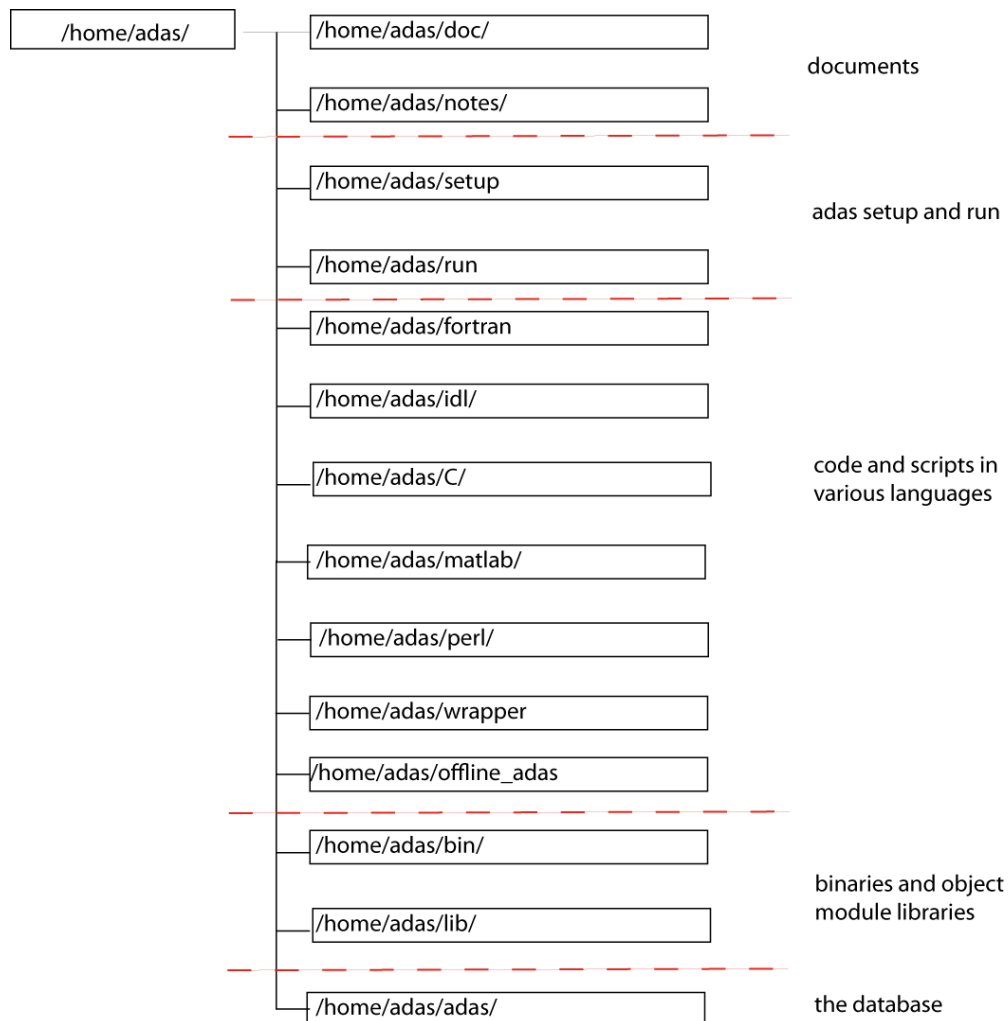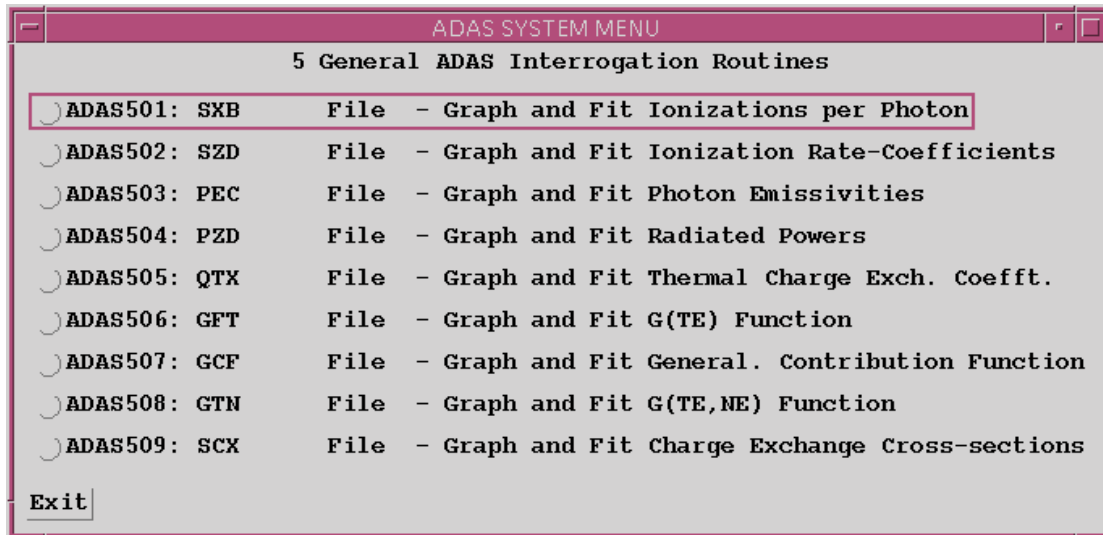# Lecture 1b   Computational overview of ADAS

The ADAS suite comprises mainly IDL and FORTRAN code and runs under UNIX. Tested systems include Solaris, DEC, HP, AIX and Linux. Pre-requisites for an installation of ADAS are ~ 5.0Gb disk space; F77 and C compilers; IDL (fully licensed – ADAS will not run in IDL demo mode); a PDF viewer such as Acrobat reader. Installation is carried out and managed by the ADAS manager (Dr. Allan Whiteford). ADAS is usually installed in the */home* directory of an account with user name '*adas*'.

The ADAS distribution has the directory structure shown below.

/home/adas/	
/home/adas/doc/	documents
/home/adas/notes/	
/home/adas/setup	adas setup and run
/home/adas/run	
/home/adas/fortran	
/home/adas/idl/	
/home/adas/C/	code and scripts in various languages
/home/adas/matlab/	
/home/adas/perl/	
/home/adas/wrapper	
/home/adas/offline_adas	
/home/adas/bin/	binaries and object module libraries
/home/adas/lib/	
/home/adas/adas/	the database

The interactive ADAS suite comprises in the region of 85 programs. They are arranged in 8 series reflecting distinct regions of atomic physics purpose. The menu selection for series 5 is shown below.

```
┌─────────────────────────────────────────────────────────────────────┐
│ ─                      ADAS SYSTEM MENU                        ▪ □   │
├─────────────────────────────────────────────────────────────────────┤
│              5 General ADAS Interrogation Routines                   │
│ ┌─────────────────────────────────────────────────────────────────┐ │
│ │○ ADAS501: SXB     File  - Graph and Fit Ionizations per Photon  │ │
│ └─────────────────────────────────────────────────────────────────┘ │
│  ○ ADAS502: SZD     File  - Graph and Fit Ionization Rate-Coefficients │
│  ○ ADAS503: PEC     File  - Graph and Fit Photon Emissivities        │
│  ○ ADAS504: PZD     File  - Graph and Fit Radiated Powers            │
│  ○ ADAS505: QTX     File  - Graph and Fit Thermal Charge Exch. Coefft. │
│  ○ ADAS506: GFT     File  - Graph and Fit G(TE) Function             │
│  ○ ADAS507: GCF     File  - Graph and Fit General. Contribution Function │
│  ○ ADAS508: GTN     File  - Graph and Fit G(TE,NE) Function          │
│  ○ ADAS509: SCX     File  - Graph and Fit Charge Exchange Cross-sections │
│                                                                       │
│ ┌────┐                                                                │
│ │Exit│                                                                │
│ └────┘                                                                │
└─────────────────────────────────────────────────────────────────────┘
```

The IDL, FORTRAN, C and MATLAB codes and associated sub-routines (>1000) are organized hierarchically according to series and maintained under CVS. /adaslib subdirectories contain subroutines common to codes at their hierarchical level. Series 1 code subroutines names commence with the letter 'a' followed by the numerical (hexadecimal) value of the particular code. The structure is shown below in the FORTRAN case.

. . .

Note the sub-directories of the top level /fortran/adaslib/ subdirectory according to sub-routine character. Also note the /xxdata/ subdirectory which contains important sub-routines for getting data from the ADAS database int your own FORTRAN programs. The /idl/ subdirectory structure is similar, but note some extras in the top level /idl/adaslib/ sub-directory. There are subdirectories for graphical user interface procedures and read_adf and write_adf procedures which you will find useful. Source IDL code is open, but FORTRAN code is restricted. FORTRAN shared object module libraries are available to user codes.
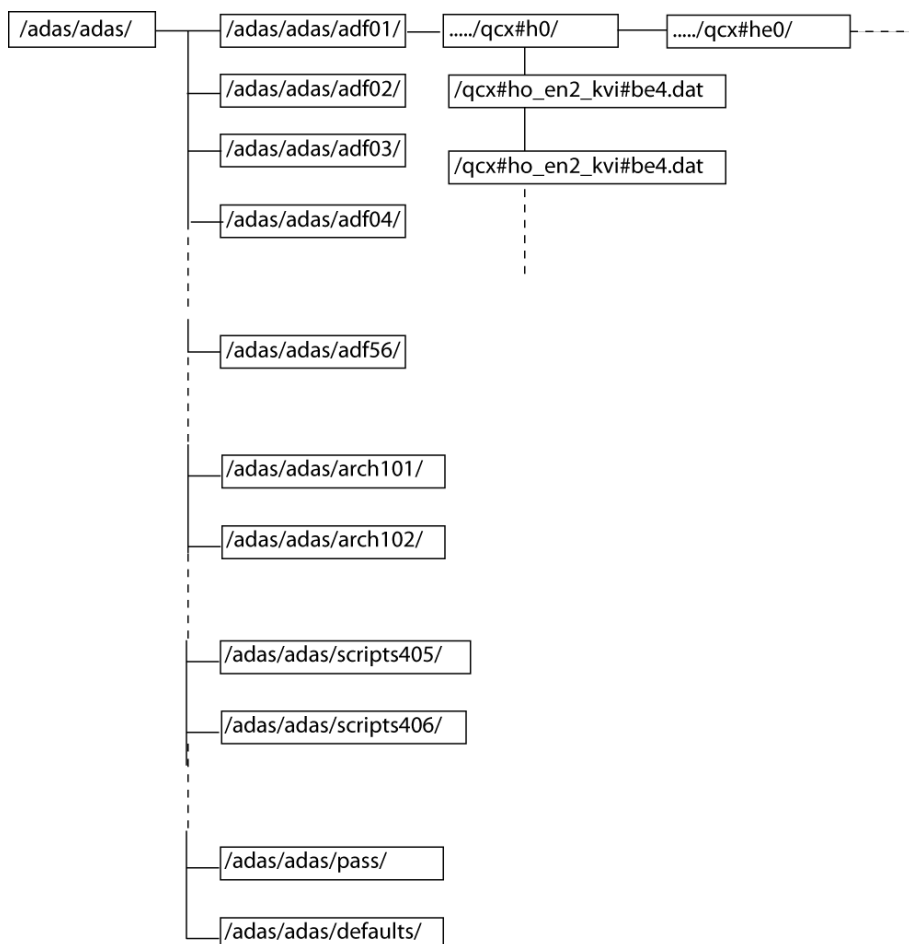
ADAS data

The subdirectory */home/adas/adas/* contains the central ADAS data archive. In also includes sub-directories */pass* of 'passing files' and */defaults* of 'defaults' files for use by the user *adas* in testing the distribution. The latter two file categories are also required in each individual ADAS user's file space. The primary data themselves are stored in sub-directories according to ADAS data format number, e.g. *adf04*. There are currently 56 data formats whose layout and organization is precisely specified. These are listed below. It is recommended that each user sets up a personal data space as /home/<uid>/adas/ which parallels the central ADAS structure. ADAS codes are designed to go automatically to the correct ADAS data format either in the central or user space.

adf01	bundle-n and bundle-nl charge exchange cross-sections
adf02	ion impact cross-sections with named participant
adf03	recombination, ionisation and power parameter sets
adf04	resolved specific ion data collections
adf05	general z excitation data collections
adf06	general z recombination/ionisation data collections
adf07	direct resolved electron impact ionisation coefficients
adf08	direct resolved radiative recombination coefficients
adf09	direct resolved dielectronic recombination coefficients
adf10	iso-electronic master files
adf11	iso-nuclear master files
adf12	charge exchange effective emission coefficients
adf13	ionisation per photon coefficients
adf14	thermal charge exchange coefficients
adf15	photon emissivity coefficients
adf16	generalised contribution functions
adf17	condensed projection coefficients
adf18	cross-referencing data
adf19	zero-density radiative power data
adf20	G(Te) functions
adf21	effective beam stopping coefficients
adf22	effective beam emission coefficients
adf23	state selective electron impact ionisation coefficients
adf24	state selective charge transfer cross-sections
adf25	driver data-sets for ADAS204 calculation
adf26	bundle-n populations of excited states in beams
adf27	driver data-sets for ADAS701 calculations
adf28	driver data-sets for ADAS702 post-processing
adf29	driver data sets for ADAS707 calculation
adf30	driver data-sets for ADAS708 post-processing
adf31	feature files for satellite line spectral simulation
adf32	driver data-sets for ADAS802 calculations
adf33	driver data-sets for ADAS803 postprocessing
adf34	driver data-sets for ADAS801 calculations
adf35	spectral filter data
adf36	feature files for series limit spectral simulation
adf37	non-Maxwellian distribution function files
adf38	Seaton - opacity photo-excitation
adf39	Seaton - opacity - photo-ionisation

adf40	envelope feature photon emissivity coefficients
adf41	driver data-sets for offline ADAS8#1 calculations
adf42	driver data-sets for ADAS810 calculations
adf43	GTN photon emissivity functions
adf44	F_GTN envelope feature emissivity functions
adf45	feature files for continuum emission
adf46	BBGP driver datasets for dielectronic recombination
adf47	-
adf48	direct resolved radiative recombination coefficients
adf49	universal z-scaled CXS n and nl resolved xsects
adf50	-
adf51	-
adf52	-
adf53	-
adf54	promotion rules - structure
adf55	promotion rules – dielectronic recombination
adf56	promotion rules - ionisation

Further layers of sub-directories are assigned as necessary for different species etc. The sub-directory and final data set naming is designed to give some indication of content. The final data sets themselves are all ascii and have the extension *.dat*. The figure below shows the layout.

For central ADAS, sub-directories, *arch101*,…, *scripts405*, … contain only samples. Such data is normally personal to a user.

ADAS documentation

ADAS documentation is now most easily accessed via the web pages from www.adas.ac.uk and on through OPEN-ADAS. The documentation is also present on every ADAS sites in PDF format so is available for viewing electronically and for printing. It is placed in the */.../adas/doc/* directory under several headings. A schematic is shown below.

```
/adas/doc/
                          /doc/bulletin/
                          /doc/manual/
                          /doc/datastatus/

                          /doc/usernotes/
                        /doc/adas-and-atomic-calculations-course/
                      /doc/adopted_laboratory_wavelengths/
```
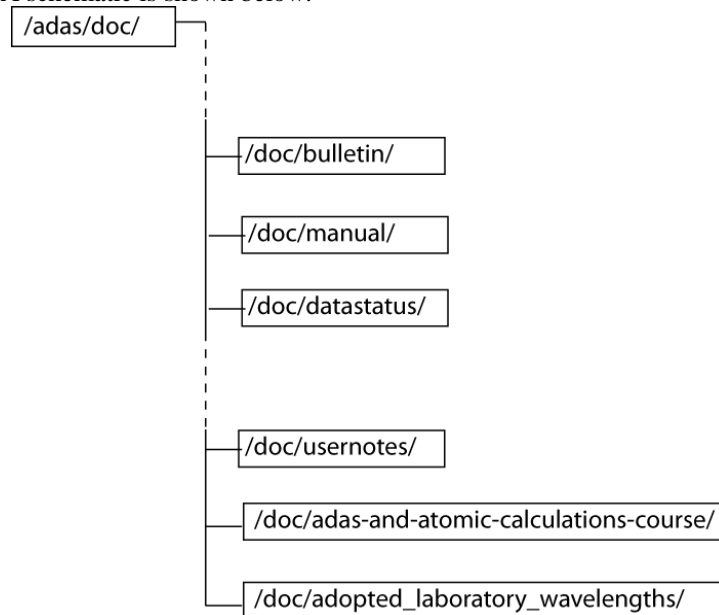
The principal Unix-IDL-ADAS manual is comprehensive, organised in chapters and sub-chapters connected to the ADAS series and named as */.../adas/doc/manual/chap\<i\>-\<nn\>.pdf* where \<i\> denotes chapter and \<nn\> denotes the sub-chapter number. It is unfortunately a bit out-of-date now. There are major appendices, in particular appendix B contains full descriptors and current states of the ADAS data formats. Bulletins are currently issued about once per year and are named according to date of issue. They contain information of bug fixes, new data and descriptions of newly added codes.

There are a number of shorter special manuals, which describe particular types of activity within ADAS, such as charge exchange spectroscopy or influx spectroscopy. These are also a bit out of date now. They include

flx-manual	influx spectroscopy
bms-manual	beam emission spectroscopy
cxs-manual	charge exchange spectroscopy
ion1-manual	basic ionisation balance studies
ion2-manual	advanced ionisation balance studies
opac-manual	opacity studies
spec-manual	spectral analysis
cds-manual	atomic modelling for solar analysis

The content of the Datastatus documents, named as */.../adas/doc/datastatus/adf\<nn\>.pdf* where \<nn\> is an ADAS data format number, are now present in appendix B of the main user manual. There may be additional files such as data reviews conducted by ADAS participants.

A substantial number of ADAS tutorials have been presented at laboratories in Europe and the USA. The tutorials are named as */.../adas/doc/\<lab\>\<yr\>-tut/\<section\>.pdf* where \<lab\> is a mnemonic for a laboratory and \<yr\> is a two digit year number. They are divided into sections in which a sub-area is summarised with viewgraphs followed by simple learning exercises with ADAS.
Some of these older tutorial files are 'postscript' .

Initial ADAS user set-up

There are a number of steps which a user must take in order to prepare his/her environment for ADAS properly.

A directory called 'adas' must be created in the user's home directory as */home/<uid>/adas/*. A setup script should then be executed from the newly created directory. The appropriate setup script for a user's site can be found in the central ADAS file space. The steps at Strathclyde are

        cd adas
        ./adas_strathclyde.csh

The setup script (a) creates sub-directories with in the user's *adas/* directory space; (b) adds entries to the user's *.cshrc* or *.profile* files to set up the user's environment for IDL and ADAS; (c) sets the user's ADASUSER environment variable which is the pathway to the newly created user's *adas/* directory.

Important directories are

        adas/defaults/ - directory where the user defaults for each ADAS program are stored. The defaults file for an ADAS series code remembers the user entries at the last run of the code.
        adas/pass /   -directory for storing output files from ADAS codes, called 'passing files'.

There a number of important entries in the *.cshrc* file. Values at Strathclyde are

      setenv ADASUSER /home/<uid>/adas
      source /packages/rsi/idl/bin/idl_setup   sets up default IDL path
      source /packages/adas/idl_adas/adas_setup   amends IDL-PATH for ADAS
                                         defines ADASCENT – path to central ADAS archive
                                         defines ADASFORT – path to FORTRAN executable

Working with interactive ADAS widgets

A number of IDL screens are common to many of the separate ADAS codes in the interactive series. These include the file selection screen on input, the table editor screen used for entry of user values for parameters, graphical input of user data pairs, screens for graphical output, graph display adjustment and graph retention. Code ADAS501 uses these screens and is suitable for practice . The following sub-sections summarize the main features and how to work with these screens. Programs of series 5 make use of data from archived ADAS datasets and initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output. Start ADAS501 from the interactive ADAS menus

File selection

The first window has the appearance shown below

1. Data root shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Note that each type of data is stored according to its ADAS data format (*adf* number). Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas,* to use this facility.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

3. Available sub-directories are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
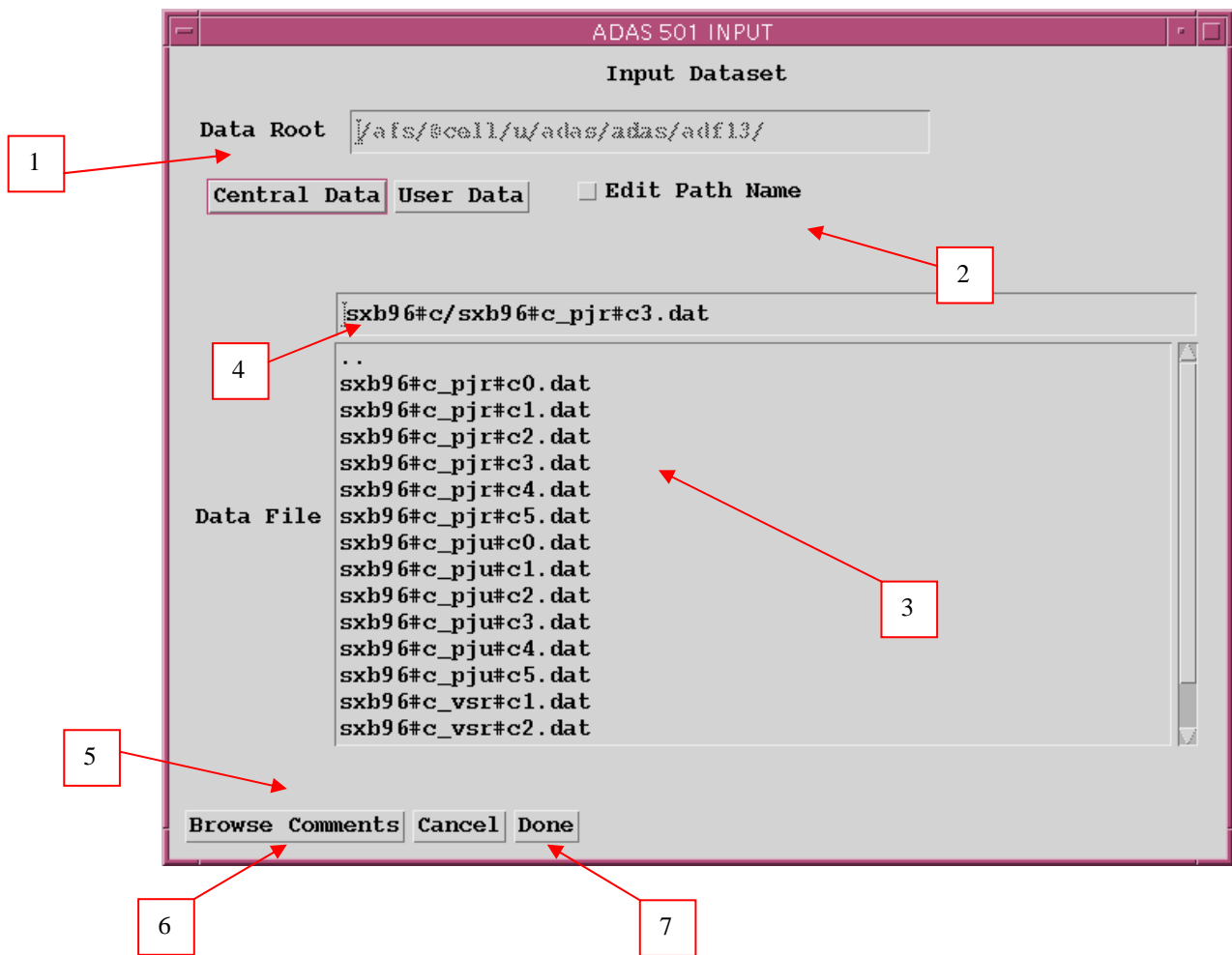
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

Processing options

The next window is called the processing options screen and has the appearance shown below
1. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being analysed is also shown. The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.

2. The output data extracted from the datafile, in the case of ADAS501, an 'emissivity coefficient', may be fitted with a polynomial. This is as a function of temperature. Clicking the *Fit polynomial* button activates this. The accuracy of the fitting required may be specified in the editable box. The value in the box is editable only if the *Fit Polynomial* button is active.

3. Spectrum lines for which emissivity coefficients are available in the data set are displayed in the line list display window. This is a scrollable window using the scroll bar to the right of the window. Click anywhere on the row for a line to select it. The selected line appears in the selection window just above the line list display window.

4. Your settings of electron temperature/electron density pairs (outputs) are shown in the temperature/density display window. The temperature and density values at which the emissivity coefficients are stored in the datafile (inputs) are also shown for information. **Note that you must give temperature/density pairs, ie. the same number of each as for a model.** The underlying datafile has a two-dimensional storage as a function of temperature <u>and</u> density.

5. The program recovers the output temperature/density pairs you used when last executing the program. Pressing the *Default Te* or *Default Ne* buttons insert a default set of temperatures or densities equal to the input values. A choice of particular density or particular temperature respectively from the input sets is allowed on a 'pop-up' window.
6. The Temperature & Density Values are editable. Click on the *Edit Table* button if you wish to change the values. A 'drop-down' window, the ADAS Table Editor window, appears as shown below:
7. ADAS501 has a more sophisticated graphical method for Te/Ne pair selection. Activate the *Value Selection by Display* button. The detailed operation of the widget is described in Chap1-00 of this user manual.

Output options

The **third window** is called the output options window and has the appearance shown below
1. As in the previous window, the full pathway to the file being analysed is shown for information. Also the *Browse comments* button is available.
2. Graphical display is activated by the *Graphical Output* button. This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.
3. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

4. Hard copy is activated by the *Enable Hard Copy* button. The File name box then becomes editable. If the output graphic file already exits and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
5. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
6. The *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt'may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
7. The graph is displayed in a following **Graphical Output** window described below.

Graphical output

The final graph display window has some additional controls
1. Printing of the currently displayed graph is activated by the *Print* button.
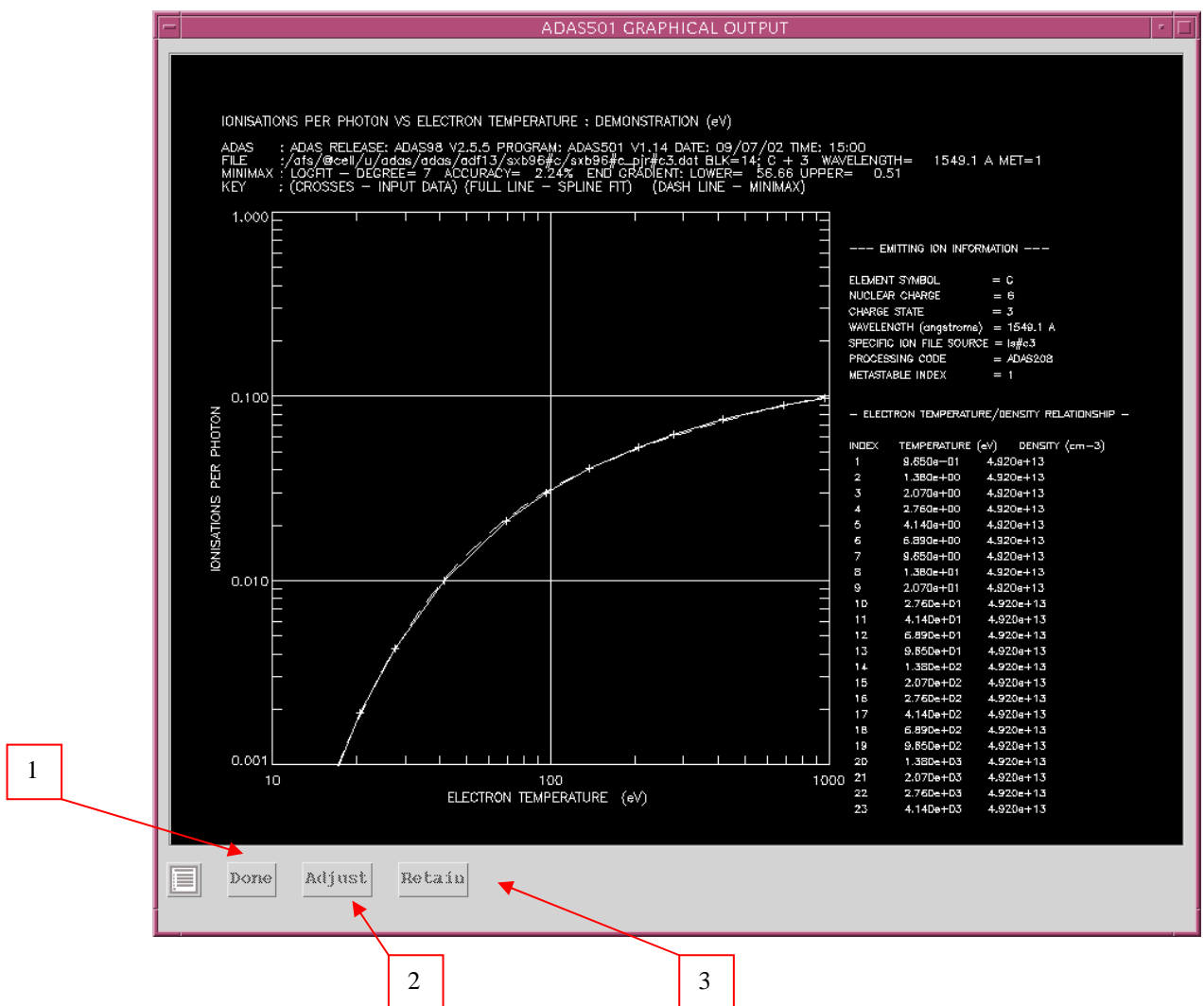
2. Activate the *Adjust* button to pop-up the Graph Adjust window. It's operation is described in Chap1-00 of this user manual.
3. Activate the *Retain* button to pop-up the Multiplot window. This widget permits superposition of graphs from multiple passes through ADAS501 and hence graph comparison. The detailed operation of the widget is described in Chap1-00 of this user manual.

Table Editor

A necessary operation in interactive ADAS is entry of user values into a table. Since this is common to many ADAS programs, a special window has been developed to assist in this task. A typical appearance of the **Table Editor** window is shown below
1. The values in italic font are your input data. Click in any of these boxes to edit the number within it. The workstation cut, paste and copy keys operate. Press the *return* key on the keyboard to record any change. This is the normal editing mode.

2. The set of round and square buttons below the table are designed to help in some editing tasks. You must be careful to remember the sequence of operations since it is different from that on personal computers. **Activate** the appropriate button, **position** the mouse text cursor or drag over required digits, **press** the *return* key on the keyboard to complete the sequence.

3. The *Default* round button is the reset to normal editing mode. The *Delete* button allows deletion of the value in a box, leaving an empty box; the *Remove* button allows deletion of a value with the column then being pushed up; the *Insert* button creates a new empty box, pushing the column down. These buttons stay active until you click *Default*.

4. The *Copy* and *Paste* round buttons operate for the next immediate action only.

5. Square buttons have a continuing effect until an alternative is pressed. The *Row_skip* button causes a jump to the next editable box in a row when the *return* key on the keyboard is pressed; *Column_skip* causes jumping to next box in a column. *Scroll up* moves the whole window down. Note that the window only shows ten values in a column, but the whole table may be longer that this.

6. Preferred Temperature units for working with may be chosen. Changing units causes the Inputs from the file to change to the new units. It **does not** change any Output values already typed in. It merely interprets Output values in the selected units.

7. Press the *Done* button to record the changes and return to the screen from which Table Editor was initiated. The *Cancel* button prevents the new values being substituted on return.