mar18-02 **ADAS Bulletin**

In the light of changes, restrictions and possible removal of some legacy facilities in future IDL releases, we have been concerned to replace some of our older practices which now generate warnings. Ricky has worked through all the codes amending these items. To avoid any confusion with these changes and the large release of new codes which is now due, we are going to upgrade ADAS in two steps. With this bulletin, we are putting out ADAS release 2.5.5. It is the usual error correction release but including the IDL changes mentioned above. We shall give this release about 2-3 weeks to settle down and then issue the big new code upgrade. It will be version 2.6.1 and there will be a new version of the ADAS Manual to accompany it.

Corrections and additions to codes

C.1 The subroutine *cxpmat.for* in */…/idl_adas/fortran/adaslib/* had its variables declared in a non standard way which caused compilation problems with the *g77* compiler – corrected.

C.2 The modified comments in the *read_adf* routines have been regularised.

C.3 In *ml_gauss.for*, real*8 variables were used to index arrays. In the *mlfit* and *lsfun2* FPCOUNT and FPCOUNT2 have been set to integer. This has been corrected. Note that the variables were only used to index arrays and there appears to have been no actual computational errors ensuing.

C.4 On testing the 'absoft' compiler in the 'ansi standard f77' mode, the following items turned up and were corrected.

adas211 - replace all the routines as most of them had legacy listing information in columns 72—80 . Also, *bdcf4*, *gama6*, *phase*, *wig6j*, *zeff* and *zeffl* had the definition REAL FUNCTION zeff*8. These are changed to REAL*8 FUNCTION zeff etc. (see also C.6 below.

adas507 - *bwno* in *e7ispf.for* array is not used and it is an illegal sizeable variable in any case. This caused trouble with the 'absoft' compiler.

C.6 Note that the absoft f77 compiler does not like code beyond column 72. The -W switch can be used. If the -W option is used to avoid keeping the code within columns 7-72 all the old mainframe relic card numbering in columns 73-80 must be removed. The *adaslib* directory has been cleaned up in this manner.

C.7 In *adas211* the opportunity has been taken to rectify several features.

- the progress bar has been centred.
- space put before % completed figure.
- default output files are now *adas211_adf04.pass* and *adas211_adf08.pass* rather than *data04.pass* and *data08.pass*.
- junk at the end of lines in output files has been removed.
- automatically include name of producer.
- A more serious fix is that it now traps for transition energies larger than the ionisation potential. The code stops with a warning message rather than trying to continue.

C.8 Similarly, *adas212* also had a few annoying features.

- automatically include name of producer.
- replaced the drop down list of yes/no for adding DR to R lines with an exclusive button pair. This is more consistent with other ADAS codes
- the proper font size is now used in the progress bar widget and the message is centred the bar.

C.9 In *read_adf11.pro* the values of *iprt* and *igrd* must be passed as long integers to the *call_external* C routine. The conversion is now done automatically.

C.10 The comments in *adas603_get_hdlike.pro* were incorrect and have been updated. Also the variables passed to the C code are checked.

C.11 There was a syntax error in the *adas414* and *adas415* output routines. If menu button was pressed on these screens the programs would crash. All this was due to a missing apostrophe.

C.12 In *adas405* and *adas406* the hydrogen temperature and density can (legitimately) be zero which causes trouble if their logarithm is taken. This has been trapped. Note that there is no trap for electron temperature and density as these should be non-zero.

C.13 In *adas405* and *adas406* , the maximum Z has been increased to 82 to accommodate lead.

C.14 *adas407* has been altered to create *adf03* files from a directory of *adf04* files without the intervention of the user. When the program is launched a selection screen offering 'Automatic' or 'Interactive' use is displayed. Pressing 'Interactive' brings us into the old program. The new branch puts up a screen asking for *adf04* directory location, element and min/max ion stages, and the *adf03* and *paper.txt* output locations.
In order to make the minimum of changes there is a new fortran code associated with the automatic branch - *adas407_auto.for*. Therefore the compilation script has beem changed also. Note that an extra structure is stored in the defaults file which will necessitate deletion of any old ones.

C.15 Some more changes have been made to *read_adf04.pro*.
- add filename to structure which returns all info.
- properly calculate energy/kT for calculating Burgess x value.
- remove attempts to 'correct' configuration with *norm_config*.
- do not fail if collision strengths are 0.0 in *adf04* file.

Corrections and updates to data

D.1 Some discrepancies followed synchronising the new SCCS tagged central ADAS data with the collection at JET.
- *adf27/helike/mom93#fe* should be *adf27/helike/mom93#he*
- *adf21/bms93#a* directory has no meaning and is removed.

D.2 There is a more up to date version of Don Griffin's Li0 *adf04* file, namely,
/adf04/lilike/lilike_dcg01#li0.dat

D.3 The *belike adf09* files calculated by James Colgan, which were pulled at the last minute from the release 2.5.4 are now included, namely,
/adf09/jc00#be/….
Note the following:
There was a problem running the post processor on this sequence.
The LS differences are very small, so re-labelling will suffice.
In the IC case, the only significant differences appear to be on the bundled-n=4 and the bundled-nl=4l. The data for parents 1 and 2 has been wrongly binned, but the sum over the two parents looks o.k. Since Nigel Badnell is fairly sure of the scope of the inaccuracy of the adf09 file, it was decided to go with just patching rather than rerunning everything.

D.4 The helium-like *adf09* (and *adf27/adf28*) sets from Manuel Bautista are now available, namely,
/adf09/mb00#he/…
/adf27/helike/mb00#he/…
/adf28/helike/mb00#he/…

D.5 There has been a correction to neutral hydrogen *adf04* file. See corrigendum in J Phys B – in press.
/adf04/hlike/hlike_ha00#h0ls.dat

D.6 Revised *adf04* files for neutral helium have been placed as follow:

- */…/adas/adas/adf04/helike/helike_hps02he_t1.dat* type 1 file

- */…/adas/adas/adf04/helike/helike_hpsl02he.dat*	type 3 file, low temperature set
- */…/adas/adas/adf04/helike/helike_hpsh02he.dat*	type 3 file, high temperature set
- */…/adas/adas/adf04/helike/helike_hps02he.dat*	type 3 file, standard temperature set

Note that these new data sets originate from reappraisal of electron impact excitation and ionisation cross-section data up to 2002. See the */adas_excel/he0_electron_impact_xsects/* spreadsheet directory for more information (released only on request). The original preferred data are combined to make up an *adf04 – type 1* file. The conversion to a Maxwellian averaged *adf04 – type 3* file is done by the code *adas809.for*. This will be made generally available in ADAS release 2.6.1.

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