Tutorial session 2 examples

1. ADF04

1.1. Explore the /.../adas/adas/adf04 database. Note that a summary of the data base is given in the ADAS User manual *appxa-04.pdf*.

2. ADAS201 Test Case

- 2.1. Move to your sub-directory /.../<uid>/adas/pass. Graph and text hardcopy will consequently appear here. Start ADAS [type adas] and go to the ADAS2 series sub-menu. Start ADAS201
- 2.2. Click on *Central Data*, the data root to data class ADF04 should appear dimmed in the window above. Click on the directory name *adas*#7 in the datafile list window. Note the designations. The 'ic' denotes J-resolved intermediate coupling system. 'ls' denotes a term resolution system. The 'n' case is a special bundled –n system for the hydrogen-like ion. The degeneracy ensures very strong mixing by ion collisions which can be assumed complete.
- 2.3. Select *cop98#7_ic#n3.dat*. Click the *Browse comments* button. Information on the content and quality of the data set can be reviewed.. Click *Done* to restore the Input window. Click *Done* and the ADA201 Processing window appears.
- 2.4. You may select to have a polynomial fit by clicking *Fit polynomial* button, and selecting a accuarcy (%) in the adjacent active editable box..
- 2.5. Activate the *Select Temperatures for output file* button to obtain a numerical tabulation of results. Either edit in the temperatures you wish or click the *Default Temperatures Values* button.
- 2.6. Click on the *Done* button to proceed to the Output options window and *Graphical Output*.
- 2.7. Select Post-Script and Enable Hard Copy and assign an output graph file.
- 2.8. Click on the button for *Text Output*. And route output to *paper.txt*, the standard text output File Name. Then click *Done*.
- 2.9. The graph appears in the next window. Click on *Print* to send a copy of the graph file. Click *Done* to return to the Output Options window. Click on *the Exit to Menu* icon at the bottom left corner to restore the ADAS5 series menu. *paper.txt* is not viewable with an editor until you exit.
- 2.10. You may wish to examine the *paper.txt* file to see its format.

3. Additional exercise

3.1. Restart ADAS201 and again select the adas#7 sub-directory. Select the *cop98#7_ls#n3.dat* file. Browse the comments. Note that this file is obtained by bundling the level resolved 'ic' file you fist chose into terms. This procedure you will observe in the comments was done by ADAS209. You may wish to try ADAS209. The operation is described in the ADAS User manual Chap3-09.

4. ADAS811 Test case

- 4.1. ADAS811 is a new and more sophisticated interrogation code on ADF04 files. It allows not only display of single collision rates but comparison of such data from different ADF04 files. [Note this code uses the configuration information and quantum numbers to match transitions between different files. If you use a non-standard (that is not *ADAS Standard* or *Eissner*) form, the code will fail to match it is quite sensitive.
- 4.2. For this test we shall compare a high grade assessed boron-like ion of oxygen (adas#8/cop98#8_ls#o3.dat with a much older impact parameter cross-section based data set (copss#b/copss#b ss#o3l.dat) built on a SUPERSTRUCTURE calculation.
- 4.3. Select the first data set in the in the upper part of the Input window. The second data set is selected in the lower part and uses a more standard Unix file selection so that files can be tested during construction when not located in your ADAS space. You can choose a third file if you wish (e.g. the Born baseline *copmm#8/ls#o3.dat*).
- 4.4. There is only a further display screen which incorporates selection and controls. At this stage we are only concerned with electron impact excitation data. This is the default *e-exc* in the Type of Plot. The Type of e-exc plot is selectable. Note the usual Upsilon (gamma) and excitation rate coefficient, but also the Burgess C-plot.

- 4.5. At the top of the window, select the file whose transitions youn wish to step through. The code will attempt to match transitions from the other file to it which may nit be successful indeed the transition may not exist in the other files.
- 4.6. Note the tape recorder controls at the bottom. The upper and lower indices of a particular transition may be entered in the editable boxes. Then click *Show*.
- 4.7. We find it convenient to have the files open in an editor as we do the examination.
- 4.8. Note the cursor is active for reading of values.
- 4.9. *Print* will send the displayed transition to a file (via a pop-up dialogue). Be cautious of using the *Print All* button there may be a lot of electron impact excitation transitions.

5. ADAS205 Test Case

- 5.1. Move to your sub-directory /.../<uid>/adas/pass. ADAS205.
- 5.2. Click on Central Data. Select the Be-like oxygen case adas#8/cop98#8 ls#o4.dat.
- 5.3. Click on the *Default Temperatures button* and *Default Densities* button.
- 5.4. Click on the *Selections* button for metastable states. A pop-up list of all the levels appears. Click on the button beside the first level. Note that it darkens. It is a click on/click off button. Then click on its *Done* button to restore the full Processing options window.
- 5.5. Click on the *Done* button to proceed to the Output options window.
- 5.6. Click on the button for *Graphics* to display the graphics choices then click on the button for *Graphical Output*. Select *Graph Temperature* by clicking on the one you wish in the list. Choose the fifth one [1e5]. Click on the *Text* button to display the output data set choices. Click on the *Contour File* button and enter *contour.pass* in the File Name editable window. Then click *Done*. The graph pops up. There are several graphs to look at. Finally click *Done* to restore the Output options window. Click the *Exit to Menu* icon to finish up. Finally click on the *Exit* button on the sub-menu and main menu windows to exit ADAS.
- 5.7. Note the files created includes the collection file *contour.pass*. You may wish look at its format.

6. ADAS207 Test Case

- 6.1. Move to your sub-directory /.../<uid>/adas/pass. Make sure you have a contour.pass file there. Start ADAS and go to the ADAS2 series sub-menu. Click with the mouse on the seventh button in adas2 series for ADAS207. The Input window for ADAS207 pops up.
- 6.2. Click on *User Data*, the data root to you /pass sub-directory should appear in the window alongside. Click on *contour.pass* in the file list window. It appears in the selection window.
- 6.3. Click *Done* and the ADAS207 Processing window appears.
- 6.4. Click on the *Selections* button for the 1st composite line assembly. The window with the full list of lines pops up. Click on the buttons alongside the lines you wish for the numerator of the line ratio. These are on/off buttons. Note a button is darkened when activated and the program remembers the choice you made if you have had a previous run. Select transition 2 for the test. Click the *Done* button.
- 6.5. Click on the *Selections* button for the 2nd composite line assembly. The window with the full list of lines pops up. Click on the buttons alongside the lines you wish for the numerator of the line ratio. Select transition 26 for the test. Click the *Done* button.
- 6.6. Click on the *Done* button to proceed to the Output options window.
- 6.7. Click on the button for *Graphical Output*. Click on the *Diagnostic Contour Plot* button. This brings up contour plot choices. Click on the *Default Contour Scaling* button if not already selected. Then click *Done*. The graph pops up.
- 6.8. An object of such a plot is to detect diagnostic line ratios, that is ratios senitive to density or temperature. Note that the contour plot gives an overview but is coarse.

Example 7

6.9. Experiment with the same data set in ADAS205 but edit in a relevant range of electron temperatures and densities for the density sensitive region. Proceed to form the *contour.pass* file. Now run ADAS207 with this *contour.pass* file. Try adding more lines to the two composites or changing the lines.

Example 8

- 6.10. Repeat the above but at the metastable selection in the ADAS205 Processing options window, select the first and second levels. Follow through the consequences to ADAS207. Remember to obtain a contour output file from ADAS205.
- 6.11. Note that with two metastables, we have the opportunity to shift their relative number densities from that in equilibrium. Generally a dynamic ionisation balance provides this, but note that disequilibrium can confuse an apparent density sensitivity.