DECON

Update 5 July 2017

DECON is a customized package running under Mantid for the deconvolution of S(Q) data. Whilst it was developed for S(q) or rather S(theta) it can be used for powder diffraction.

Details on Mantid can be obtained from its website where there is a web based user manual. In Mantid there is the Help menu.

1 Mantid setup

In order to run DECON, Mantid needs to be setup:

- *View > Preferences...*

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

- *Manage Directories* icon (finger pointing at folder) :

- RAW files go into the *Data Search Directories* box but is not used by Decon & the 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. 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 *Information*.

2 Python

There are 2 ways of running Python:

iPython - this is a window for command line running of Python. It is launched from *View > Launch IPython Console*.

Script Window is launched from *View > Script Window*. Python scripts can be written & edited in the window and then *Executed*.

3 Algorithms

The package consists of a set of algorithms. There are 2 'basic' algorithms and a set of 'wrapper' workflow algorithms specific to instruments or techniques. These wrapper algorithms run the basic algorithms. The wrappers also provide options of Plottin data and Saving results.

3.1 DeconCalculateDerivatives

Input is a workspace containing the data eg S(theta). The data is smoothed and the result appended to the input workspace. The derivatives are calculated using the smoothed data and and the results are in the output workspace.
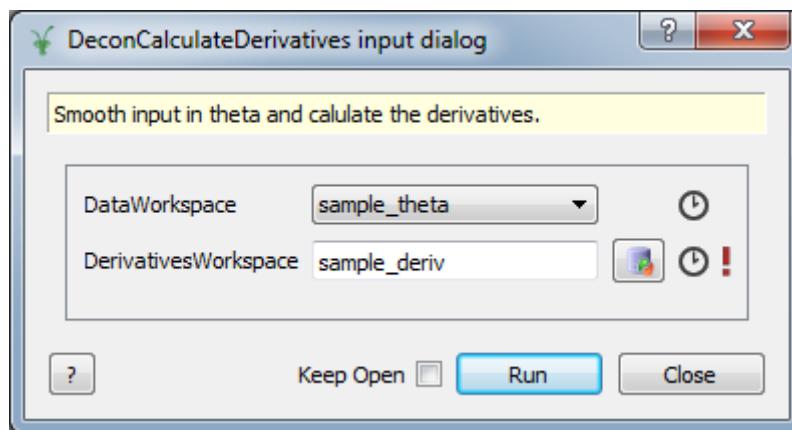
3.2 DeconApplyCorrections

Input are the 3 workspaces for data, derivatives and moments. The corrections are calculated and applied to the data. There are several output workspaces with names created by adding a suffix to the data workspace name :

_theta_used is the form of data used for the corrections – smoothed or unsmoothed

_coeff : moments 1 to 4 are normalised to M0. The coefficients (combinations of moments) are calculated and put into this workspace as 4 histograms.

_corr : the coefficients are multiplied by the derivatives and put into this workspace as 4 histograms. The input data has successive corrections subtracted and the results are in workspace *<sofq_name>_result* as 4 histograms.

_result : The input data has successive corrections subtracted and the results are in this workspace as 4 histograms.

*_corrected_ : the correction terms are truncated at the cutoff point, the selected number of terms subtracted from the input data and the input data above the cutoff point spliced on. The result is in this.

Input parameters are :

- UseSmoothData : tick if the smoothed data is used for the corrections

- Number of terms to use : number of correction terms to use for final output

- Cutoff : tick if corrected data is to be cutoff at high angle

- CutoffPoint – if Cutoff is True, corrected data above this value will not be used
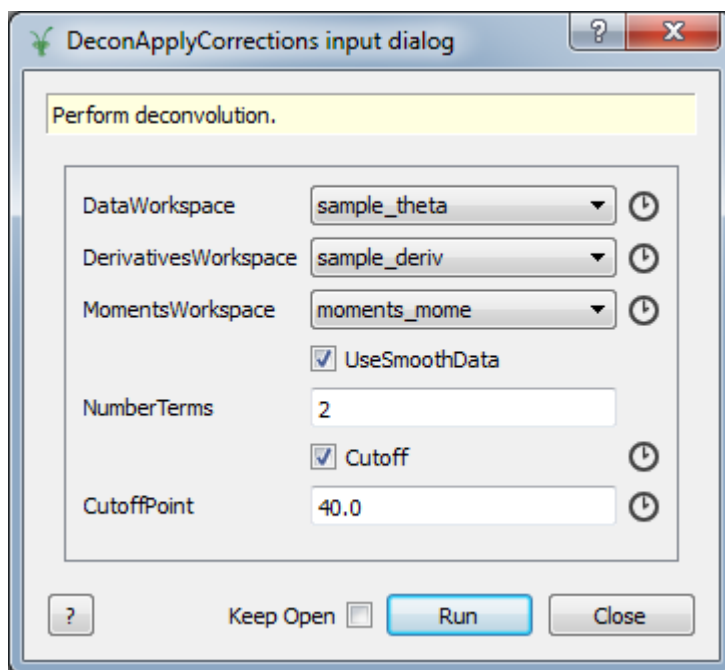

3.3 DeconD4LoadSofQ

This is part of the wrapper for reading D4 data.

The input parameters are:

- FilePath : full path name for the input file.

- Wavelength : for Q input only, lambda to convert to 2theta

- Zero : zero angle correction

If type is Q the file *<file_name>.soq* is read into the workspace *<file_name>_Q* and is converted into 2theta in workspace *<file_name>_theta.* If the type is Angle, the file *<file_name>.sot* is read into the workspace *<file_name>_theta* as the first histogram.
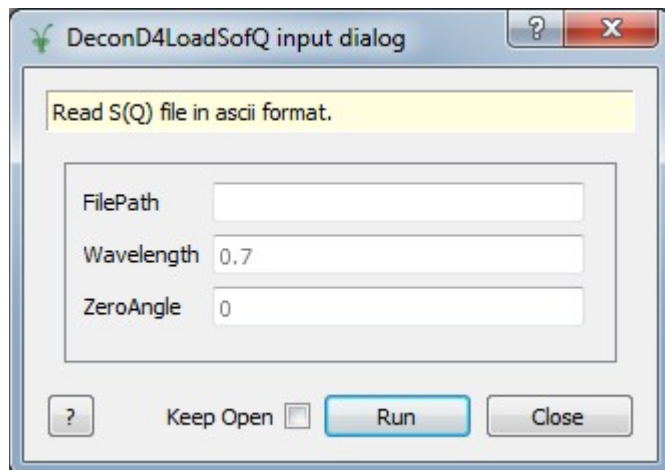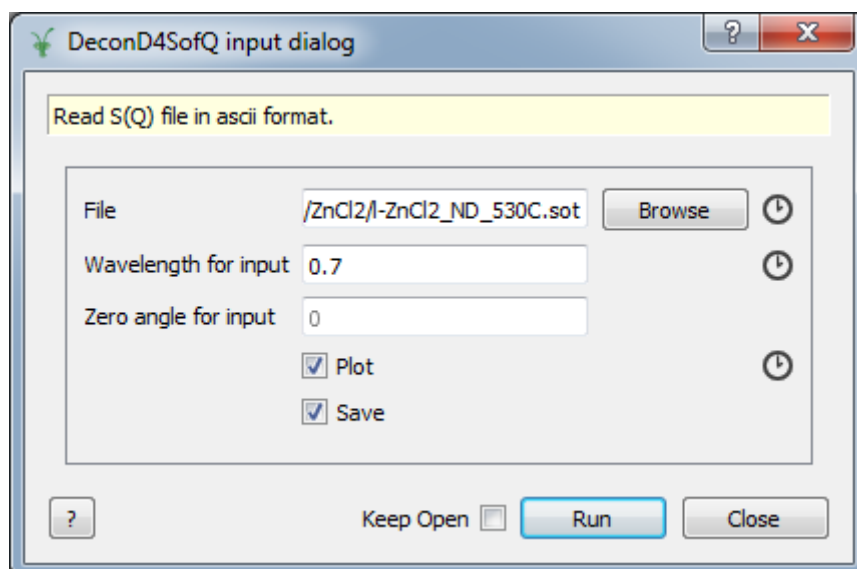

3.4 DeconD4SofQ

This is the main wrapper for input D4 data.

The input parameters are:

- Structure file name : assumes the extension is *sot* for Angle or *soq* for Q

- Wavelength for input : for Q input only, lambda to convert to 2theta

- Zero angle for input : zero angle correction

The ascii file is read using the algorithm DeconD4LoadSofQ.

For both types of input (theta or Q), if smoothing is performed the result is the second histogram of the *<file_name>_theta* workspace and the difference in the third.

The first 4 derivatives are calculated and put into workspace *<file_name>_deriv* as 4 histograms.

Plot gives a graph of input data with smoothed version, if performed and another of the 4 derivatives.

The header text info and Smooth option are written to the *Sample Log.*

3.5 DeconD4Moments

This is a wrapper type algorithm for D4 moments which just reads the moments ascii file to create the workspace.

The input parameters are:

- Moments file name : assumes the extension is *mom*

- Freeze : tick for the freeze option

- Freeze point : if Freeze is True, the freeze point in 2theta

The file *<mome_name>.mom* is read into workspace *<mome_name>_mome* as 5 histograms. Values for angles less than the freeze point are set to the value at the freeze point.
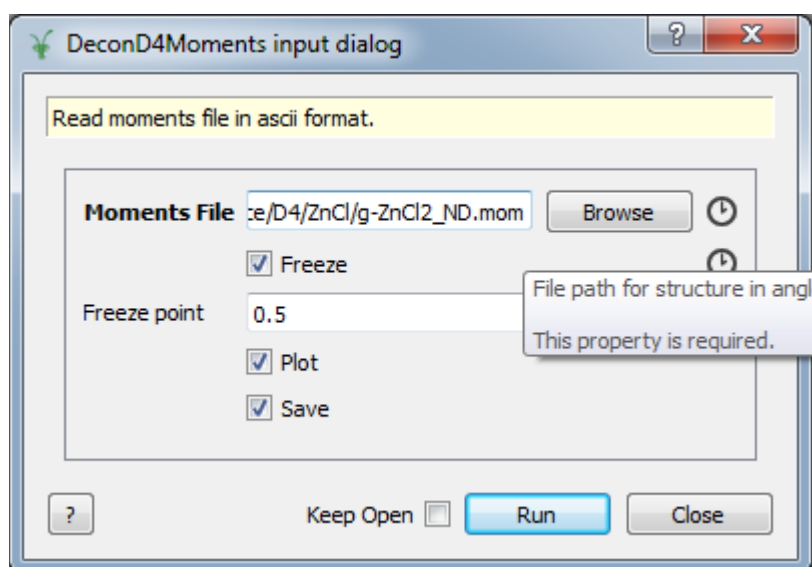
Plot gives a graph of M0 and another of M1-4.

The header text info and Freeze parameters are written to the *Sample Log.*

3.6 DeconD4Result

This is a wrapper type algorithm for D4 which converts the result in theta back to Q.

The input parameters are:

- CorrectedWorkspace : name of input workspace containing the results in angle

- QWorkspace : name of output workspace for the results in Q

- *Wavelength : lambda to use for output conversion to Q*

- ZeroAngle : zero angle correction for output conversion to Q

- RebinOption : None, Interpolate or Spline

- RebinQrange : origin of range either New or Snap to original Q range (if input was in Q)

- RebinQinc : if rebin range is New, the Q increment & the range is *0,deltaQ, Qmax*

If Rebin has been selected, the final S(Q) in rebinned either by interpolation or spline and either to New Q-range or Snapped back to Q-range of input S(Q) if it exists.
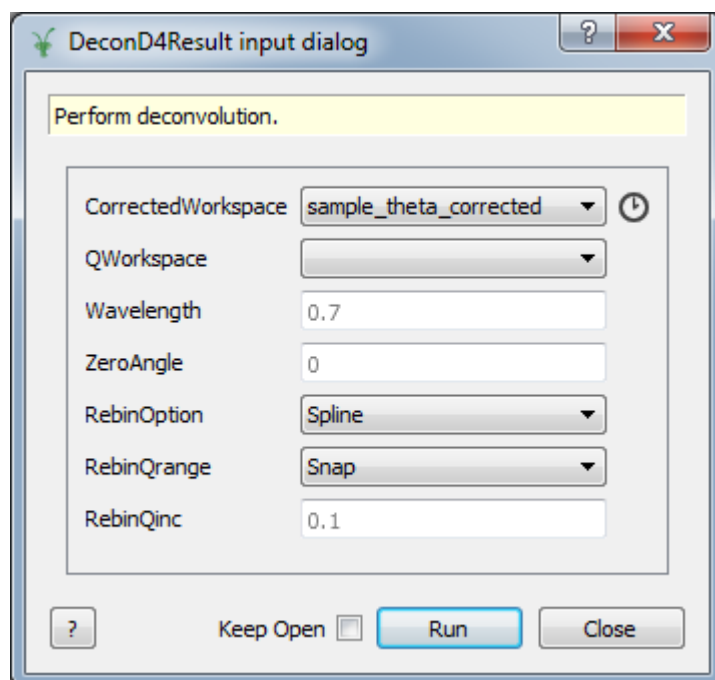
The header info for the S(theta) & moments are copied to the *Sample Log* of the various workspaces and all the options & parameters are also added.

3.7 DeconD4Correct

This is the wrapper for applying the corrections to D4 data. It uses the algorithm DeconD4Result.

The S(theta) & moment input can be either the existing workspace or read from a previously created NXS file.

The input parameters are:

- S(theta) Input : whether Workspace or Nxs file

- S(theta) Workspace : name of workspace if workspace used

- S(theta) File : name of file if file used. Browse may be used

- Derivatives Input : whether Workspace or Nxs file

- Derivatives Workspace : name of workspace if workspace used

- Derivatives File : name of file if file used. Browse may be used

- Moments Input : whether Workspace or Nxs file

- Moments Workspace : name of workspace if workspace used

- Moments file name : name of file if file used. Browse may be used

- QWorkspace : name of output workspace for results in Q

- Use Smooth S(Q) : tick if the smoothed data is used for the corrections

- Number of terms to use : number of correction terms to use for final ouput

- Cutoff : tick if corrected data is to be cutoff at high angle

- Cutoff point – if Cutoff is True, corrected data above this value will not be used

- Wavelength for output : lambda to use for output conversion to Q

- Zero angle for output : zero angle correction for output conversion to Q

- Rebin option : None, Interpolate or Spline

- Rebin Qrange : origin of range either New or Snap to original Q range (if input was in Q)

- Rebin Qinc : if rebin range is New, the Q increment & the range is *0,deltaQ, Qmax*

DeconD4Correct input dialog

Perform deconvolution.

S(theta) Input	File ▾	🕐
S(theta) Workspace	▾	
S(theta) File	D4/Example/sample_theta.nxs	Browse 🕐
Derivatives Input	File ▾	🕐
Derivatives Workspace	▾	
Derivatives File	/D4/Example/sample_deriv.nxs	Browse 🕐
Moments Input	File ▾	🕐
Moments Workspace	▾	
Moments File	I/Example/moments_mome.nxs	Browse 🕐
QWorkspace	sample_Q	🖳 🕐
	☑ Use Smooth S(Q)	🕐
Number of terms to use	2	
	☑ Cutoff	🕐
Cutoff point	45.0	🕐
Wavelength for output	0.7	🕐
Zero angle for output	0.151	🕐
Rebin option	Spline ▾	🕐
Rebin Qrange	Snap ▾	🕐
Rebin Qinc	0.1	
	☑ Plot	🕐
	☑ Save NXS format	🕐
	☑ Save ASCII format	🕐

Keep Open ☐   Run   Close

?

Plot gives graphs of original & corrected data in theta and Q.

If *SaveAscii* has been selected, an ascii file of the final corrected S(theta) & S(Q) are created with the extensions *.stc* & *.sqc* respectively.

4. Installing DECON

The DECON package consists of the following files:

 Python algorithm files (extension py) : *DeconCalculateDerivatives, DeconApplyCorrections, DeconD4SofQ, DeconD4Moments, DeconD4Result & DeconD4Correct*

The algorithm files go into the directory *../plugins/python/algorithms/WorkflowAlgorithms*.

The algorithms can be started in 2 ways:

- type the algorithm name into the *input box.* As a character is input a drop-down menu is displayed of algorithms beginning with the characters typed. Select the algorithm and *Execute*.

- in the menu of algorithm categories, expand *Workflow*, then expand *DECON* and finally double-click on the algorithm.

All algorithms have a graphic user interface for input. Some have control options with tick boxes:

- *Plot* activates the plotting of customised graphs

- *Save* activates the creation of NXS files of the workspaces. In *DeconCorrect* there are 2 options S*ave NXS* and *Save ASCII* for ascii data.

5 Mantid utilities

5.1 Plots

Double-clicking on an item in the window opens a window with edit options. Examples include: changing scale ticks & axis limits; removing & adding curves; changing to logarithmic values.

5.2 Workspaces

The output of routines is stored in a Workspace whose name appears in the Workspace window.

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.

Plot Spectrum ...   - plots the specified histograms/spectra with or without error bars.

Sample logs ..   - lists parameters stored such as the text lines from the data file, options selected & variables input.

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.