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Atomic Data and Analysis Structure

User manual

Special edition for opacity studies

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IDL-ADAS

Version 1.1

23 June, 1998

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Introduction

The Atomic Data and Analysis Structure (ADAS) is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas and for assisting in the analysis and interpretation of spectral measurements. The structure has both interactive and non-interactive capabilities. The interactive part provides immediate display of important fundamental and derived quantities used in analysis together with a substantial capability for exploring parameter dependencies and diagnostic predictions of atomic population and plasma models. The second part is non-interactive but provides a set of subroutines which can be accessed from the user's own codes to draw in necessary data from the derived ADAS database.

Objectives of opacity modelling

The main objective of this manual is to describe a set of codes in ADAS which provide some assistance in modelling the re-absorption of emitted photons in a plasma. The first effect of the re-absorption is that the escaping intensity from the plasma is less than the integrated emission along the line-of-sight. Consequently all spectral diagnostics which assume free photon escape (optically thin plasma) will be invalid in such plasmas. A secondary effect is that that the population distribution of the absorbing atom or ion states is also altered. The single ADAS code provided at this time uses the escape factor approach to evaluate these effects. Escape factor models have bee used since the 1940's and are a relatively simple approach to accounting for such re-absorption. They work by evaluating a quantity called the 'escape factor' which corresponds to the probability of a photon escaping from the plasma. Escape factors are functions of column density, and so if a spectral line ratio is known , the column density of the plasma can be deduced. The other uses of escape factors are to calculate opacity modified populations for the excited states of the atom or ion in question, and to assess whether spectral lines will be optically thin and thus useful for other diagnostics (eg. differential emission measure). For a comprehensive solution to photon re-absorption, it is necessary to solve the equations of radiative transfer. This is a much more complex problem and an escape factor approach often provides a reasonable approximation.

General organisation

The various ADAS routines are essentially of two types, namely those which are interrogative on the ADAS database (both fundamental and derived parts) and those which execute atomic modelling calculations. The latter may relay substantial quantities of data for further processing or for addition to the derived database.

In the interrogative codes, the principle objective has been to allow graphical display of any part of the database. All codes satisfy this quick look and check facility. In ADAS interrogation codes, cubic spline interpolation is performed on the source data from the database. These interpolated values are given as convenient printer tabulations. Atomic modelling codes generally create output data sets as well as normal tabular output. These files are structured according to the requirement of the ADAS data base or for further ADAS programs. It is anticipated that the user will edit these files into standard ADAS named files when establishing a personal database after being satisfied of their correctness.

ADAS as a whole is organised into the seven code series shown below. In technical terms there objectives are as follow: ADAS1 is concerned with fundamental, that is essentially individual reaction data. This is to be distinguished from the composite effects of many processes which are the subject of ADAS2-ADAS5. ADAS2 is concerned with evaluating excited populations of specific ions in a plasma environment and then their radiation emission. It relies on availability of a reaction rate data collection for the ion in the ADAS database although ADAS has some provision for generating an approximate collection of such data when this is not so. ADAS3 is of special interest for charge exchange spectroscopy and beam emission spectroscopy in fusion applications. ADAS4 is concerned with the ground and metastable populations of ions in a plasma and particularly their preparation and calculation for establishing the ionisation state in equilibrium and dynamical plasma models. It therefore operates with generalised collisional dielectronic recombination and ionisation coefficients, associated power loss coefficients and metastable fractions. It also mediates a transfer from an iso-electronic sequence storage of data which is the preferred choice for atomic data preparation and manipulation to an iso-nuclear sequence storage preferred for applied studies in dynamical plasma models. ADAS5 provides a set of general programs interrogating data collections in the derived database. The ADAS data classes addressed are those which have been found of particular importance for reduction of calibrated observed data. ADAS6 series is concerned with fitting and analysis of the spectral data stream from observations. It includes dedicated fitting codes for particular types of spectral feature. ADAS7 series is dedicated to the fundamental calculation of dielectronic recombination, ionisation and excitation/auto-ionisation data including their organisation for applications. ADAS7 series also includes modelling and analysis codes extended to treat the doubly excited populations and associated emissions occurring because of these processes.

Series	*Content*
ADAS1	Entry and validation of fundamental atomic data
ADAS2	Excited state populations of ions in a plasma
ADAS3	Charge exchange related emission
ADAS4	Recombination, ionisation and radiated power
ADAS5	General interrogation programs
ADAS6	Data analysis programs
ADAS7	Creating and using dielectronic data

There are 29 distinct data types in the ADAS databases. Each data set type has its layout and content precisely described. These prescriptions are called ADAS data formats or *adf*s and must be rigidly adhered to in preparation of personal data for use by the ADAS package. A full description of all the ADAS data formats is given in appendix B of the main manual. These formats apply both to fundamental and derived data. The most important here is

ADF04	resolved specific ion data collections

ADAS on a Unix workstation

The interactive ADAS is intended for use by the non-specialist but informed user. It is implemented as a shell command on the Unix workstations. Some preliminaries are necessary. It is assumed that the user has basic knowledge of Unix command structure and experience of a typical ‘desktop’.

Initial checks

cd /.../<user identifier>	Change to your home directory /.../ denotes the root path to user directories.
ls	Check file and directories present

If the directory /adas is not present create it.

mkdir adas	Make you personal adas database top directory
cd adas	Move into the directory adas
mkdir defaults	Make a defaults directory if it does not exist
mkdir pass	Make a passing file directory if it does not exist
mkdir scripts405	Make a script file directory for ADAS405 if it does not exist
mkdir arch101	Make an archive file directory for ADAS101 if it does not exist

Sub-directories for various ADAS data formats may be created here if you wish to make up a personal adas database and they are not already present. For example

mkdir adf04	Create an ADF04 sub-directory

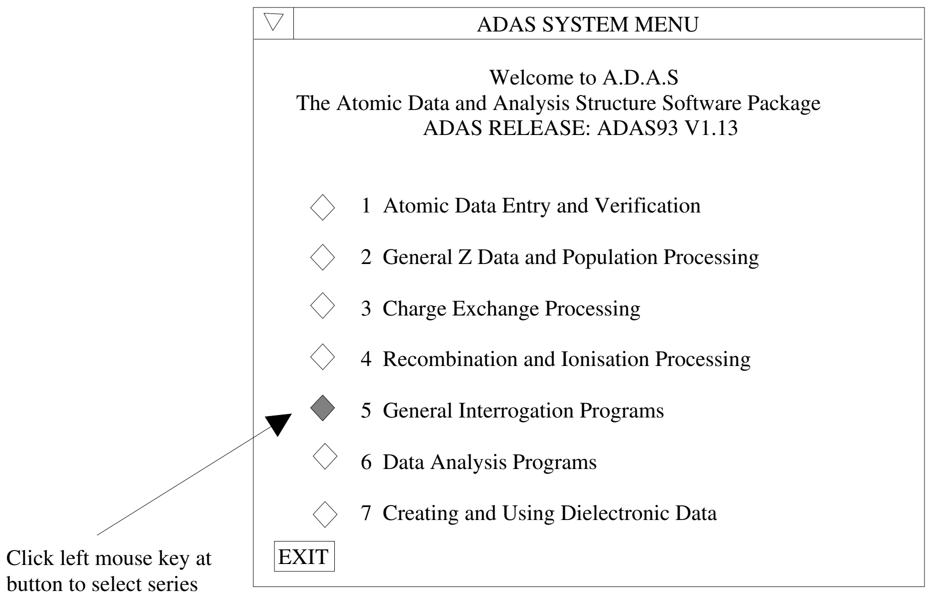
Central ADAS data has the directory path */.../adas/adas* on the SOLG DEC ALPHA workstations. You can look at them.

/.../adas/adas/adf04/belike	move to a Be-like specific ion file sub-directory
ls	list data files available
cat belike_jl1990o.dat	list a particular file for O^{+4} prepared by J. Lang

Starting ADAS

cd /.../<user identifier>	return to your home directory
adas	start ADAS

The top level ADAS selection menu should be displayed as below



Central ADAS documentation

Documentation is placed in the */.../adas/docs directory* under three headings

1. *Bulletins:* files named as /.../adas/docs/bulletin/<date>.ps
   where <date> is of the form <month><day>-<year> [eg. **nov18-94** (this bulletin)].
2. *Usernotes:* files named as /.../adas/docs/usernotes/<library code>/<code name>.ps

   where <library code> is the associated Fortran library name [eg. **adaslib** , **adas2xx**, etc.]
   and <code name> is the Fortran subroutine name [eg. **ssxb**, **xxssxb** etc.]
3. *Manual:* files named as /.../adas/docs/manual/chap<i>-<nn>.ps
   where <i> denotes chapter number from the ADAS User Manual and <nn> denotes the sub-chapter. The manual has been split into these sub-chapters for easy of interrogation.

All these files are 'postscript' files.

To look at the files, activate a CDA viewer tool:

dxvdoc bring up CDA viewer window

Button select FILE FORMAT choice *PS*

Double click on directory names to move to required sub-directory

Click on required file to select it

Button select *OK*

To terminate CDA viewer

Button select *FILE* at top left of window

Button select *EXIT* on drop down menu.

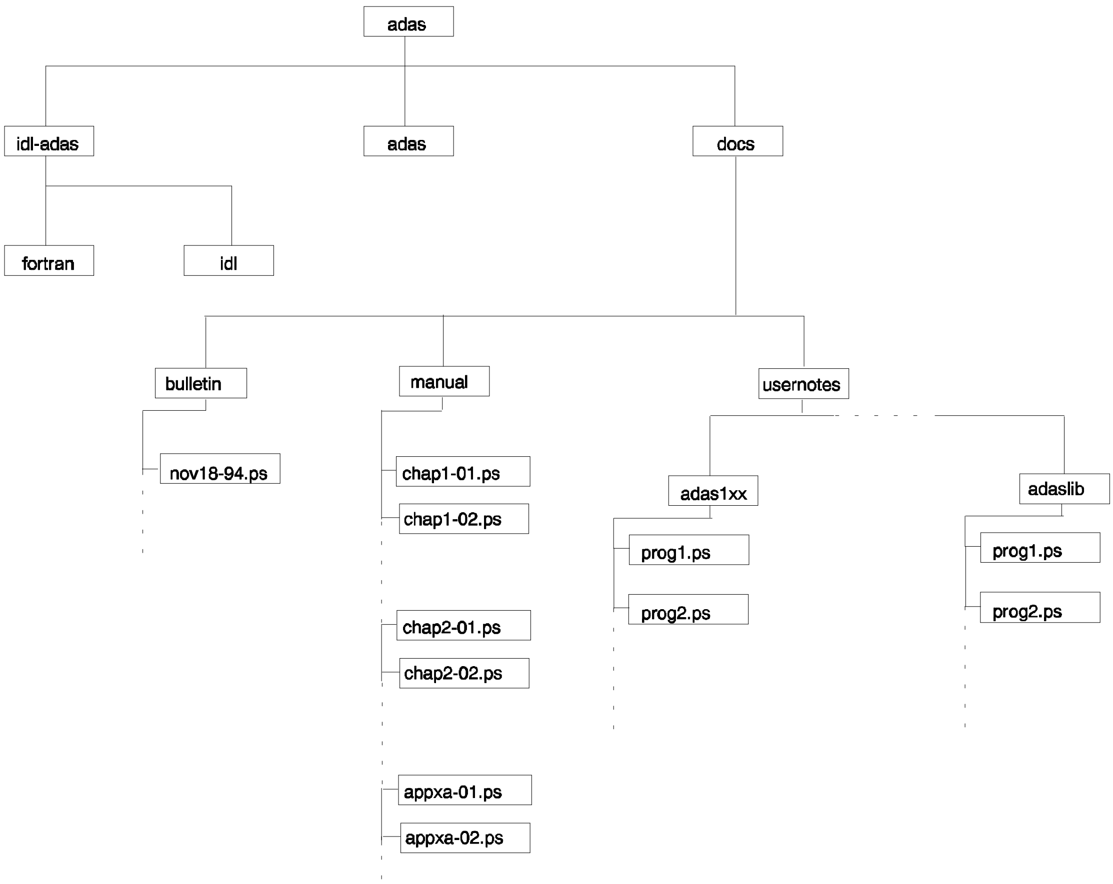


Table Editor

A necessary operation in interactive ADAS is entry of user values into a table. Since this is common to many ADAS programs, a special widget has been developed to assist in this task.

To avoid repetition in the description of each code, a summary of how to use **Table Editor** is given here. A typical appearance 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 triangular 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. The *Default* triangle button is the reset to nomal 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*. The *Copy* and *Paste* triangle buttons operate for the next immediate action only. 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. 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.

3. 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.

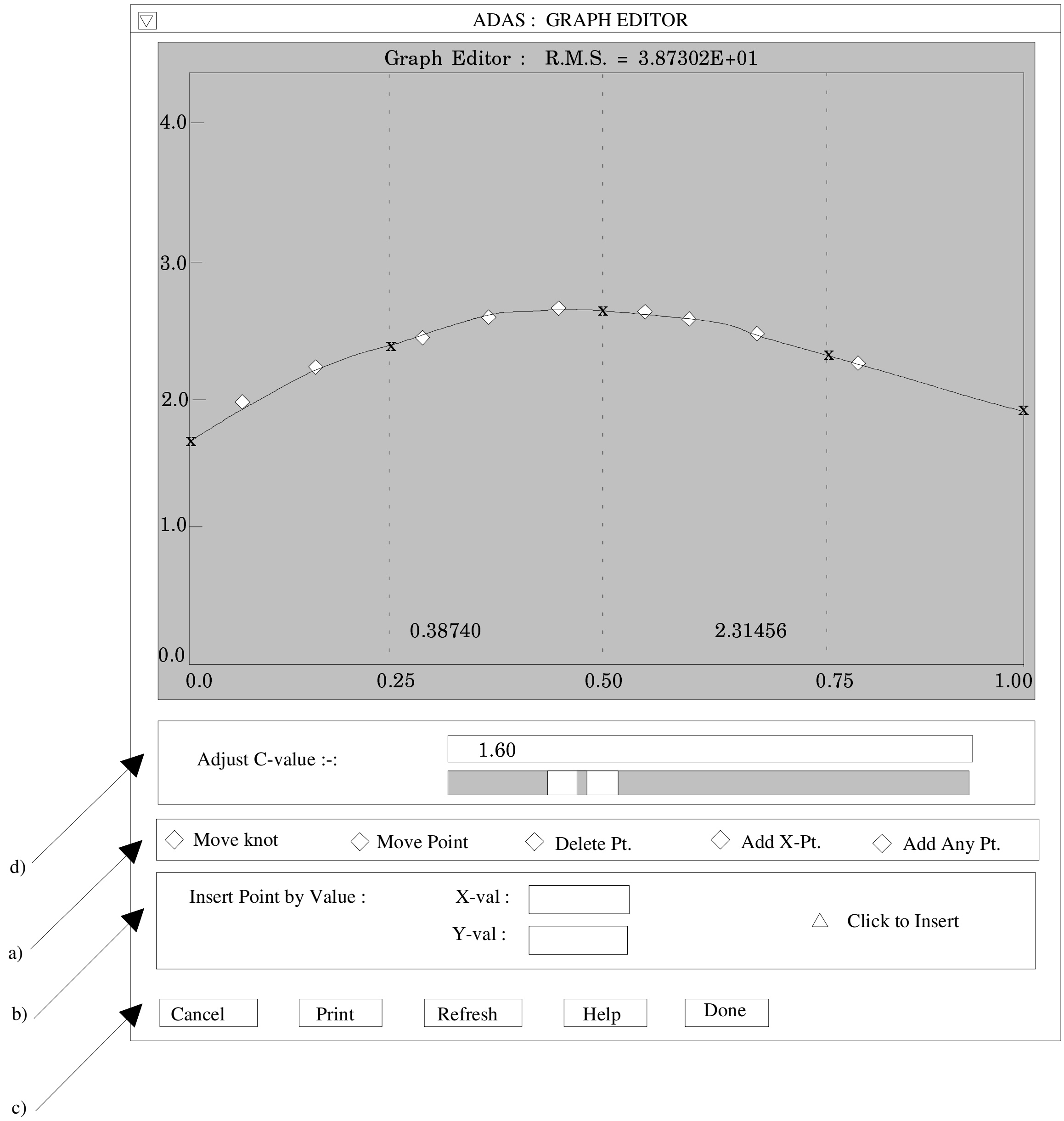
Graph Editor

In the fundamental data entry and verification sections of interactive ADAS, flexibility in adjustment, deletion and insertion of points on a displayed comparative graph is useful. Since this is common to a number of ADAS programs, a special widget has been developed to assist in this task. A summary of how to use **Graph Editor** is given here. A typical appearance (in fact from ADAS101) is shown below.

1. Input values are displayed as circles. The points can be modified by using the buttons a) beneath the graph in association with the mouse. In the table editor for ADAS101, a least squares spline fit is made to these tabular points. The spline passes through five special knot points which are distinguished in the Graph Editor as crosses. An extra button is present for this case to allow the knot points to be moved vertically.

2. To move a point, click the *move a point* button. Then use the *left* mouse button to pick and drag a point to a new position. Note that the x-ordering of points should be maintained although not forced by the editor. Each point has a small active zone around it for picking by the mouse. Terminate point moving operations by pressing the *right* mouse button. To delete a point, click the *delete a point* button. Then click the *left* mouse button with the pointer over the point to be deleted. Terminate point deletion operations by pressing the *right* mouse button. To add a new point in the x-ordered position between two existing points, click the *add X-point* button. Then click the *left* mouse button with the pointer at the position where the new point is to be inserted. Terminate point insertion operations by pressing the *right* mouse button. For completeness, the capability for adding a point anywhere is given although physically unreasonable. The operation is

slightly different. Click the *add anywhere* button. With the *left* mouse button pick a point after which you wish the new point added. Press the *left* mouse button with the pointer at the insertion point. Multiple insertions may be made by continuing to click the *left* mouse button. Click the *right* mouse button to terminate this particular insertion. Press the *right* mouse button a second time to terminate insertion operations.



3. To insert a point by value use sub-window b).

4. The buttons at c) provide the usual *cancel*, *print* and *done* options. In addition the *help* button displays some information on using the graph editing facilities. The original data and graph can be restored by clicking the *refresh* button. Note that after leaving the graph editor window with the *done* button, the modified and or additional points replace the original user input data. Further actions depend on the particular ADAS program which launched Graph Editor. Thus for ADAS101 with the ADAS analysis option, if any points are modified, the program cycles back for reanalysis. With the Burgess analysis option, movement only of the spline knots does not force reanalysis.

5. The graph editor for ADAS101 also includes a slider to adjust a parameter ‘C’ which affects the plot.