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AIDA - A Graphical User Interface for the ATLAS Program Package

W S Howells

December 1997

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AIDA

A Graphical User Interface for the ATLAS program package

W S Howells

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Also on http://sutekh.nd.rl.ac.uk/wsh/aida/

Contents

1. Introduction	2
1.1 General	2
2. Data Input	2
2.1 Introduction	2
2.2 Buttons	2
2.3 Input boxes	3
3. Windows	4
4. NORM	7
5. Background	9
6. FingerPrint	10
7. CORAL	12
8. VanSm	14
9. Analyse	16
10. Placzek	18
10.1 Atom option : Platom	18
10.2 Ideal Gas option : PlacID	19
11. H/D substitution	21
12. McGofR	24

1. Introduction

1.1 General

AIDA is a GUI (Graphical User Interface) using a WIMP (Window Icon Mouse Pointer) environment to provide a user-friendly means of launching the Batch jobs in the Atlas program suite. It carries out all the operations presently provided by the Atlas Batch menu (using the command A_B). This manual is a guide to the menu system only - for descriptions of the programs themselves the user should refer to the Atlas manual.

The programs use the Tcl/Tk computer language with further extensions from Tix. For further information on these languages the user should refer to the appropriate manuals. Use of the window interface requires a fast computer and it is recommended that this package should only be run on an Alpha computer.

2. Data Input

2.1 Introduction

Options and data can be specified in one of two ways:
a) by pointing to an area on the screen and pressing the mouse button which will be referred to as pressing a button or clicking.
b) typing a value for a variable.

2.2 Buttons

There are four types of button:

i) main button. These are large and have a text label on them. By pressing them a specific command/operation is initiated. In this package they are confined to three types of operation and the buttons are colour coded and mainly positioned along the bottom of the window.
The three types are :
a) Help - blue. On pressing, a new window appears containing text describing the operations performed from the window containing the Help button.
b) Go forward - green. These are called either Run or Continue. The first type initiates the task described in the window; the second is usually used when the window is no longer needed. In both cases the window is closed.
c) Go back - red. These are normally called Stop or Cancel. When used the operations defined in the window are not carried out and the window is closed.

ii) radio button. This refers to a series of buttons of diamond shape of which only one can be active and is coloured red. On starting up, this marked button will be the default option. Each button has an associated text label. To change on option, point and click on the new option

which will then turn red and the previous option turns white. The buttons linked together will all be situated either on the same line or within the same frame.

iii) check button. This has a square shape and is a straight forward on/off button for a single option. The on state is red and on startup signifies the default option, if there is one.

iv) Drop down menu button. These buttons are usually within the main part of the window and incorporate a drop-down menu of text labels. Clicking on the button brings up the menu and the option can then be chosen by clicking. The new choice will then become the value of the label.

2.3 Input boxes

Variable values are typed into a specific box which has a descriptive label. If the caret is not already positioned in the box, the pointer must be positioned inside it and clicked. Input MUST be terminated either with the Return key or the Tab key. In most cases the input cursor then moves to the next appropriate input box or, if it is the last box in the window, carries out the command defined by the Run (green) button. The position of the caret within the box can be moved by using the cursor keys and characters can be removed with the Delete key. After editing a value, the entry must still be terminated with a Return or Tab.

A variable retains its value until changed. If a particular variable is used in several programs, then once defined will become the default for subsequent programs. For example, when a vanadium run number is defined in VanSm it becomes the default value in Analyse.

A further version of input box, called a ComboBox, has a drop-down menu of fixed values and the menu is activated by clicking on the down-arrow to the right of the box. The value required is chosen by clicking on it. A different value may be typed in if necessary.

In some routines an entry box for a run number has a button next to it labelled Browse (described in Section 3).

3. Windows

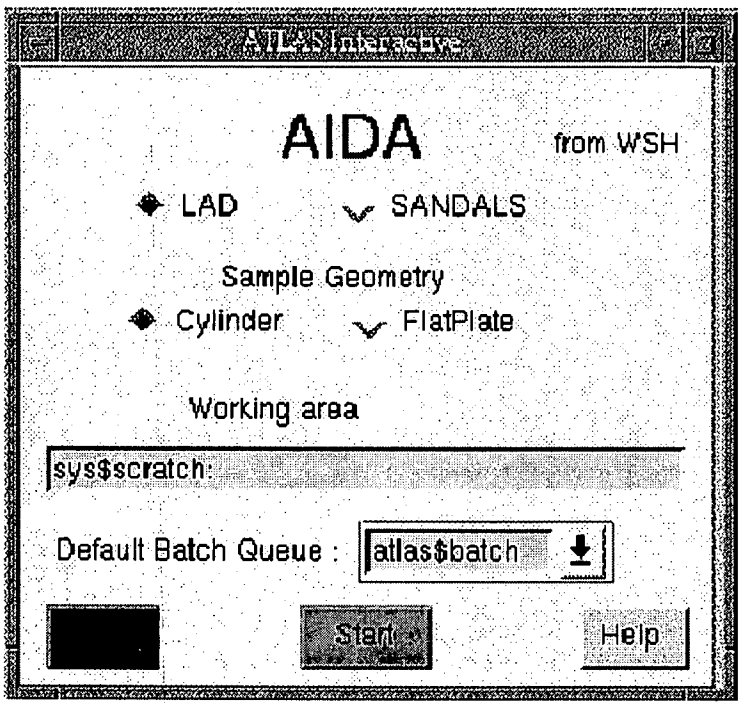
These appear at various stages of operation and can be iconised if required.
There are two main types :

i) Program Menu windows - are specific to a program or option and only appear for that option and are closed when finished. The three main windows described below are not closed until AIDA is shut down. Buttons in these windows will perform the task or operation specific to that window.

ii) Message windows - just show a text message and the window is closed when no longer required.
The Help pages for example contain black text and a scroll-bar.
Error messages have their own style of window with red text. An example is one which states that a file does not exist.
Information windows have the message in blue text. An example is the last window to appear in an option which states that the Batch job has been submitted and gives the names of the files created (this window has a label Finale).

The standard windows show all the text within the one window, but a NoteBook style window contains several 'pages' which are selected by clicking on the appropriate 'tab' arranged along the top of the window (like a card index).

The StartUp window appears when the program is started with the command AIDA.



Below the AIDA banner are the first two sets of radiobuttons to specify the instrument (LAD or SANDALS) and the sample geometry (Cylindrical or FlatePlate). These two options will remain in force for all further programs and until they are changed.

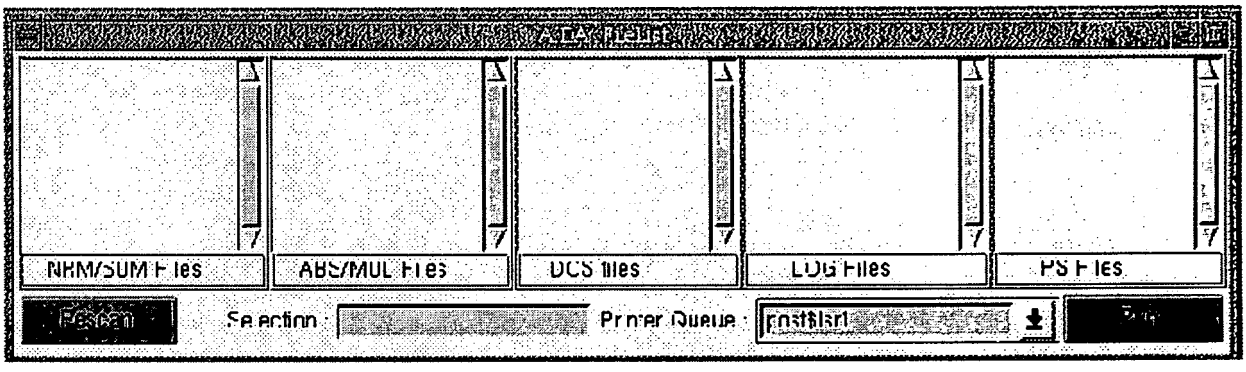
Many of the options have different sets of parameters for the two instruments, if a parameter is not in use then its text will be light grey instead of black and any buttons or input boxes will be inhibited.

The Working Area is the disk and directory in which the files to be used (other than RAW files) are stored and where the new files (except LOG files) will be created. The default value is the directory from which AIDA has been launched. This means that AIDA can be started from one directory and use files from another directory (or computer). The value can be changed at any time during an AIDA session and it remains in force until the next change.

The Default Batch Queue can be defined at this point, but can be changed for each individual option if required.

On pressing the Start button, two new windows appear :

i) the FileList window.



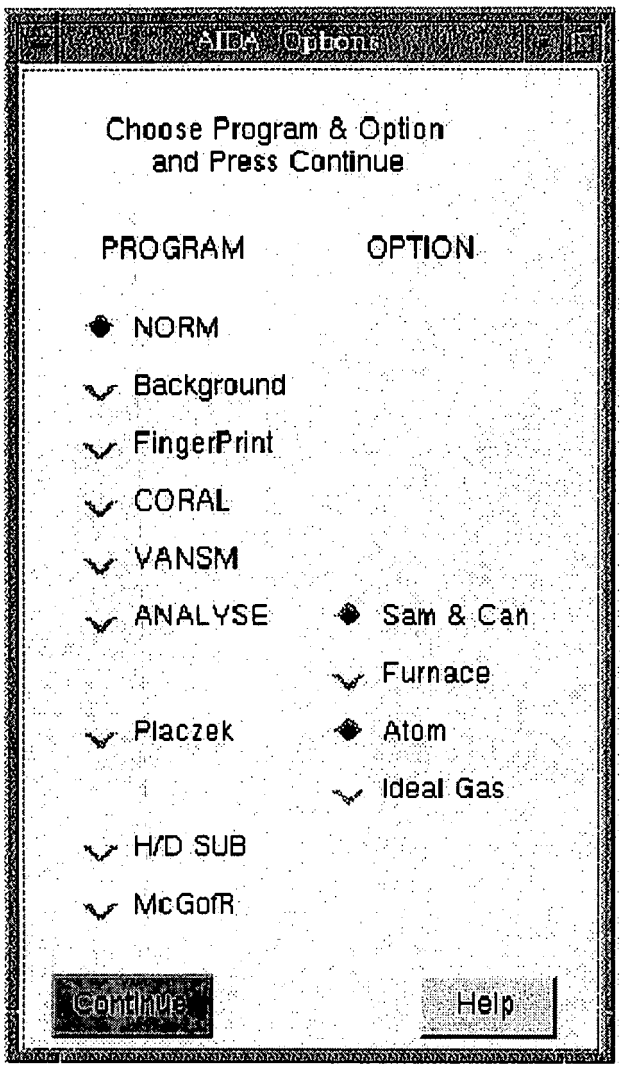
This contains 5 panes and will list in each pane the files in the Working Area with the extensions specified at the bottom of the pane. For the LOG files, the directory is the user's scratch disk directory.

In order to update the lists click on the Rescan button.

A file can be selected by clicking on its name which then appears in the Selection box. It can then be sent to a printer by clicking on the Print button. The printer can be chosen with the ComboBox style entry. (Only LOG files or PostScript files should be sent to a printer - all others are binary files!)

A variation on this window is opened from the Browse button. Clicking on the button brings up a window with a single pane (similar to the Filelist window) in which are listed all the files with the extension indicated. The extension will be specific to that particular entry. Clicking on the chosen file results in that name appearing in the Selection box. If the Select button is now clicked the corresponding run number will appear in the entry box.

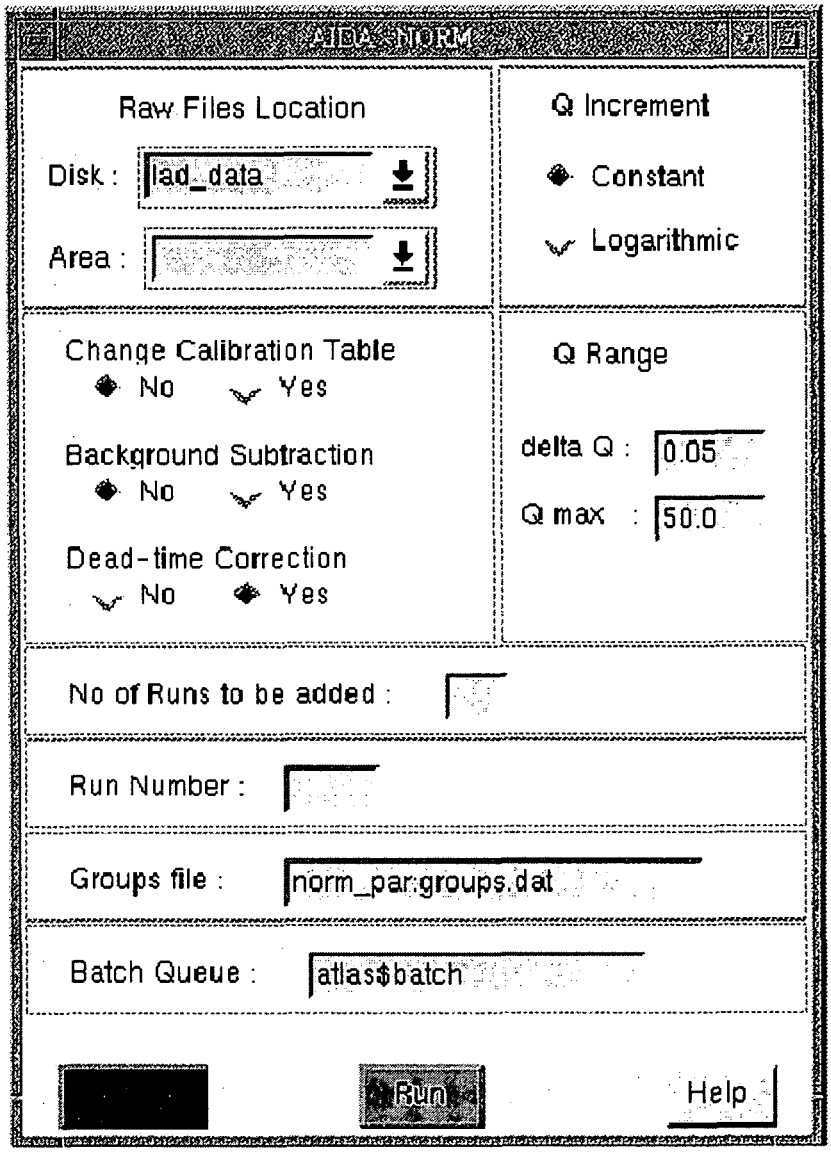
ii) the main Option window contains a menu of the options available and correspond to those that are available in the VMS command system using A_B.



To run a program click on the appropriate radiobutton and then the Continue main button.
The Analyse and Placzek programs each have two variations with their radiobuttons.
After clicking, the window for the specified program will then appear.

In the rest of this manual comments will only be made about points which are specific to AIDA.

4. NORM



Frame 1-left: The RAW files location defaults to lad_data or sls_data as usual - if the RAW files for the run numbers specified are not in that area there will be an error message.
The disk and directory may be specified using the input boxes with the usual selection available as a drop-down menu.

Frame 1-right: Radiobuttons are provided to specify whether the Q increment is constant or logarithmic.

Frame 2-left:
Radiobuttons are provided to specify :
whether to change the calibration table
whether to carry out a background subtraction as provided by the Background program
whether to apply dead time corrections

Frame 2-right: the Q range is specified by inputing the Q increment (delta Q) and Q maximum. The default values in the input boxes depend on the Q increment setting defined in frame 1-right.

Frame 3: specifies the number of runs to be added. If the number of runs is set to 1 the input caret moves to the Run Number input box in frame 4.
If the number of runs is greater than 1 a new window appears with an entry box for each run. On terminating entry to a box, the caret moves to the next box, except for the last box in which case the window is closed and the caret moves to frame 5 .

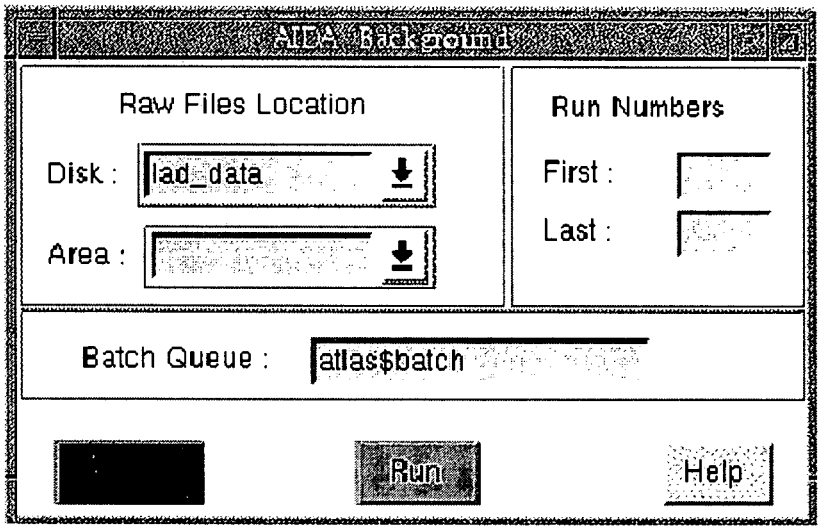
Frame 5: defines the Groups file and defaults to norm_par:groups.dat.

Frame 6 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

The values for number of runs and run number together with all the other options, when defined, become the default values for the next time NORM is run. So if NORM is to be run with the number of runs equal to 1 several times, only the run number needs to be changed (but do not forget to terminate the entry).

5. Background



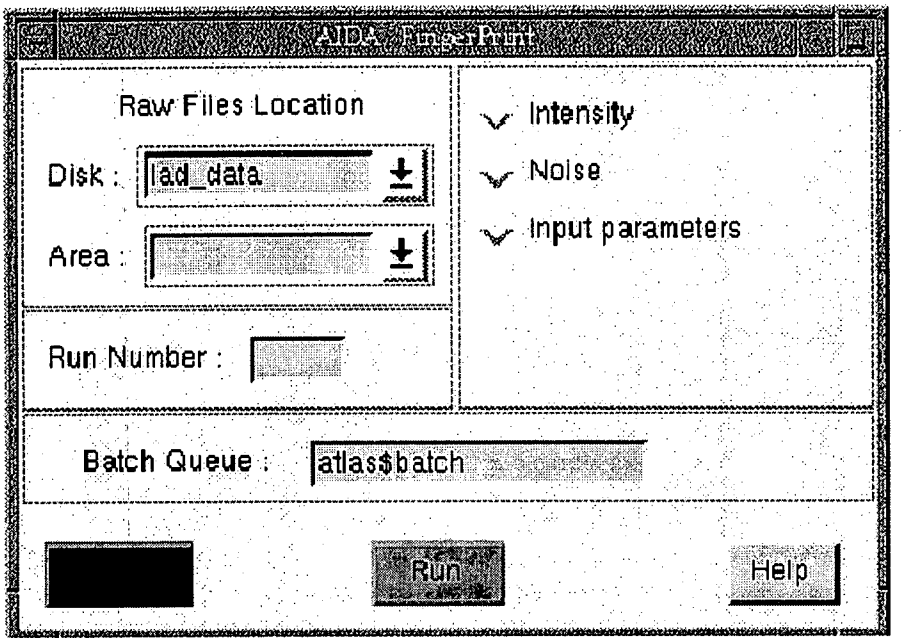
Frame 1-left: The RAW files location defaults to lad_data or sls_data as usual - if the RAW files for the run numbers specified are not in that area there will be an error message.
The disk and directory may be specified using the input boxes with the usual selection available as a drop-down menu.

Frame 1-right: defines the numbers of the first and last runs to be processed.

Frame 2 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

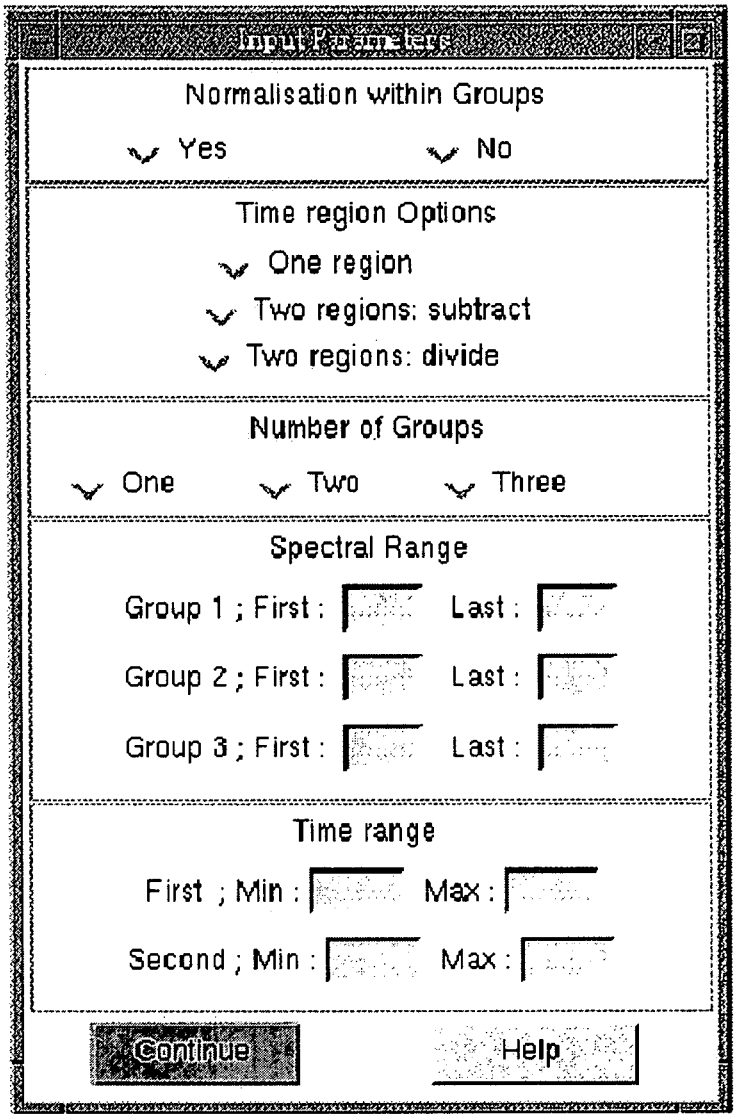
When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

6. FingerPrint



Frame 1-left: The RAW files location defaults to lad_data or sls_data as usual - if the RAW files for the run numbers specified are not in that area there will be an error message.
The disk and directory may be specified using the input boxes with the usual selection available as a drop-down menu.

Frame 1-right : has radiobuttons to give a choice between using a file as input or typing values for the parameters.
Three options are available for the type of calculation :
i) intensity - the sum over all channels
ii) noise - to check on detectors
iii) input parameters - in this option an extra window appears to define the type of operation and for input of grouping and time ranges.



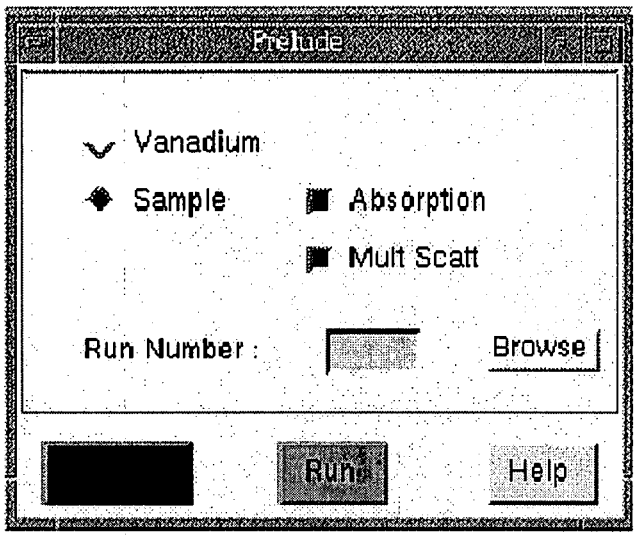
Frame 2 : is for the run number.

Frame 3 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

7. CORAL

CORAL starts off with a Prelude window which has :



i) radiobuttons to select sample or vanadium corrections
ii) checkbuttons for the sample option to define which corrections (absorption and/or multiple scattering) are required to be calculated.
iii) the run number - which can be input either by typing in the entry box or found using the Browse button

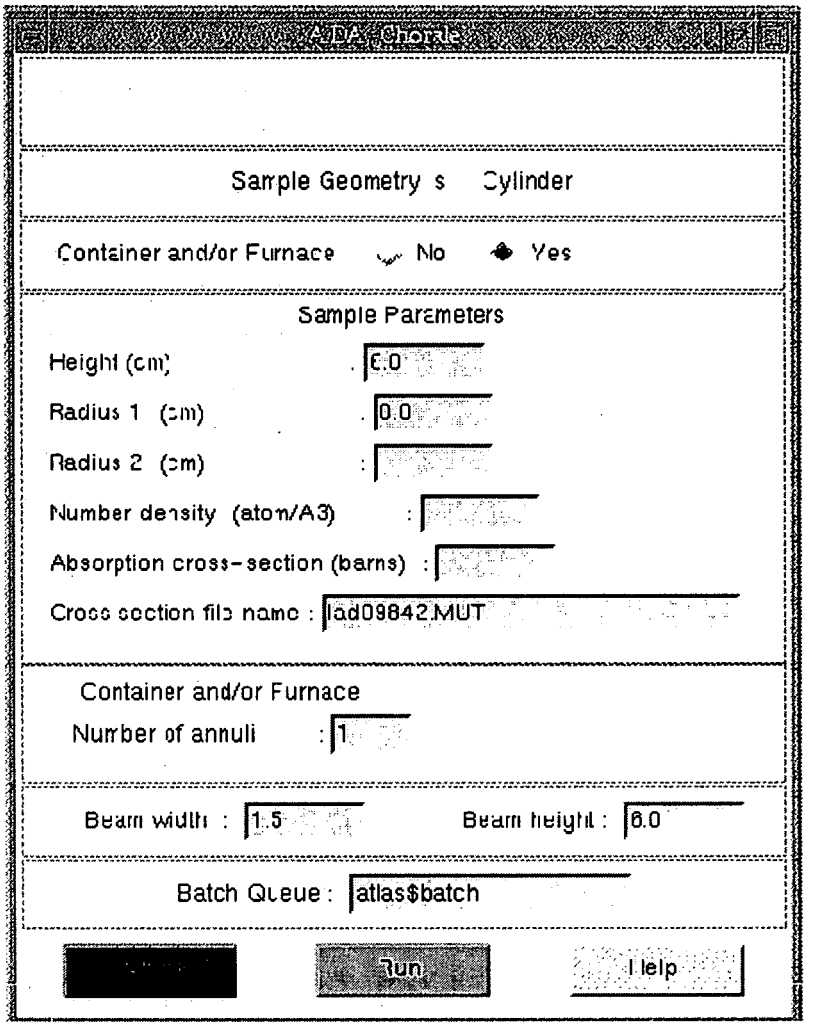
The routine then checks whether AIN and MIN files already exist before closing and opening the main Chorale window.

Frame 1 : If AIN or MIN files exist then this will show the message Data from File in blue and the entries in the subsequent boxes will be those from the file. Otherwise it will be blank and the entries will be blank or default values.

Frame 2 : is a message frame indicating the Sample geometry as defined in the StartUp window.

Frame 3 : has a radiobutton to define whether a Container and/or Furnace is present.

Frame 4 : contains the Sample parameters. The cross-section file name will default to <runnumber>.MUT.



Frame 5 : is for the Container/Furnace. If no container is present this frame will be grey and inhibited. For a container, the entry box is for the number of annuli (cylinder) or layers (flat) - the default value is 1. This entry must be terminated in order to bring up the Container window for its parameters, which when closed returns to the Chorale window.

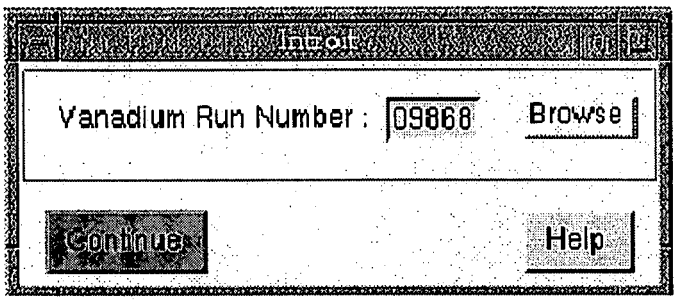
Frame 6 : for the cylinder option this is the beam width and beam height; for the flat plate option it is the angle of the sample to the beam.

Frame 7 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

8. VanSm

VanSm begins with an introductory Introit window.



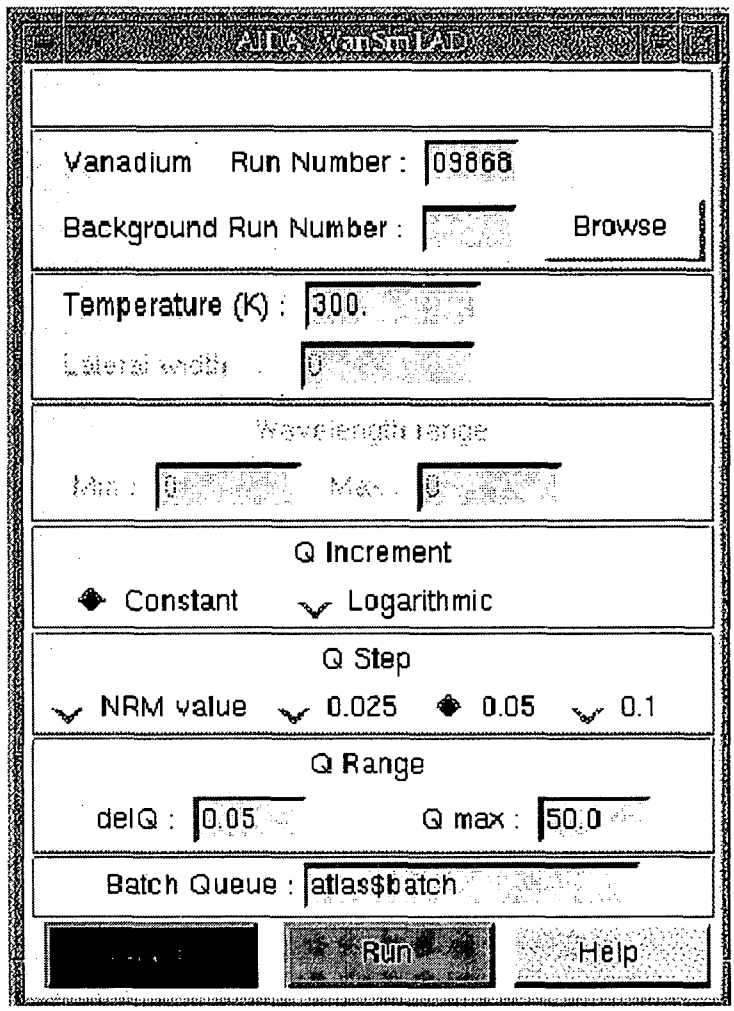
The input in this window is :
i) the vanadium run number - which can be input either by typing in the entry box or found using the Browse button.

The routine checks for the existence of a VANB_DAT file before closing and opening the main VanSm window.

Frame 1 : If the VANB_DAT file exists then this will show the message "Data from File" in blue and the entries in the subsequent boxes will be those from the file. Otherwise it will be blank and the entries will be blank or default values.

Frame 2 : is for the vanadium and background run numbers. The vanadium value will be that given in Introit while the background number can be input either by typing in the entry box or found using the Browse button. The program will check for the existence of the NRM/SUM, MON and REF files. If a file does not exist an error message will appear.

Frame 3 : the main box is for the temperature. If the instrument is SANDALS then the second box is for the lateral width - this is grey and inhibited for LAD.



Frame 4 : is only for SANDALS and defines the wavelength range. It is grey and inhibited for LAD.

Frame 5 : has radiobuttons to define the Q increment as constant or logarithmic.

Frame 6 : has radiobuttons to define the Q step. The values (other than the NRM/SUM option) will depend on the Q increment option defines in frame 5.

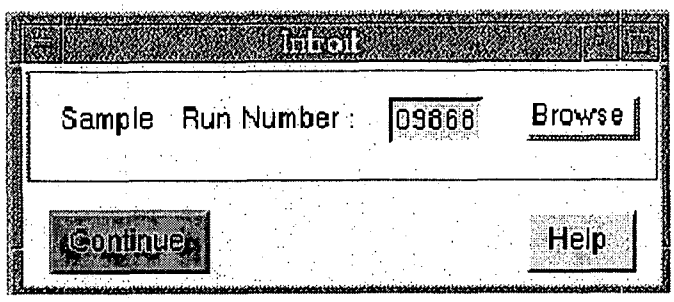
Frame 7 : is for input of the Q range. The default for del Q is that defined in frame 6 and the Q max is 50.

Frame 8 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

9. Analyse

In the main menu, the Option : Sam & Can or Furnace must be defined.
Analyse must be run after Coral and begins with an introductory Introit window.



The input in this window is :
i) the sample run number - which can be input either by typing in the entry box or found using the Browse button.

The routine checks for the existence of a ANAB_DAT file before closing and opening the main Analyse window. The routine also assumes that runs have the extension NRM/SUM and that the vanadium is SMO. It checks for the existence of these files and the ABS and MUL files. If any file does not exist then an error message will appear.

Frame 1 : If the ANAB_DAT file exists then this will show the message Data from File in blue and the entries in the subsequent boxes will be those from the file. Otherwise it will be blank and the entries will be blank or default values.

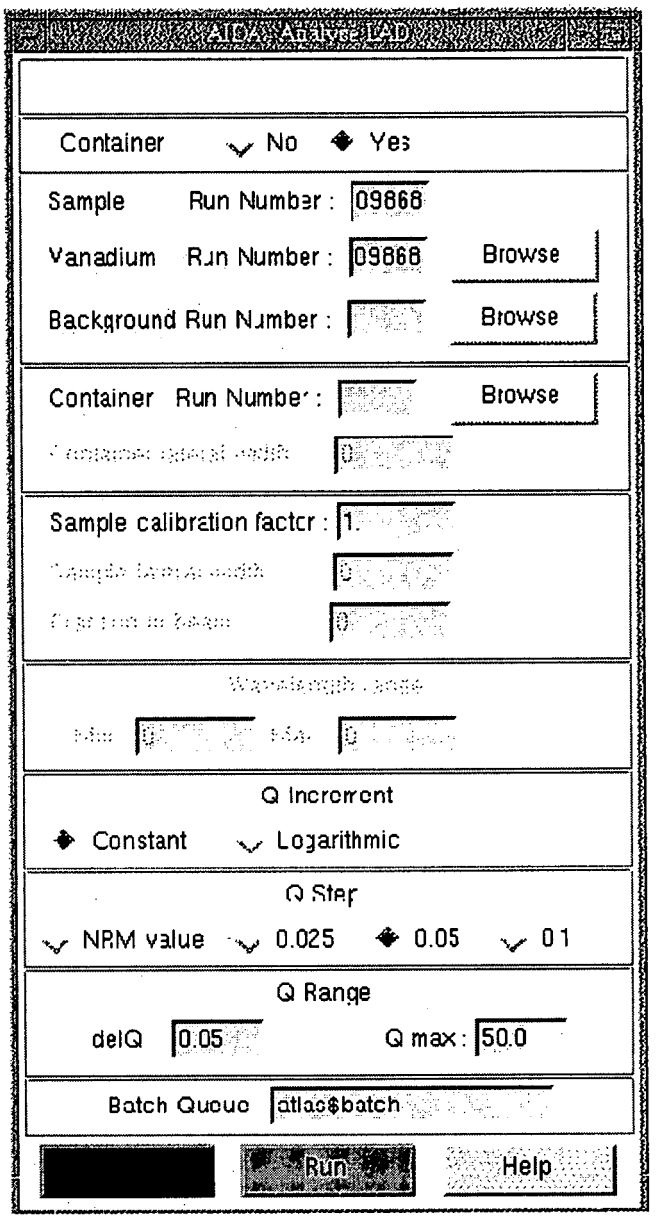
Frame 2: provides radiobuttons to select Container option

Frame 3 : is for the sample, vanadium and background run numbers. The sample run number will be that given in Introit. If VanSm has been run during the current session then the vanadium run number will be that given in VanSm; otherwise it can be input by typing in the entry box or found using the Browse button. The background run number can be input either by typing in the entry box or found using the Browse button.

Frame 4 : is for the container run number. If not selected the text will be grey; otherwise the container run number can be input either by typing in the entry box or found using the Browse button. For SANDALS there is an entry box is for the container lateral width - this is grey and inhibited for LAD.

Frame 5 : is for input of the sample calibration factor (defaulted to 1.). For SANDALS there are entry boxes for for the sample lateral width and the fraction in the beam. They are grey and inhibited for LAD.

Frame 6 : is only for SANDALS and defines the wavelength range. They are grey and inhibited for LAD.



Frame 7 : has radiobuttons to define the Q increment as constant or logarithmic.

Frame 8 : has radiobuttons to define the Q step. The values (other than the NRM/SUM option) will depend on the Q increment option defines in frame 7.

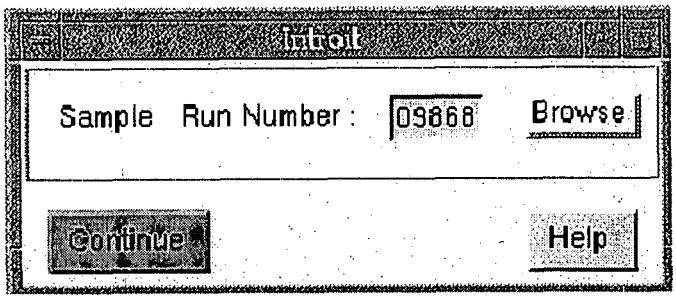
Frame 9 : is for input of the Q range. The default for del Q is that defined in frame 8 and the Q max is 50.

Frame 8 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

10. Placzek

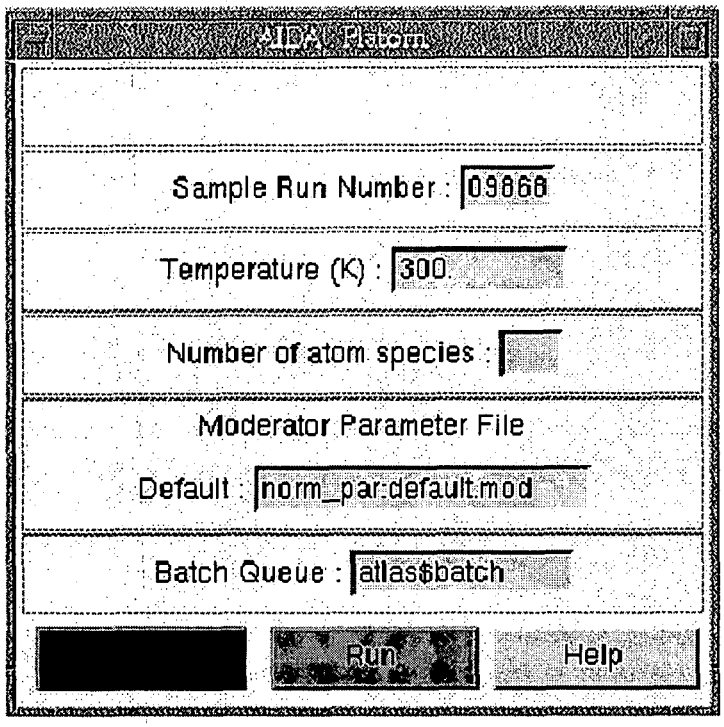
In the main menu, the Option : Atom or Ideal Gas must be defined.
Placzek begins with an introductory Introit window.



The input in this window is :
i) the sample run number - which can be input either by typing in the entry box or found using the Browse button.

10.1 Atom option : Platom

The routine checks for the existence of a PATB_DAT file before closing and opening the main Platom window.



Frame 1 : If the PATB_DAT file exists then this will show the message Data from File in blue and the entries in the subsequent boxes will be those from the file. Otherwise it will be blank and the entries will be blank or default values.

Frame 2 : is for the sample run number.

Frame 3 : is for the temperature.

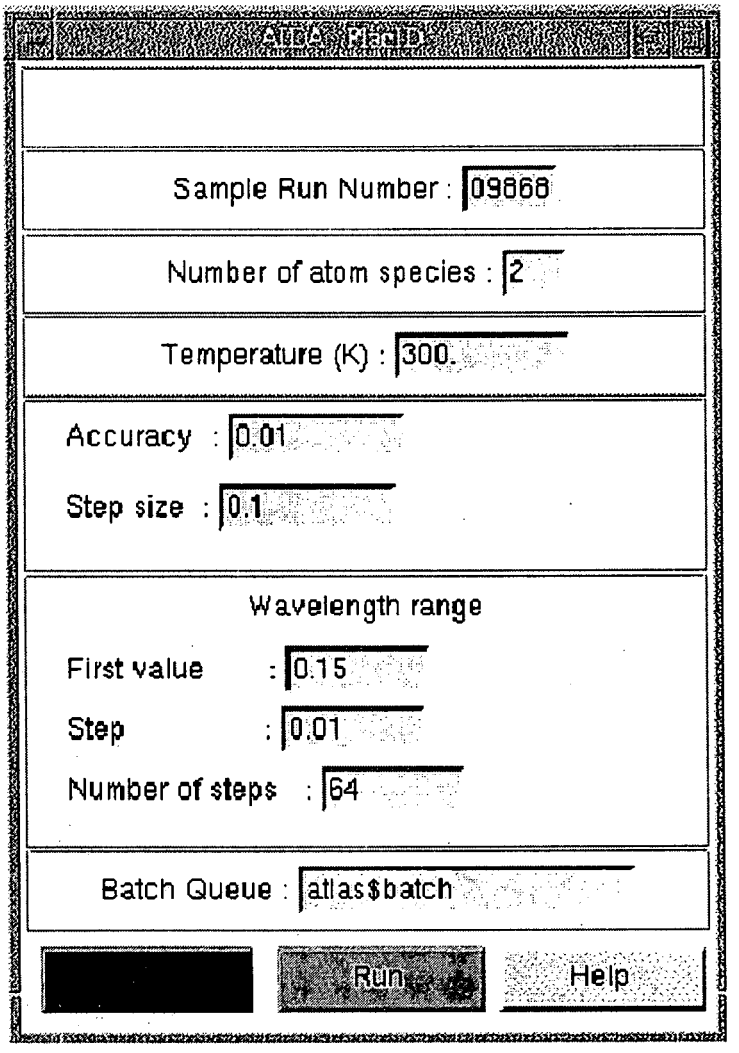
Frame 4 : defines the number of atom species. When the number is entered a new window appears with entry boxes for each species for its fraction, atomic mass nad scattering cross-section. On completion this window closes and imput returns to the Platom window.

Frame 5 : is for the moderator paramters file name and defaults to the methane option.

Frame 6 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

10.2 Ideal Gas option : PlacID



The routine checks for the existence of a PIDB_DAT file before closing and opening the main PlacID window.

Frame 1 : If the PIDB_DAT file exists then this will show the message Data from File in blue and the entries in the subsequent boxes will be those from the file. Otherwise it will be blank and the entries will be blank or default values.

Frame 2 : is for the sample run number.

Frame 3 : defines the number of atom species. When the number is entered a new window appears with entry boxes for each species for its fraction, atomic mass nad scattering cross-section. On completion this window closes and imput returns to the PlacID window.

Frame 4 : is for the temperature.

Frame 5 : is for the values of the accuracy and step size.

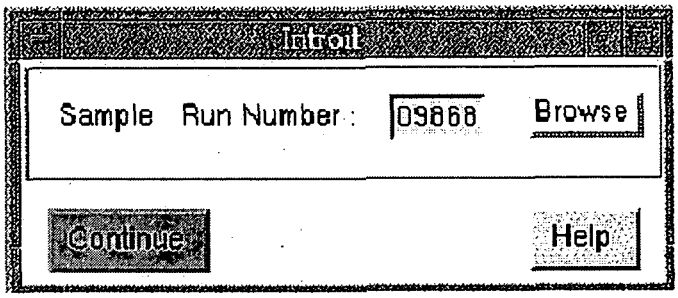
Frame 6 : is for the wavelength range defined by the first value, the step and the number of steps.

Frame 7 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

11. H/D substitution

HDsub begins with an introductory Introit window.

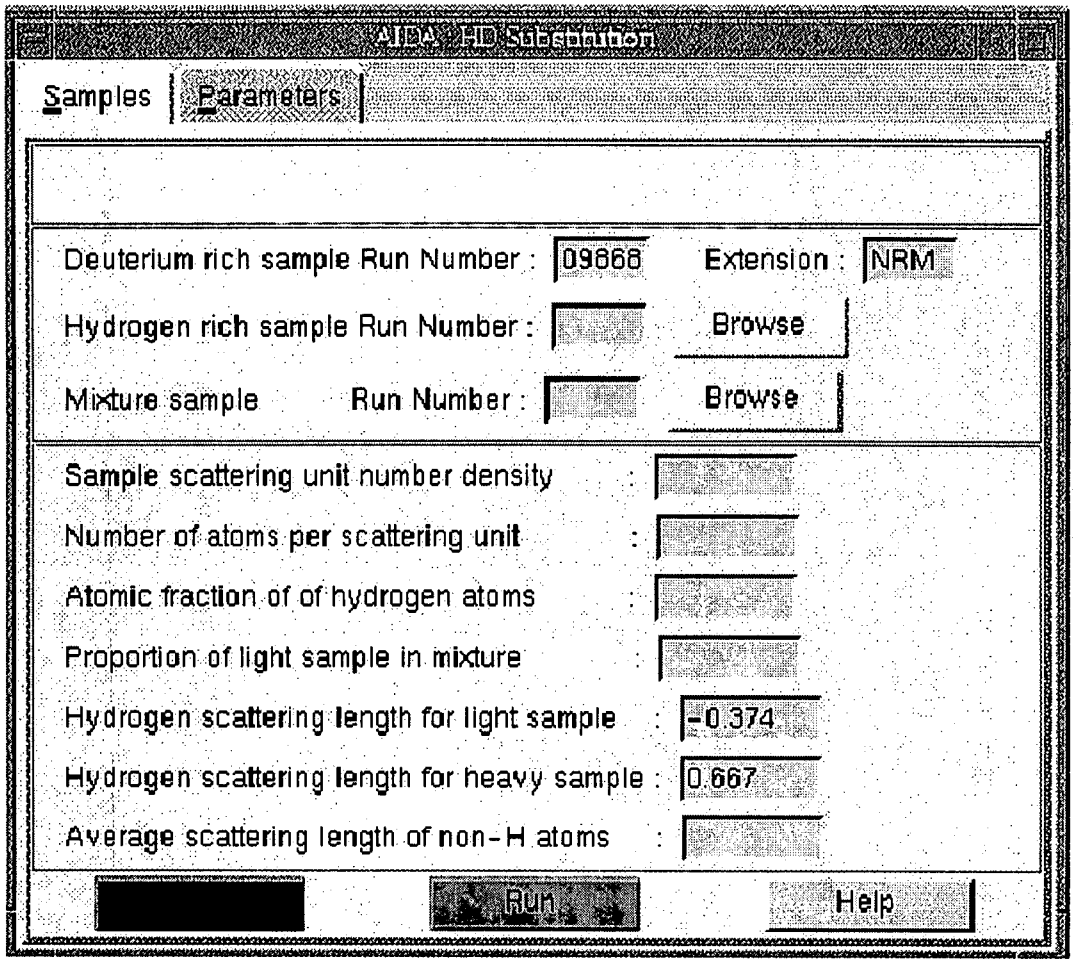


The input in this window is :
i) the sample run number - which can be input either by typing in the entry box or found using the Browse button.

The routine checks for the existence of a HDSB_DAT file before closing and opening the main HDsub window.

This window is in NoteBook form with 2 choices : Samples and Parameters.

PAGE 1 : The Samples page. This is the one used most often.



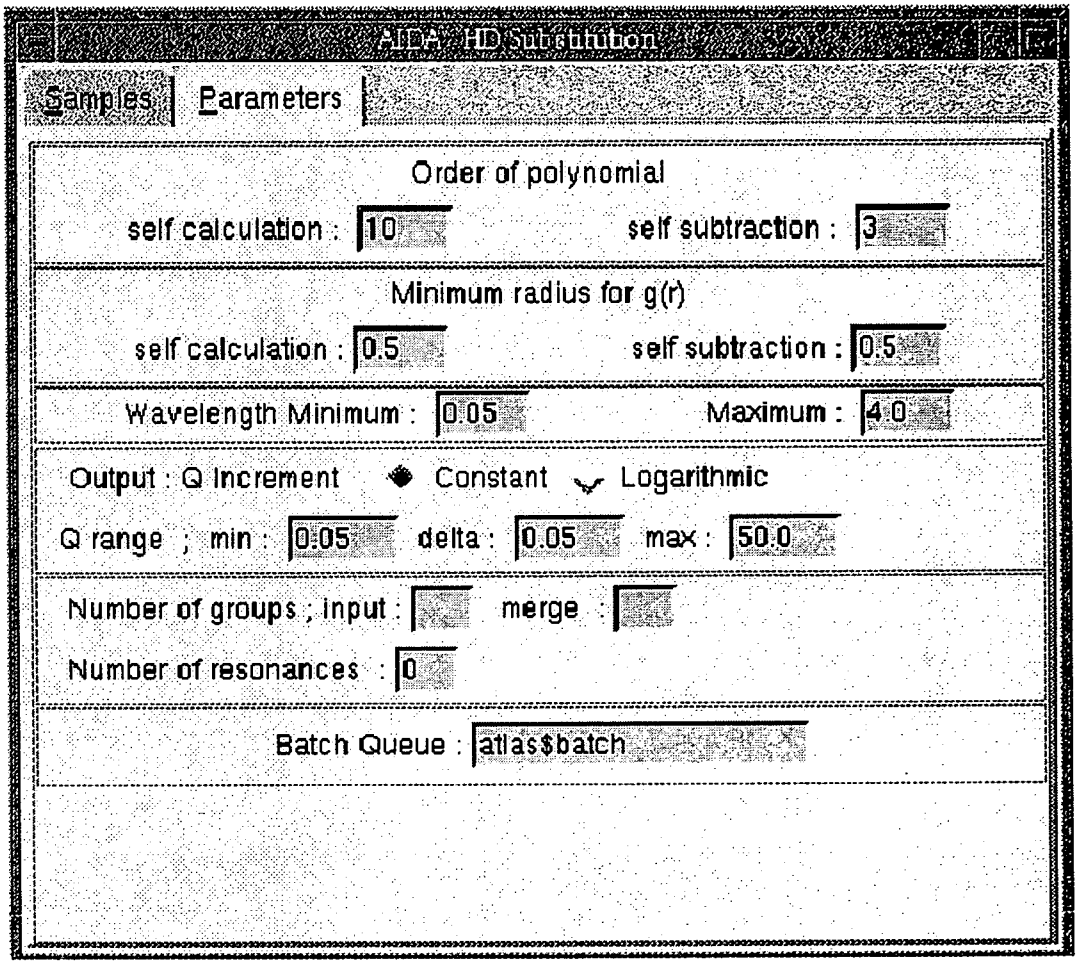
Frame 1 : If the HDSB_DAT file exists then this will show the message Data from File in blue and the entries in the subsequent boxes will be those from the file. Otherwise it will be blank and the entries will be blank or default values.

Frame 2 : is for the run numbers and the extension. The deuterium rich sample run number will be that given in Introit. The hydrogen rich and mixture sample run numbers can be input either by typing in the entry box or found using the Browse button.

Frame 3 : is for details of the samples.

The main button bar is along the bottom of this page only.

PAGE 2 : the Parameters page. Once set up this needs not to be changed or the default values can be used.



Frame 1 : defines the order of the polynomial.

Frame 2 : defines the minimum radius of g(r).

Frame 3 : defines the wavelength range.

Frame 4 : defines the Q range.

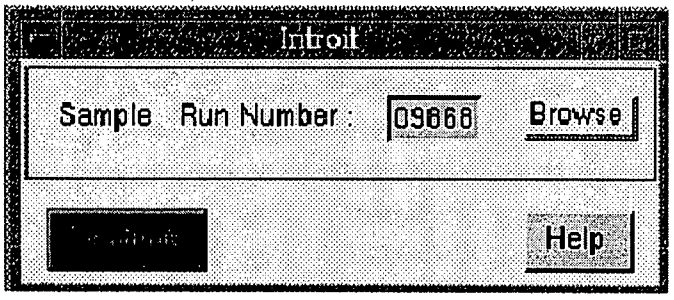
Frame 5 : defines the groups and resonances. The input value defines the number of groups in the input file. When a value is inserted in the merge box, a new window appears to define the groups to be used in the merging. If the number of resonances is greater than 1, a new window appears to input the minimum and mximum wavelengths for each resonance.

Frame 6 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.

12. McGofR

McGofR begins with an introductory Introit window.

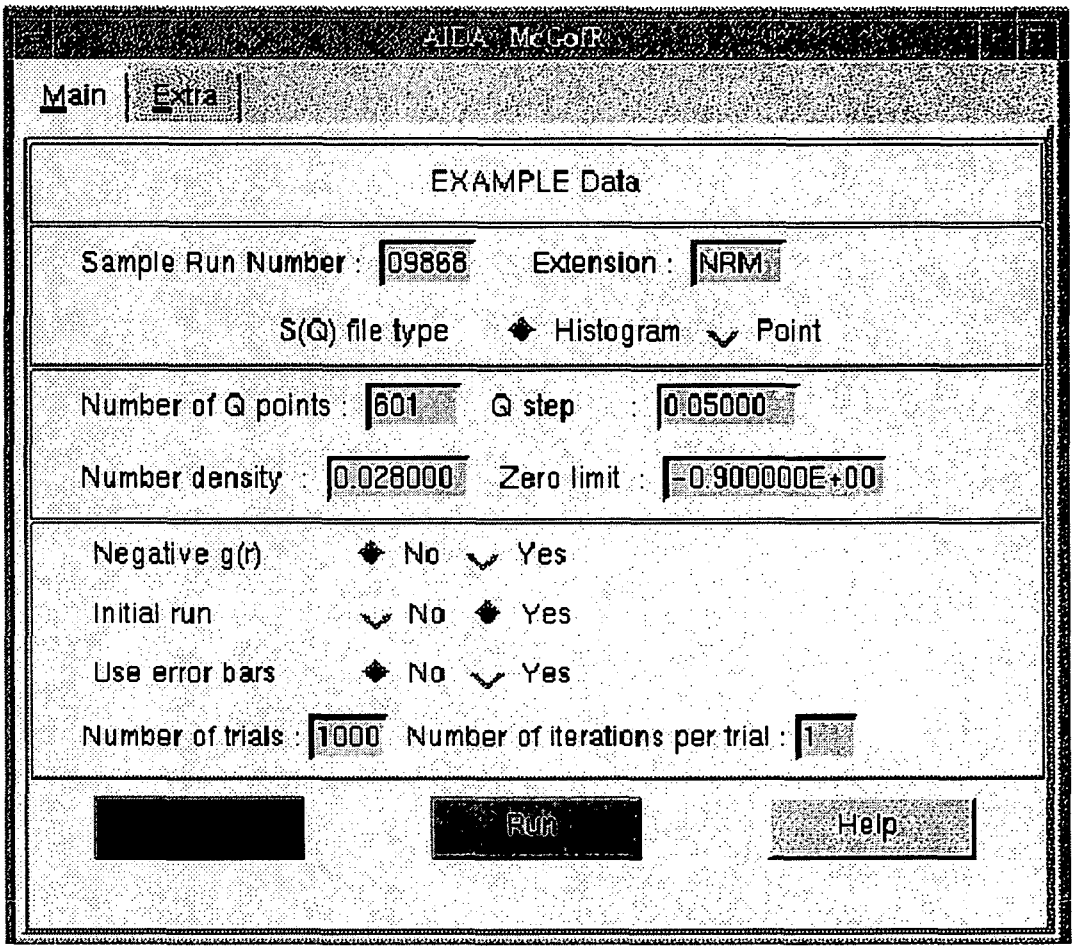


The input in this window is :
i) the sample run number - which can be input either by typing in the entry box or found using the Browse button.

The routine checks for the existence of a INP file before closing and opening the main McGofR window.

This window is in NoteBook form with 2 choices : Main and Extra.

PAGE 1 : The Main page. This is the one used most often.



Frame 1 : If the INP file exists then this will show the message EXAMPLE Data in red and the entries in the subsequent boxes will be those from the file. Otherwise it will be blank and the entries will be blank or default values.

Frame 2 : is for the sample run number and the extension. The sample run number will be that given in Introit. Radiobuttons define whether the S(Q) data is in histogram or point format.

Frame 3 : defines the Q range, the number density and the limit of S(Q) for Q=0.

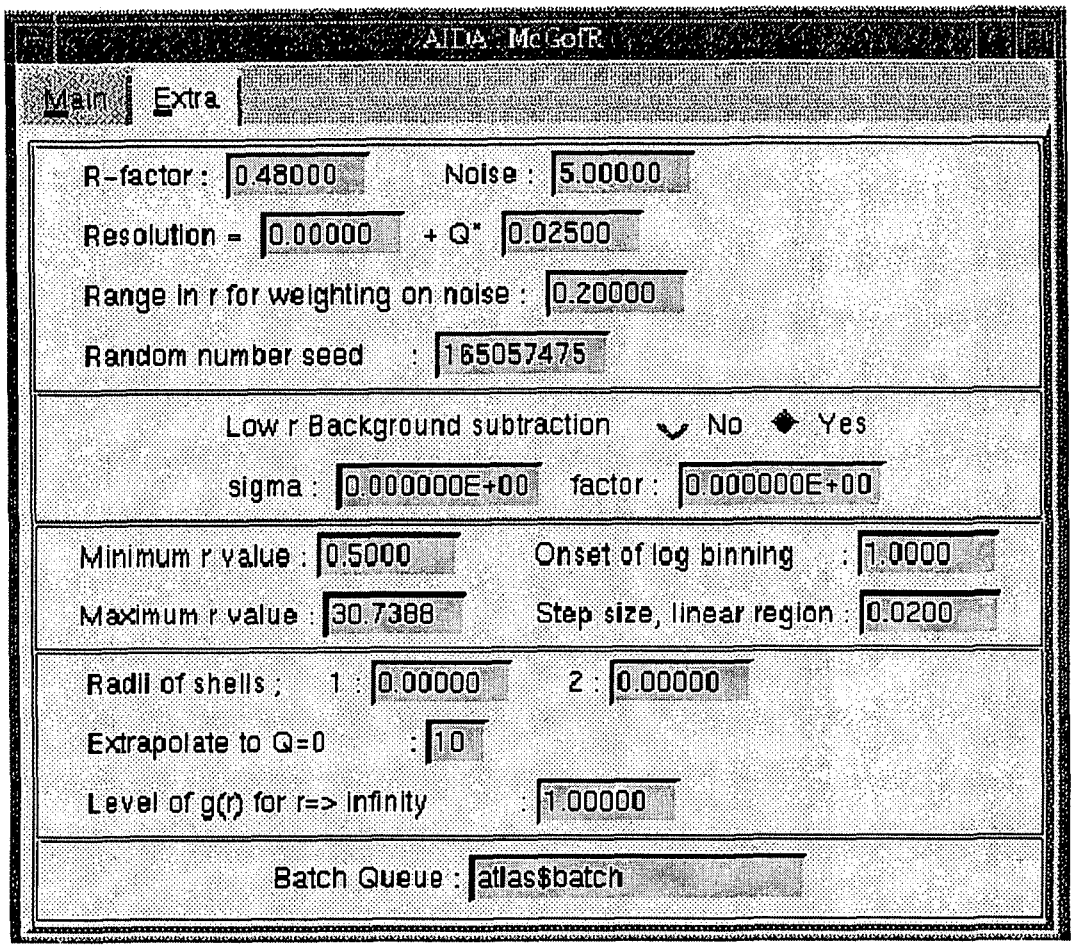
Frame 4 : has sets of radiobuttons to define :

whether g(r) is to go negative
whether it is the initial run
whether to use error bars

Then there are entry boxes for the number of trials and the number of iterations per trial.

The main button bar is along the bottom of this page only.

PAGE 2 : the Extra page. Once set up this needs not to be changed or the default values can be used.



Frame 1 : defines the R-factor, resolution and the random number seed.

Frame 2 : has radiobuttons to choose low r background subtraction and the associated parameters.

Frame 3 : defines the r range.

Frame 4 : defines the shells, the extrapolation to Q=0 and the level of g(r) as $r \rightarrow \infty$.

Frame 5 : If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted the Finale message window appears with the filenames of the Command file and the LOG files.