible eigenvalue range of (> -4000kK) was not sufficient. We have relaxed the permissible value to > -20000kK. (kK - kilo Kaisers!).

Note that the interactive version may fail for complex configurations, or for ions with very many configurations. This is due to internal dimension settings. Use the offline version for these cases.

C.5 Allan found an error in *xxtcon.pro* which gives rise to a problem when running ADAS801 and using eV, rather than K or reduced, as temperature input. This has been corrected.

C.6 The maximum dimensions in *read_adf04.pro* have been increased to make it useful for reading the large *adf04* files associated with intermediate-coupling (IC) high Z data. This can be set in IDL and is passed through to *xxdata_04.for* without the need to recompile - sometimes things work properly!

C.7 For IDL v5.5 and above we have switched to using the inbuilt *file_info* procedure to get file attributes. Allan has determined that this can be significantly faster than the current method where *file_acc* spawned unix commands.

C.8 When drawing graphs in widgets, we now make IDL perform backing store by default. This should ensure that the graphs are not lost if other windows are moved in front of them. Kurt Behringer drew our attention to this problem.

C.9 We have sorted out the problems with some of the '99' He beam *adf21* stopping data – a consequence incidentally is that we now have an *xxdata_21* in both fortran and IDL.

-The *read_adf21.pro* routine now returns all the data in a structure if *all=all* is specified. There are some restrictions: only one file is allowed and the other options, such as interpolating, are bypassed. *read_adf22* gets these updates as well.

- ADAS304 and the library routine, *cxbms.for*, have been updated to use the new routine. *c4data* now return a 'subroutine deprecated' message.
- The interactive ADAS304 returned an error when trying to access the '99' He data. These are stored as, eg. */.../adas/adf21/bms99#he_fast/gcrc11/gcrc11#he_c6.dat* for fast beams and C^{+6}. ADAS304 can now read these files if the data root is edited to include the */bms99#he_fast* part and the member is given as *gcrc11*.
- For the new *bms97#h_fast data*, *c4chkz* was altered to test for a '_' in the filename. This routine demands consistency between the filename and the ion charge. Why this is desirable is not immediately obvious but we have left that as it is for the moment.

C.10 An IDL version of *xxsple* has been added. This allows for interpolation/extrapolation with the standard ADAS end conditions. See the routine for a listing.

C.11 In *read_adf14.pro* the mismatch between the IDL and fortran variables is fixed. There is no longer a limit of twenty-four temperatures.

C.12 In ADAS810 the treatment of *plt*, the total line power, for both total and filtered versions, has changed. The *plt* is now the sum of all transitions and is not subject to a minimum A-value restriction. The filtered version is determined by the *adf35* filter and not the wavelength interval as before.

- The previously inaccessible options in the interactive code, that is to input a filter, now been activated.

C.13 The progress bar as provided by the *adas_progressbar* routine did not show the correct percentage on screen. The fact that it was out by one was noticeable for a few event tasks. It has been corrected.

C.14 A library routine was missing from *xxdtes.pro* which caused problems when converting Eissner configurations. This mostly affects ADAS811. A new compilation script fixes this.

C.15 There was a discrepancy between the *adf40* file produced by ADAS810 (interactive and offline versions) and that expected by ADAS509. This has been resolved and the sample files in *adas/adf40* have been amended.

C.16 The *offline_adas/adas8#1* now comprises all of the files and not just empty sub-directories. The fortran routines are the same as the interactive codes but dimensions may be different.

- Up to 380,000 transitions are now possible. Note that in the interactive code, this is set to 120,000.
- The offline version has the same code updates as ADAS801 and ADAS810.
- Note there is a new *adas4xx* directory in the offline code.
- Failure to converge in the *rcn* SCF calculation terminates the offline version.
- The copy from central script has been dropped.

C.17 ADAS407 has been modified to cope with the configurations from high Z ions. Lots of internal dimensions have been substantially increased. The size of *adf04* files which can be handled is now in line with those produced by the offline ADAS8#1 code.

- The automatic branch can now cope correctly with the final H-like case. Previously it omitted this.
- The change to up to ten allowed metastables (why?) caused a subtle bug to be revealed. The *ndmet* dimension is passed through the *cw_adas_sel_sel* routine but this changes its type (integer to long) and its value in the H-like case only. This caused the fortran to hang later on.
- The *gdiel.for* routine has been restructured in keeping with ADAS conventions.

C.18 The type B parameterisation work also affects ADAS408 but more work still need to be done. The changes are:

- *xxdata_03* returned the incorrect type for the ground state effective principal quantum number *v0* in type B radiative recombination.
- Type B ionisation was faulty and gave incorrect rates out by 4 orders of magnitude!
- The excitation-autoionisation correction has been switched off until we are satisfied that it works. Note that ADAS407 does not deliver these parameters.
- Type B radiative recombination power is not implemented. If *prb* files are required we recommend using Type A for radiative recombination. Dielectronic recombination is not affected and either parameterisation can be used.
- The *d8vgol.for* routine has been restructured in keeping with ADAS conventions.
- The *d8gpca.for* routine has been restructured in keeping with ADAS conventions. The *ncut* and *eij* input arguments were altered within the subroutine but the calling routine did not expect this. We use internal variables for these quantities. An incorrect energy was used to evaluate the contribution from levels with n>10.
- An extra options button has been added to the output. This allows the more expert use to decide which of the recombination processes are sent to the *acd* and *prb* file. Radiative and dielectronic recombination can be separated along with bremsstrahlung for the *prb* output. Note that the power coefficients only apply to the non-filtered case. The same output filenames are used and no subsequent checking will be done. Exercise appropriate caution!

C.19 Yet another IDL run time version of an interactive code is included – this time *run_adas310.pro*.

C.20 The *adf04* bundling code, ADAS209, did not cope with the larger specific ion files associated with heavy species. Internal changes now permit up to 1000 levels and arbitrary length statistical weights in the output. *xxdata_04* can read these flexibly-formatted files.

- The *adasdev.for* routine was an unnecessary extra layer. It is now incorporated into *adas209.for*.

C.21 ADAS402 has been simplified. Now it just plots/tabulates the requested ionisation stage process from the selected *adf11* file. Until now it also plotted the other stages at a fixed density which made for confusing graphs. This context checking plot should be done elsewhere. If there is great demand for this feature we can re-instate it as an expert option.

- The noticeable changes are that the temperature and density choices must be made and the confusing nearest density input field is gone.

C.22 A minor bug has been fixed in ADAS207 by Martin Torney. This was a fault in the multiple line selection.

2. Corrections and updates to data (ADAS v2.7 to ADAS v2.7.1)

D.1 A H-like *adf04* file for Ar^{17+} is required to make an *adf15* for transport analysis. An LS resolved version is already in the *copsm#h* directory. As the levels are degenerate it was bundled and stored as *copha#h_bn#97ar.dat* following Harvey's naming template.

- The *pec* files for the transport analysis are archived in the *adf15/transport* directory and have the template name *transport_llu#<el><iz><ic>.dat*. The *ic* is optional depending on whether the file is J resolved or not.
- A warning message is included in the comments that theses files are not part of the GCR project and that there may be significant variability in the data quality between ionisation stages of the same element.
- The 'llu' prefix is to reinforce that these are low level metastable unresolved population calculations.

Data included: Ar^{14+}, Ar^{15+}, Ar^{16+}, Ar^{17+}, Fe^{24+} and Fe^{25+}

D.2 We also require data for molybdenum. We have Sampson data but it needed to be regenerated from its primitives. Files added to central ADAS are for Li-like $Mo^{39+,}$ Be-like Mo^{38+} and F-like Mo^{33+}. *adf15/transport pec*s are provided for $Mo^{38+,}$ Mo^{39+} as well as Na-like Mo^{31+} .

Note the Li-like file is a superset of the one already present.

D.3 More rogue files have been found:
- In the *adf10/prb96* directory, the backup file *adf04/nlike/nlike_rf97#n0.dat%* should not be present. Its presence causes ADAS403 to fail.

*** remove *adf10/prb96/pj#prb96_c24.dat*
*** remove *adf04/nlike/nlike_rf97#n0.dat%*

D.4 The *adf09* N-like Xe data files have incorrect names. Change these as follow:

*** *dmm00#n_xe44icr22.dat* to *dmm00#n_xe47icr22.dat*
*** *dmm00#n_xe44icr23.dat* to *dmm00#n_xe47icr23.da*t

But these are now in fact superceded - see D.10 below.

D.5 Ian Jenkins noticed that the '93' He beam stopping coefficients for B, N and Ne had incorrect formatting in the first line. This has been corrected.

D.6 More serious problems were found in the '99' He stopping data which affects the 1-1 and 3-3 metastable coefficients. Data for Li^{3+}, B^{5+}, N^{7+}, F^{9+} and Ne^{10+} was incorrect for both slow and fast beams. An absence of fundamental cross section data in the input was at fault - as ever garbage into a code results in garbage out! Fortunately the 'good' data covered the most likely elements found in tokamak plasmas (H, He, Be, C, O) and so probably no damage was done. The behaviour of the stopping coefficients is sufficiently well behaved that interpolating the good data gives acceptable coefficients for the remaining elements.

Ultimately these data will be revisited and re-calculated properly but this 'fix' should be sufficient not to introduce too great an error.

The adf26 population files for the incorrect data have been removed.

The associated beam emission coefficients for the problem species have been removed. Extrapolating these may be more problematic than the stopping coefficients.

D.7 Tritium has been added as a separate element in the '96' *adf11* datasets. This is to introduce a *ccd96* T with D donor file. As the H-H *ccd* file does not represent a CX recombination (at least from one thermal population), it is set to 0.0 everywhere.

The ionisation, recombination and power coefficients have been copied from the H files.

The *ccd96_t.dat* file was generated from the ORNL CX cross-section using ADAS509. The associated file for cross sections to low energy is

adf24/scx#h0/scx#h0_ornl#h1.dat

and the thermal rate file is

adf14/tcx#h0/tcx#h0_t1.dat

A dummy *pls96_t.dat* is provided but it has all values set to zero.

D.8 The configuration information for Ta^{26+} to Ta^{2+} in the *adf00/ta.dat* dataset was wrong. The ionisation potentials were correct.

D.9 The discrepancy between the *adf40* files produced by ADAS810 and that expected by ADAS509 has been resolved and the sample files in *adas/adf40* have been amended.

D.10 The completion of datasets from the DR Project continues.

- Data for the B-like sequence from Zikri Altun has been added. Driver *adf27* and *adf28* are also available.
- More N-like data from Dario Mitnik. New data for Cl^{10+}, F^{2+}, Mg^{5+} and Ne^{3+}. Some of the older data has been revised. Although this goes against our 'no unnecessary change' principle, these data are not in widespread use yet so it is just about permissible.

D.11 The stopping data for H beams by the light species (H to Ne) does not extrapolate well above ~100keV/amu. A new directory, suitable for proposed ITER MeV beams is archived in *adf21/bms97#h_fast/* with filenames of the form *bms97#h_fast_<el><n>.dat.*

D.12 The first results of the high Z work are now being archived in ADAS. New *adf04/copmm#NN* collections of LS and IC coupled specific ion file are provided.
In this release we include:

adf04/copmm#42/ls#mo<N>.dat
adf04/copmm#42/ic#mo<N>.dat

More will follow in the next release.

D.13 On the *adf09* dielectronic recombination data, some reworking and replacement of data by Nigel has led to two author's initials appearing in two iso-electronic sequence directories. We have assigned new directories which reflect both author's initials. The corrections apply to some 2-2 parent transitions in *adf09/jc00#li/* and *adf09/jc00#be/*. The replacement directories are *adf09/nrbjc00#li/* and *adf09/nrbjc00#be/* and you will notice the nrb initial on some of the 2-2 members.

D.14 *adf09/oic00#c/* and *adf09/nrb00#*c/ have been merged into *adf09/oiznrb00#c/* but in this case there was no duplication and replacement of datasets.

HPS
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