Midas Indirect Data Analysis Software (MIDAS)

Mantid release 2.6 – Aug 2013

MIDAS is a customized package running under Mantid for the analysis of data from Indirect Inelastic instruments such as IRIS & OSIRIS. It is based on the MODES OpenGenie package.

Details on Mantid can be obtained from its website where there is a web based user manual.
In Mantid there is the Help menu while in the MIDAS package the manual can be accessed from the Interfaces via a Help button marked with ?.

Mantid setup

In order to run MANTID, Midas needs to be setup:

- *View > Preferences...*

  Mantid > Instrument : set *Facility* to ISIS & *Default Instrument* to IRIS or OSIRIS

  General > Confirmations : this controls what happens when you try to close a window such as a plot.

- *Manage Directories* icon (finger pointing at folder) : add folder for RAW files in the *Data Search Directories* box & work directory in *Default Save Directory*
  These may not apply straight away so exit & start again.

- *View* > *Manage Custom Menus...* will open a new window. The right-hand box *Custom Menus* will have an item *&Interfaces*, click on the little arrow to open up its menu. The only ones required are *Convert to Energy, Indirect Data Analysis* and *Indirect Diffraction*. Click on an item not required to highlight it & then the << button to remove it.

- *View* > *Results Log*. A box labelled *Results Log* will appear. Information on the running of a routine will be in blue; error messages in red. To activate this right-click in the box and for *Log Level* select *Notice*. Eventually this will be controlled with the *Verbose* option on the Interfaces.

MIDAS

The package has a selection of customised *Interfaces* each with several *Tabs*. Each tab runs a routine which is the equivalent of a MODES program.

Several tabs have a small embedded plot (miniPlot) which shows the data with horizontal or vertical coloured lines. These lines either just show information or are interactive and can be moved with the cursor. In both cases the position of the line is linked to the value of a variable in a box usually on the left of the plot. Results are usually plotted in individual windows.

Files created in the work directory are usually in the Nexus format with the extension nxs. The naming convention is different to that in MODES which uses the extension to define the type of data.

In MIDAS the file name will describe this type. In MODES, most of the routines take the run-number as input: in MIDAS, files are selected by typing its name or using the Browse button. When browsing files the usual selection criteria apply – using ctrl or ^ to pick multiple files.

In some tabs the Input type can be selected to be either File or Workspace. When the latter is selected a drop-down list appears of suitable workspaces.

Workspaces

The output of routines is stored in a Workspace whose name appears in the Workspace window. The naming convention is that it starts with *<instrument><run-number>_<analyser><reflection>* where *<run-number>* does not have leading zeroes & *<instrument>* depends on whether the run-number is in 5 digit or 8 digit format; for 5 digit *<instrument>* is the 3 character abbreviated form whereas for 8 digit it is the full name. The name then follows with words/codes specifying the type – the routine that created it & any options. The name may then end with a pseudo-extension – for example, *_red* for reduced data from *EnergyTransfer*, *_res* for resolution, *_iqt* for I(q,t) and *_sqw* for S(Q,w).

When a Workspace is saved to a nxs file the file name is the WS name with the extension *.nxs*.

Double-clicking on the WS name will open up the workspace table showing the x,y,e values under their tabs. The data is usually in histogram form so that the number of x-values is the number of y/e-values plus 1. The columns correspond to the x-values, are numbered from 0 and are often referred to as bins. The rows are the histograms also numbered from 0, correspond to the angles/groups/Q and are often referred to as spectra, numbered from 1. In some workspaces the histogram is given a hidden different value such as Q.

Right-clicking on the WS name brings up a menu of operations that can be performed on the WS, such as:

Show Data - opens the WS table.
Show Instrument - opens a 3D display of the instrument layout.

Plot Spectrum ... - plots the specified histograms/spectra with or without error bars.
Show Image Viewer - produces a contour plot with horizontal & vertical slices for cursor position.
Color Fill plot - gives a contour plot.

Show detectors - opens the detector table showing eg the detector angles.
Sample logs .. - shows the logged variables.

Right-clicking on the WS table also gives a menu of operations. In particular, rows or columns can be selected & highlighted and the menu then allows plotting. *Plot bin* is used for the columns and *Plot spectrum* for the rows.

Convert to Energy

An overview is given in http://www.mantidproject.org/Indirect

- *Energy Transfer*

MODES routine ICON/IONIAN. For input of raw file names : either Browse or type in name OR type in run-numbers (for many runs use ‘,’ to separate runs and ‘-‘ between 2 run-numbers for a sequence).

New options:

Scale the intensity by multiplying with a specified factor eq for absolute normalisation.

Read the SE log files so that a temperature, say, can be used in a subsequent program like ElWin.

http://www.mantidproject.org/Indirect:EnergyTransfer

- *Calibration*

MODES routine Calib in the top half of window. Select raw file & plot to activate miniPlot. Select time ranges by typing in boxes or using cursor plotted lines (blue for peak; green for background)

MODES routine ResMEM in the bottom half. This creates the equivalent of the PG002.res (eg) file. Tick box, plot & adjust parameters.

http://www.mantidproject.org/Indirect:Calibration

- *Diagnostics*

MODES routine Slice (time). Select file, plot & adjust parameters.

http://www.mantidproject.org/Indirect:Diagnostics

- *S(Q,w)*

Convert data into S(Q,ω) on a specified Q, ω grid

http://www.mantidproject.org/Indirect:SofQW

Indirect Data Analysis

An overview is given in http://www.mantidproject.org/IDA

- *Elwin*

MODES routine Int>Elwin.

Now reads a temperature parameter - currently default 'sample'. It first checks the Log parameters in the Workspace. If not there, it looks for a log file to read and if that does not exist, it uses the run-number instead.

Three workspaces & nxs files are created with a histogram for each run. *_eq1 is Intensity v Q. *_eq2 is log(Intensity) v Q^2 - primarily for use as input to msdFit. The histograms are labelled by Temperature or Run-number (last 3 digits). *_elf is a transpose of eq1 so that the histograms are in Temperature and labelled by Q.

Their names are of the form *<instrument><first-run>_to_<last-run>_e**.

New option for eq1 : Normalise to Lowest Temperature. All histograms are scaled to the intensity of the lowest Q value of the lowest temperature run. It is assumed that the temperature range either decreases or increases regularly so it determines the lowest temperature form the first & last runs.

Plotting can be as a graph, a contour & 3D plot.

http://www.mantidproject.org/IDA:Elwin

- *MSD Fit*

MODES routine Function>Msd Fit

This has been modified so the Help page is not correct. The input file (named *<inst><first-run>_to_<last-run>*_eq2) can be selected with Browse. The routine fits log(intensity) v. Q^2 with a straight line for each run specified to give the Mean Square Displacement (msd). Then it plots the msd as function of Temperature or Run-number (last 3 digits).

The fitted parameters for all runs are in **_msd_Table* and the <u2> in **_msd*.

The fitted data are in the group WS *_Result with a WS for each spectrum/histogram labelled Data, Calc and Diff where Diff is the difference between the input Data and the Calculation.

http://www.mantidproject.org/IDA:MSDFit

- *Fury*

MODES routine Function>Fury

The FT works in point mode rather than histogram mode so I(Q,t) begins with t=0 .

http://www.mantidproject.org/IDA:Fury

- *FuryFit*

  MODES routine Function>Fqt Fit

  In the miniPlot use the cursor to define StartX,StartY (blue) and Background (green). When *Plot Guess* is ticked typing in a parameter value will plot the guess of the function in red.

  The fitted data are in the group WS *_Result with a WS for each spectrum/histogram labelled Data, Calc and Diff where Diff is the difference between the input Data and the Calculation.

  http://www.mantidproject.org/IDA:FuryFit

- *ConvFit*

  MODES routine Function>Swift

  In the miniPlot use the cursor to define StartX,Starty (blue) and Background (green). When *Plot Guess* is ticked typing in a parameter value will plot the guess of the function in red. The width (FWHM) can be adjusted using a red line.

  The fitted data are in the group WS *_Result with a WS for each spectrum/histogram labelled Data, Calc and Diff where Diff is the difference between the input Data and the Calculation.

  http://www.mantidproject.org/IDA:ConvFit

- *Calculate Corrections*

  MODES routine Analyse>Acorn

  Runs a Fortran program using F2Py

  http://www.mantidproject.org/IDA:AbsF2P

- *Apply corrections*

  MODES routine Analyse>Analyse

  If just subtraction (no corrections) the output file name is *<samplerun>_subtract_<canrun>* ; if corrections are applied its name is *<samplerun>_correct_<canrun>*.

  The corrected data are in the group WS *_Result with a WS for each spectrum/histogram labelled Sample, Can and Calc where Sample & Can are the input data and Calc the corrected result.

Plot Output can be as spectra or contour or both.

The *Plot Contributions* plots of sample & can with corrected sample for the first group.

There are 2 output files: **_red* is in the reduced format ie histogram in spectrum number and **_sqw* is S(q,w) format ie histogram in Q. The former allows the file to be used in other routines, such as SofQW & Fitting. The latter is for info.

http://www.mantidproject.org/IDA:AbsCor

- *VIZ*

Mantid now has an in-built routine *ImageViewer* which is a more sophisticated version.

On the right-hand there is an option selection for type of instrument – choose *Indirect Geometry*. It may not read the value of Efixed properly – this can be changed.

The colour can be changed using the menu – Rainbow is quite good.

http://www.mantidproject.org/MantidPlot:_ImageViewer

Python algorithms

The following selection can be run from the *Algorithm > Workflow > MANTID* menu.

The Algorithm generates a simple interface for input parameters. The input can be in either a nxs file or a workspace. The names of the parameters should be obvious but holding the cursor over the parameter name will produce a box with a further description (if I've done it!). Eventually these will be customised Tabs in the main Interfaces.

1. *IDAtransmission*

   As Trans in MODES. Input is sample and background/can run-number. Plot is of sample & can normalised transmission monitor and transmission. Result WS is **_Trans*.

2. *Moments*

   Calculates the moments of S(q,w) from a sqw nxs file. The range of energy for the integration can be specified and the intensity can be scaled.

3. *MuscatData/Func*

   Multiple scattering corrections similar to Modes routine Analyse>MINUS. See WSH for details

4. *Symmetrise*

   Converts an energy asymmetric spectrum into a symmetric version. It assumes that the positive energy range is greater that the negative range. A Cut value (xCut) is input so that the energy range < -xCut is removed and the energy range > xCut is reflected about –xCut to give a symmetric spectrum. The input is a *_*red* workspace and the output a *_*sym* workspace.

5. *FuryFitMultiple*

   Runs a variation of FuryFit for a stretched exponential in which the beta value is tied to be the same for all spectra/Qvalues.

Bayes fitting Fortran programs run using F2Py. Available for Windows 32bit & 64bit in download and Linux 64bit from WSH. Eventually these will be customised tabs in IDA interface.

1. *QLines*

   Program options are : *QL* for quasilines or *QSe* for stretchedExp. *ResType* is Data for resolution as data in *_*red* file (many spectra) or Res for *_*res* file (1 spectrum). *ResNorm* to use the res file created by ResNorm. The plot output is : Probability (for QL), Intensity, FwHm (for QL it is FW11,FW21 & FW22), Beta (for QSe) and Fit (first spectrum only & for QL just for 1 peak). The WS are : *_*Prob* for the probability; *_*Parameters* grouped widths & intensities; *_*Fit* grouped Data, Fit1, Res(idual)1, Fit2, Res2. Also lpt & Ascii files as in MODES.

2. *ResNorm*

   As in MODES. Plots are of : Intensity, Stretch parameter; Fit. Output WS are : *_*ResNorm_Paras* grouped as Intensity & Stretch; *_*ResNorm_Fit* grouped as Data and Fit. Also lpt file.

3. *Quest*

   Stretched exp fitting mapped in Sigma/Beta space. The plot output is contour plots of Sigma and Beta v. Q. WS output is: *_*Qst_Fit* grouped as Sigma & Beta; *_*Qst_Contour* grouped contours of fit in Sigma/Beta space for each spectrum.

4. *JumpFit*

   Jump fit for Chudley-Elliot & Singwi-Sjolander. *QLprogram* is the program that produced the file – *QLr* for res or *QLd* for data. Plot output shows data with fit. Result is in WS *_*<fit-type>fit_<width-number>*.

ForCE – For(eign) C(hange to)E(nergy)

Reads Ascii data from non-ISIS facilities. Currently supports IN10 & IN16 with Ascii format as Raw (<*name*>.asc) or INX output (<*name*>.*inx*). Workspace created is <*Instr*>_<*name*> and Output file is <*Instr*>_<*name*>_*red*. *Plot* is as spectra or contour.

Development versions for IN13 also available.

Development routines

These are available on the server \\britannic\modes3\Midas and on the web site.

1. MolDyn

   Reads acscii files from the program nMolDyn and creates workspaces & nxs files suitable for use in the MIDAS package.

2. ESRF

   Reads ascii files of S(Q,w) and creates workspaces & nxs files suitable for use in the MIDAS package.

Worked examples

These are available on the main Mantid webpage under Examples in the menu on the left hand edge to go to http://www.mantidproject.org/Mantid_Examples

Under *Contents* go to *3 Do it yourself examples* and then choose *Indirect Inelastic Conversion to Energy* or *Indirect Data analysis*.

Script repository

The new script repository *File->Script Repository* is a tool to download/upload scripts to the Mantid script repository as a way to share scripts with other Mantid users.

When you first use the script repository it will ask you to specify where to install the repository. This can be any directory, including one where you already have some scripts.

It is envisaged that it will be used for upgraded and development files.

Glossary of MODES equivalents in MIDAS

C2E refers to the Convert to Energy interface

IDA refers to the Indirect Data Analysis interface

1. RAW

1.1 Icon	C2E: Energy Transfer tab
1.2 Demon	Indirect Diffraction interface
1.3 Calib	C2E: Calibration tab – top half
1.4 Slice	C2E: Diagnostics

2. INT

2.1 Ionian	C2E: Energy Transfer tab
2.2 Dorian	Indirect Diffraction interface
2.3 Elwin	IDA: ElWin tab
2.4 S(Q,w)	C2E: S(Q,w) tab
2.5 Bin>Ascii	Mantid algorthim: SaveAscii
2.6 Ascii>Bin	Mantid algorthim: LoadAscii

3. ANALYSE

3.1 Acorn	IDA: Calculate Corrections tab
3.2 Minus	PythonAlg: MuscatData or MuscatFunc
3.3 Trans	IDA: Calculate Corrections tab
3.4 Analyse	IDA: Apply Corrections tab

4. FUNCTION

4.1 Fury	IDA: Fury tab
4.2 Fqt Fit	IDA: FuryFit tab
4.3 Swift	IDA: ConvFit tab

4.4	MSD fit	IDA: MSD Fit tab

5. BAYES

5.1	ResMem	C2E: Calibration tab – bottom half (Not Bayes smoothing)
5.2	ResNorm	PythonAlg: ResNorm
5.3	QL function	PythonAlg: QLines
5.4	Str function	PythonAlg: QLines
5.5	QL data	PythonAlg: QLines
5.6	Stretch>bet/sig	PythonAlg: Quest
5.7	Jump fit	PythonAlg: JumpFit

6. FILE

6.1	Read Int	Mantid algorthim: Load
6.2	Write Int	Mantid algorthim: SaveNexus
6.3	Export	Mantid algorthim: SaveDASC or SaveSPE
6.4	Import	Mantid algorthim: LoadDaveGrp or LoadSPE

7. DISPLAY

7.1	Contour	WS name right-click: Colour Fill plot
7.2	Viz	WS name right-click: Show Image Viewer
7.3	3D	*no equivalent in Modes* Open the workspace and the Mantid menu will then show *3D Plot*. The menu will give Contour & various 3D plots.

Appendix A : Fit Function

This is an in-built Mantid toolkit for creating personalised fitting routines. An example is given for creating a FuryFit-like procedure. To start either run *View > Fit Function* & select the Workspace or open a Workspace and plot the spectrum/histogram to be fitted whereupon the *Fit button* (with the peak icon) is enabled. This opens the *Fit Function* window.

Select the fitting range by either moving the vertical blue lines or typing in the boxes.

From the *Display* menu enable *Plot Guess*.

Right-click on *Function* & select *Add function*. In the new window select *Background > FlatBackground*. Click on the *f0* + or arrow symbol to open up the details.

Right-click on *Function* & select *Add function.* In the new window select *General > ExpDecay*. Click on *f1* to open up the details.

Enter start values and run with *Fit > Fit*. For a sequential fit run *Fit > Sequential Fit*. In the new window select the parameter to plot, enter *Range* in format first:last and *Fit*.

In FuryFit, the background & height are linked to be = 1 - so right-click on *f1.Height*, select T*ie > CustomTie* & enter *1-f0.A0*. This option then appears in the box. Run as above.

To use a stretched exponential, right-click on *f1.ExpDecay* and *Remove*. Add the *Function General > StretchExp*. Set-up the tie and *Fit*. As an extra option, right-click on *f1.Stretching*, select *Fix* & run a *Sequential Fit*. This will keep Stretching the same for all spectra.

(As of 19 June, there is a bug in the release version of StretchExp so the NumDeriv box needs to be ticked to be True. This has been cured in overnight builds.)