Mar18-01

ADAS Bulletin

This is the first of our regular four monthly bug *ADAS code and data error & minor adjustment releases* or 'bug releases' for short. This was signalled in the last bulletin and we are now putting it into effect. I have written a more complete document about our ADAS Code and Data Practice which appears at the end of this bulletin. Note that the 'bug releases' will occur every four months. Issue of substantial new codes will be done in separate ADAS releases as and when they are ready. We are working on such an issue covering the satellite line modelling problem which we expect to be ready in about two months (Allan Whiteford and Ricky Martin are leading on this one). However the next 'bug release' will be on 18 July 2001.

It has been a very busy period, this last six months, but I think very successful. Firstly there has been the developments at JET and the opportunity for the ADAS Project to be directly involved in experiments in the C3 and C4 campaigns. We had two diagnostic experiments, D1.2 and D1.1 concerned with spectral signatures of heavy metals and mixed helium/deuterium beam injection. The first links to the heavy species plan which we adopted at the last workshop and the latter to the critical need to cross-calibrate helium beam emission and stopping against that for the better known deuterium case. It was touch and go for D1.1. Pini 6 on Octant 8 was modified for up to ~10% helium mixture at Christmas, but commissioning it and a getting a test for our experiment was achieved only the day before our session. We made the measurements successfully just two weeks ago, obtaining matching helium singlet and triplet and deuterium Balmer alpha beam emission spectra across the plasma radius at two zeffs. We are very grateful to Michael Proschek and Martin O'Mullane who were science coordinators, Mathias Brix, Klaus-Dieter Zastrow who was session leader and of course to Hans Falter and the Austrian Association who made it possible. We do now have a lot of analysis to do however. Also we have a further experiment session on 19 March to calibrate the charge exchange spectroscopy aspect of the helium beam as driver.

I can also report progress on the heavy element plan. The D1.2 experiment gave us spectral signatures for a variety of long second period heavy metals (hafnium, tantalum, tungsten, lead) in the core plasma, injected by laser ablation. Such data is essential I believe to enable us to tie down the very theoretical effort which we must make for the radiating properties of heavy species. On the theoretical side there is also progress. We have managed to win a large grant for a powerful new parallel computer system which we shall commission at Strathclyde in the next few months. Part of its time is dedicated to heavy element calculations. I have been working on a very detailed and complex plan to achieve our intentions from the workshop over a period of about four years. I shall circulate the plan to everyone soon – hoping to solicit offers to help in the calculations.

An important note before I go into the details of the current corrections. The ADAS Workshop this year is again at Ross Priory in Scotland from Sun. 30 Sept. 2001 to Tues. 2 Oct. 2001. Please mark it in your diaries. Mrs McVarish will send round initial registration forms in a week or so.

Corrections to codes

Martin has prepared the list which is as follows: (his words)

- C.1 Typo in adas801_rcn2_make.pro which only shows up when on parity is selected. Minor changes in the postprocessor ifg to account for the single parity case. Change in ifgpp to setup the extra output option of collision strengths rather than effective collision strengths.
- C.2 Minor updates to adas807 codes to make them work with neon.
- C.3 Added check to b8getp.for for expansion data which did not have any weighting factors.
- C.4 Added cxqcx.for routine to adas3xx/adaslib for accessing, and interpolating onto a requested energy range, the charge exchange cross section data in adf01 files.
- C.5 Missing comma in cdout0.for in ADAS313 causes problems with the pgf77 compiler.
- C.6 In both ml_gauss.for (ADAS602) and ml_gauss603.for the getavwdth and getheights routines declare the type of the size of the input adjustable array before the array declaration. Swap statements such that integers are defined before real*8s.
- C.7 A new read_adf01 routine is available; read_adf11 updated to access partial adf11 files as well as returning a 2D array of coefficients from the Te and ne vectors; a new read_adf08 routine;

provision of a read_adf22 routine; the processing is done with read_adf21 but this is a wrapper to provide consistent naming. Full instructions in comment section of the file header.

- C.8 New makelib3 (cxqcx.for added) and makelib5 (cut out fortran<->IDL routines, leaving the useful ones. Also remove the couple of test programs).
- C.9 A new departure run_adas405.pro is a way of generating an ionisation balance in IDL by running ADAS405 without the ADAS environment. See header for instructions.
- C.10 Error in logic in ADAS105, a5ispf.for. The subroutine used the wrong variable to gather data from IDL.
- C.11 Series 8 menu item had a misspelling of Calculation!
- C.12 Occasional problems in splining S-lines. At low Te the S value can become large (which is reduced by multiplying by exp(-E/T) which gives incorrect values for interpolated values. Correct by excluding S values GT 1.0.
- C.13 Spurious number in first column of comment block in ssxb.for has been removed. The compiler complained!
- C.14 Error in logic reading number of metastables in resolved datasets in dxrdnm.for. This error only shows up for Z GE 10.
- C.15 The incorrect adf number was used for ADAS415 adf35 is the filter functions but the code looked in adf34.
- C.16 ADAS507 has an entry in the main series 5 menu but there is no code! It is on the mainframe and it took ~2 hours to port so I have added it and the associated modifications to localize.pro and adas.pro. This came to my attention at KTH where I was asked about the passing files from 405 and 406. It was not obvious what Goft and Gcf referred to. I have changed the labels to GCF : G(Te) in both and the default passing file name to adas40X_adf16.pass (X = 5 or 6). Also the font was not set in the mass text edit widgets in 406. I have also added a warning in adas.pro if ADAS is launched under IDL v5.3.
- C.17 ADAS603 fails at JET for some cases because of an undefined base in cw_adas603_proc.pro.
- C.18 The IDL access routines read_adf13 and read_adf15 have been updated to remove the limit on the number of Te/dens pairs, to return a 2D (te,dens) array if /all is specified and to permit the input temperatures to be given in K using the /kelvin switch. The unlimited Te and kelvin options have been added to read_adf07 also.
- C.19 Some changes to ADAS208: A temporary IDL read_adf04.pro routine which should be replaced by something better later: run_adas208.pro for batch operations, much like the run_adas405 script -NOT included yet: More extensive changes to include selection of which PECs and SXBs to be written will come later: User interface changes are part of the above updates but will need more extensive testing before release.

ADAS Code and Data Practice

Hugh P. Summers

Following discussion at the ADAS 2000 Workshop, Ross Priory, some alterations are being made in the way ADAS code and data are handled and released. The opportunity is being taken in this information circular to define afresh our standard practice. The need for some change is driven by a number of issues. Firstly, the developmental aspect of ADAS has continued very strongly over recent years with quite elaborate and sophisticated new codes being added at intervals to the program suite. These new codes have been issued with a normal release. However late errors with such codes tend to show themselves once we mount them on the full range of UNIX platforms within the consortium. This has frequently lead to significant delay in a release. We wish to de-couple error fix and minor code upgrades from major new code release so that error corrections are done reasonable expeditiously. Secondly, the ADAS databases are now becoming very large and we have had continuing anxieties about maintaining the data integrity, distinguishing new data from minor data revision and about clarity on preferred data. Data control in the manner of code control via SCCS is overdue and we are now implementing this. Finally, code development is a shared activity amongst the ADAS Project members and we wish to reiterate preferred practice here so that the code integrity and universality is maintained.

1 <u>Codes:</u>

- 1.2 *Code archiving and control:* SCCS will continue to the code control and archiving system for ADAS Ricky Martin will be the sole responsible person for the master files and code entry and update in SCCS.
- 1.3 *Code development procedures:* The following defines the correct procedure for a person working on an ADAS code development.
 - 1.3.1 Verify that all reported errors are implemented in the SCCS archives This inquiry should be addressed to Ricky and is necessitated by the delay of at most four months between an error report/local bug fix to final incorporation in the SCCS archives.
 - 1.3.2 Notification to Ricky of the intended development so that he can prevent development clashes with others.
 - 1.3.3 Extraction by Ricky of all required codes and subroutines from the SCCS archive to the developer.
 - 1.3.4 Dispatch of revised codes to Ricky by the developer.
 - 1.3.5 Verification on all ADAS UNIX platforms by Ricky and implementation of any compatibility modifications by him.
 - 1.3.6 Re-check of the adjusted code by the developer.
 - 1.3.7 Entry of the final code into the master files and SCCS archives by Ricky.
 - 1.3.8 <u>Deletion</u> of the developer's personal version of the code.

The final step 1.3.8 is essential and it is failure to do this which has led to most confusion and error in new codes. The SCCS archive becomes the sole code. The developer must draw afresh from the SCCS archive as above if he/she plans any further development.

2 Data:

- 2.1. *Data archiving and control:* SCCS will be used for data archiving. Other possibilities such as CVS were reviewed by Ricky, but the conclusion is that SCCS is most straightforward and suited to the ADAS needs. Ricky will be the sole responsible person for ADAS data entry and update in SCCS.
 - 2.1.1. The complete ADAS database has been converted to SCCS, organized by *adf* number. The SCCS version number information is placed in a 'C-----' delimited area at the bottom of the comment region at the end of each data set. The SCCS data archive has been held in a test area on the ADAS system at Strathclyde.
 - 2.1.2. A validation period of four months was allocated to the new SCCS data archive. The main issue was to check whether any access subroutines are affected by the position of the version details and to make any required corrections. I trust we have now caught all the difficulties

2.1.3. The SCCS archived database version now becomes the standard release at this release 2.5.2.

- 3. Code & Data releases:
 - 3.1. ADAS code and data error & minor adjustment releases: These will take place every four months. The incremental release numbering system is of the form 'N.L.M'. The primary number 'N' (currently 2) is incremented when a new ADAS series is introduced. The secondary number 'L' (currently 4) is incremented when a significant developmental update of codes or data is included. The tertiary number 'M' is incremented with each four monthly error/minor adjustment release. This ADAS release, which is primarily corrections and modest adjustments is therefore 2.5.2.
 - 3.2. *Error notification and correction:* The following procedures will be followed in the future:
 - 3.2.1. Notify Ricky Martin (martin@phys.strath.ac.uk) or Martin O'Mullane (martin.omullane@jet.uk) of any error. A correction will be worked on by Ricky and/or Martin and rectified at the notifying site. The solution is passed to Ricky.
 - 3.2.2. Ricky will incorporate the error correction in the master files and will issue a general email message of the form '<u>ADAS code error notification</u>' or '<u>ADAS data error notification</u>' to the ADAS user list.
 - 3.2.3. The error notification messages will be accumulated and be presented again at the four monthly release in a brief error/bug fix bulletin.
 - 3.2.4. Note that rectification will take place at the notifying site immediately, but not at other sites until the next release. Immediate update can be done at any site which wishes it. This will be only in response to a request from the site for immediate update following the error notification message.
 - 3.3. ADAS development releases:
 - 3.3.1. Such releases will take place intermittently as and when the development is completed.
 - 3.3.2. Development releases will be accompanied by an update of the IDL-ADAS User manual and a full release bulletin. The later will describe in some detail the operation of any new/updated code and/or the nature of any new data.
- 4. Scan libraries:
 - 4.1. The scannable libraries of ADAS FORTRAN, C and IDL sub-routines for incorporation in users' personal programs are being moved to a */lib* directory at the top level of the ADAS files space, that is to '/.../adas/lib/'.
 - 4.2. New subroutines from ADAS co-workers for incorporation in the ADAS scan libraries should be submitted to Ricky and should include demonstration code.

5. Documentation:

- 5.1. The IDL-ADAS manual is to be converted from Microsoft Word to LATEX as soon as possible. A converter is under test. It would be helpful if designers of new codes for ADAS would also take responsibility for providing an adequate descriptive text for entry in the IDL-ADAS User manual. Items for incorporation in the manual, prepared in LATEX, should be sent to Hugh Summers.
- 5.2. The specification of scannable library subroutines in the IDL-ADAS manual will be extended with the inclusion of some sample test code where appropriate. This is an on-going task.
- 5.3. Information on ADAS preferred data and selection from the sometimes many choices of data set remains a problem. The placing of the ADAS data under SCCS control will reduce the proliferation of data sets which have modest changes one to another. The organization of the 'datastatus' document is being re-examined. This is both with a view to making preferred data more prominent within it and possibly relocating and renaming the document so that it is more obvious to users.

H. P. Summers 18 Mar. 2001