Setting Up OpenGENIE to Analyse Polaris Data

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OpenGENIE can be downloaded from the web.

- Go to www.opengenie.org, select the "Download OpenGENIE" hyperlink and choose the appropriate version.
- An auto-installer guides you through the installation process - proceeding with the default options when offered a choice will work perfectly well.

After installing OpenGENIE there are a few quick steps to follow so that you can work on your Polaris data on your own PC. These steps are all described in detail below.

1. Create a "PolOpenGenie" folder on your C:\ drive and download a set of Polaris-specific OpenGENIE scripts and data files into this folder.
2. Modify the default OpenGENIE startup file so that it loads commands for processing Polaris data.
3. Modify the "Genieinit_pol.gcl" file (which you have downloaded in step 1, above) so that it knows where on your computer to look for the RAW data files.
4. Change the default working directory to something more suitable (optional).
5. Download your Polaris RAW data files from the ISIS web site.

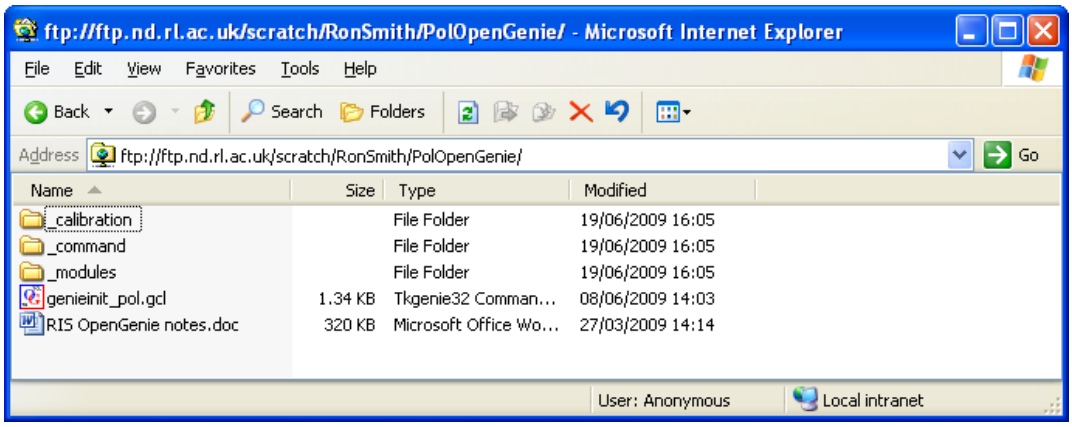
1. Create a "PolOpenGenie" Folder

First, create a "PolOpenGenie" folder on your C:\ drive, and then use a web brower to navigate to ftp://ftp.nd.rl.ac.uk and download a set of Polaris-specific OpenGENIE scripts and data files into this folder.

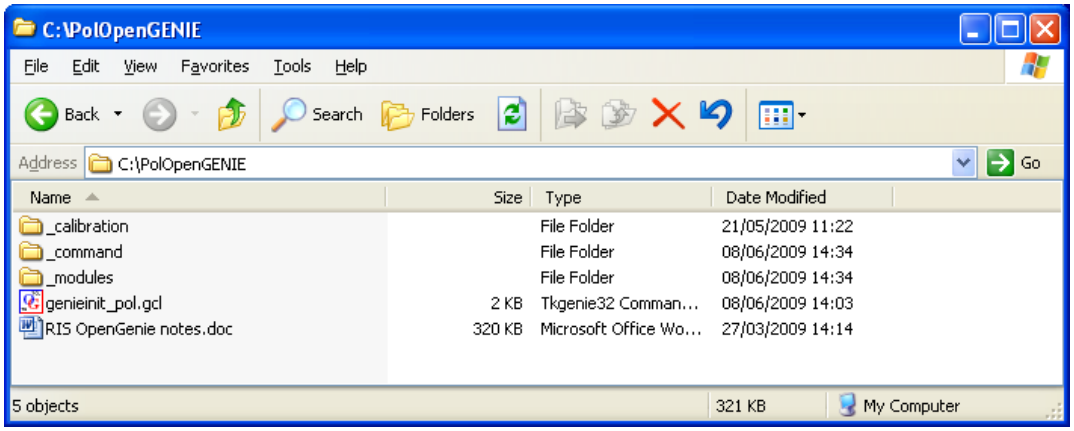
(in Internet Explorer 7 select *Page - Open FTP Site in Windows Explorer* to enable drag-and-drop copying of files/folders)

- select folder / directory Scratch
- select folder / directory RonSmith
- select folder / directory PolOpenGenie

You will now have the view shown below:
(note: the file names and dates you see may differ from those in the screen captures below as programs or data files are updated, or new ones added)



Copy these folders and files into the C:\PolOpenGenie folder you have just created. You should then have the directory / folder structure shown below on your own PC:



The _calibration folder holds standard background and vanadium data files used when normalising Polaris data. It also contains files giving details of detector positions, which are required to focus the data.

The _command folder holds .gcl script files containing OpenGENIE procedures to focus, normalise, apply attenuation corrections, write GSAS format files, etc. (note: some of these .gcl files contain more than one procedure).

The _modules folder holds the (Fortran) executable files used in some of these procedures (e.g. setup_correct, correct, and routines to write GSAS, Fullprof, etc. format data files).

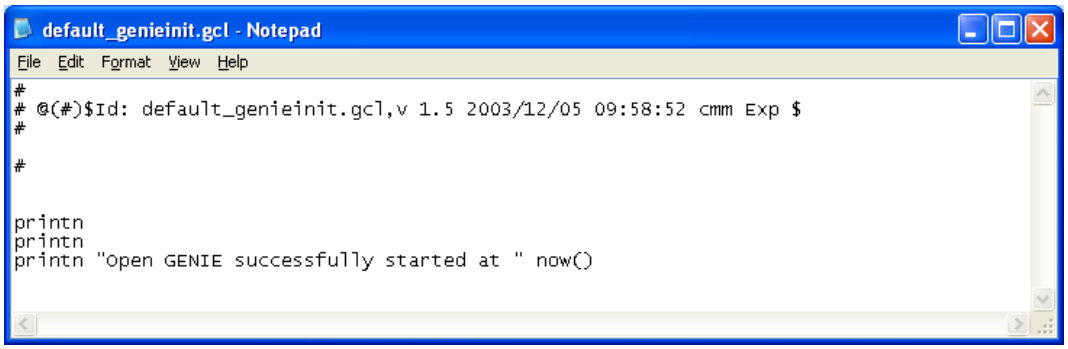
The "*RIS OpenGenie notes.doc*" file has now been replaced by this file (*Installation Notes.pdf*) and contains these installation instructions along with notes on the commands available in OpenGENIE for processing your Polaris data.

2. Modify "default_genieint.gcl" file

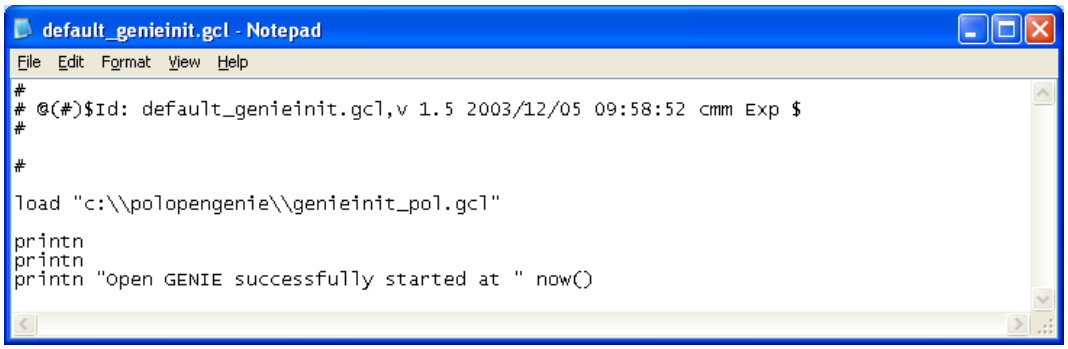
A startup file "default_genieinit.gcl" is run every time OpenGENIE is started. This file is in the location:

C:\Program Files\CCLRC ISIS Facility\Open GENIE\src\gcl\default_genieinit.gcl

The file that installs with OpenGENIE is shown below:



This file needs to have an extra line added to it so that it loads a file which defines all the commands which are needed to analyse Polaris data. Open the file in Notepad (or any other text editor) and add the line `load "c:\\polopengenie\\genieinit_pol.gcl"` to it:



(note the use of double backslash characters, which are required in OpenGENIE to indicate the single backslash character used in labelling Windows folders and directories).

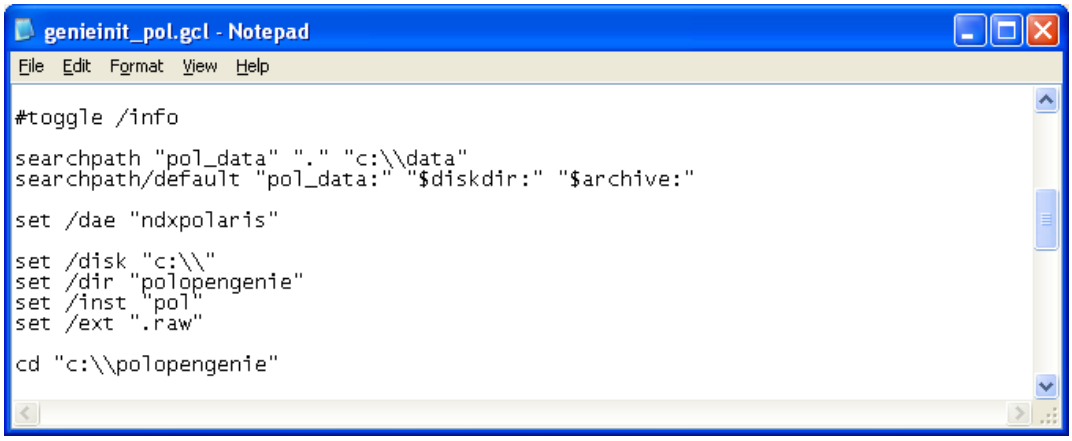
This will ensure all the focusing, setup_correct, correct, process, etc. commands and scripts which are needed to analyse Polaris data are defined when OpenGenie starts.

(you may want to make a backup copy of the original version of default_genieinit.gcl first)

3. Modify the "C:\PolOpenGenie\genieinit_pol.gcl" file

The genieinit_pol.gcl file which you will have downloaded along with the Polaris-specific files in step 1 instructs OpenGENIE to look for Polaris RAW data files in various folders on the Polaris instrument PCs and other network drives at ISIS. You won't be able to access these locations remotely, so you'll need to change a line in this file to tell OpenGENIE where on your own PC you have stored your Polaris RAW data files.

The relevant section of the file is near the top and is shown below:



The first `searchpath` line creates a label called "pol_data" which points to the current default directory ("`.`") and a folder "`C:\data`".

(again, note the use of double backslash characters, which are required in OpenGENIE to indicate the single backslash character used in labelling Windows folders and directories).

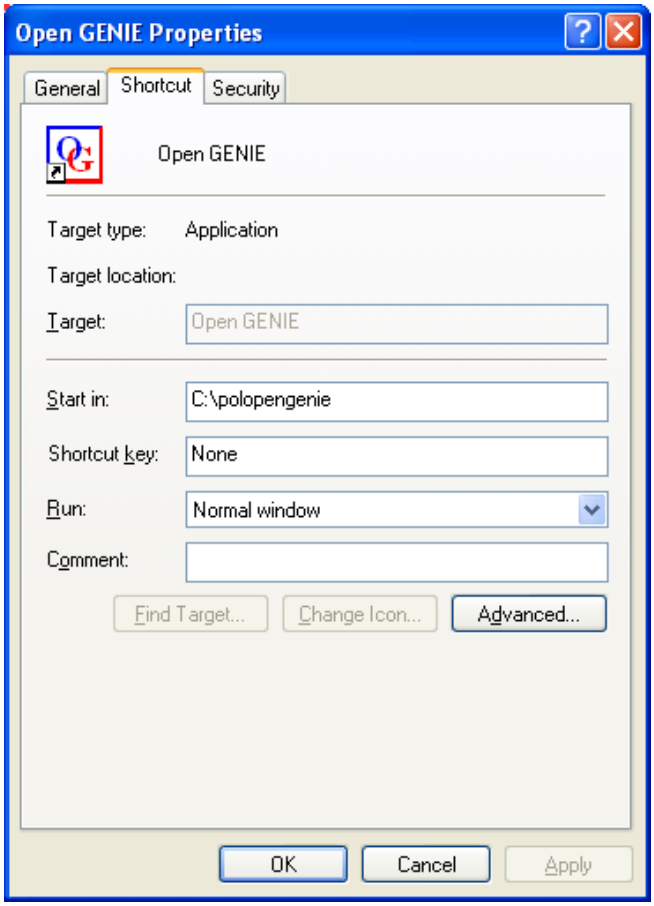
The second `searchpath` line tells OpenGENIE to look for RAW data files in "pol_data" first. If it can't find them there it then looks in the path "`$diskdir`", then looks in the path "`$archive`".

- `$diskdir` is an OpenGENIE defined label for the disk and directory path defined by the `set /disk` and `set /dir` commands (see the lines in the screen capture above).
- `$archive` is a label pointing to network drives at ISIS.

Once you have decided on a suitable location on your PC to store the RAW data files, simply replace "`C:\\data`" in the first `searchpath` line with your chosen location and delete the "`$archive`" text from the second `searchpath` line. It's probably a good idea to keep the "`$diskdir`" option on the second line.

4. Default Working Directory

Finally, it may be a good idea to change the default startup working directory where OpenGENIE will write any files created. To do this simply right-click on the OpenGENIE desktop icon, select Properties, then select the Shortcut tab and you'll see something like this:



The "Start in:" field probably points several sub-folders down within the "C:\Program Files" folder, so you may want to change this so that when you start writing data files they will be easy to find. In the example above this has been set to C:\polopengenie.

If you don't change this setting you can always use the "cd" command in OpenGENIE at any time to set (or change) your preferred working directory/folder.

Note: this step isn't actually necessary - if you look at the screen capture of the genieinit_pol.gcl file (step 3, above) you'll see it contains the line

```
cd "c:\\polopengenie"
```

which does exactly the same thing! If you want OpenGENIE to work in a different location simply change this line in the genieinit_pol.gcl file.

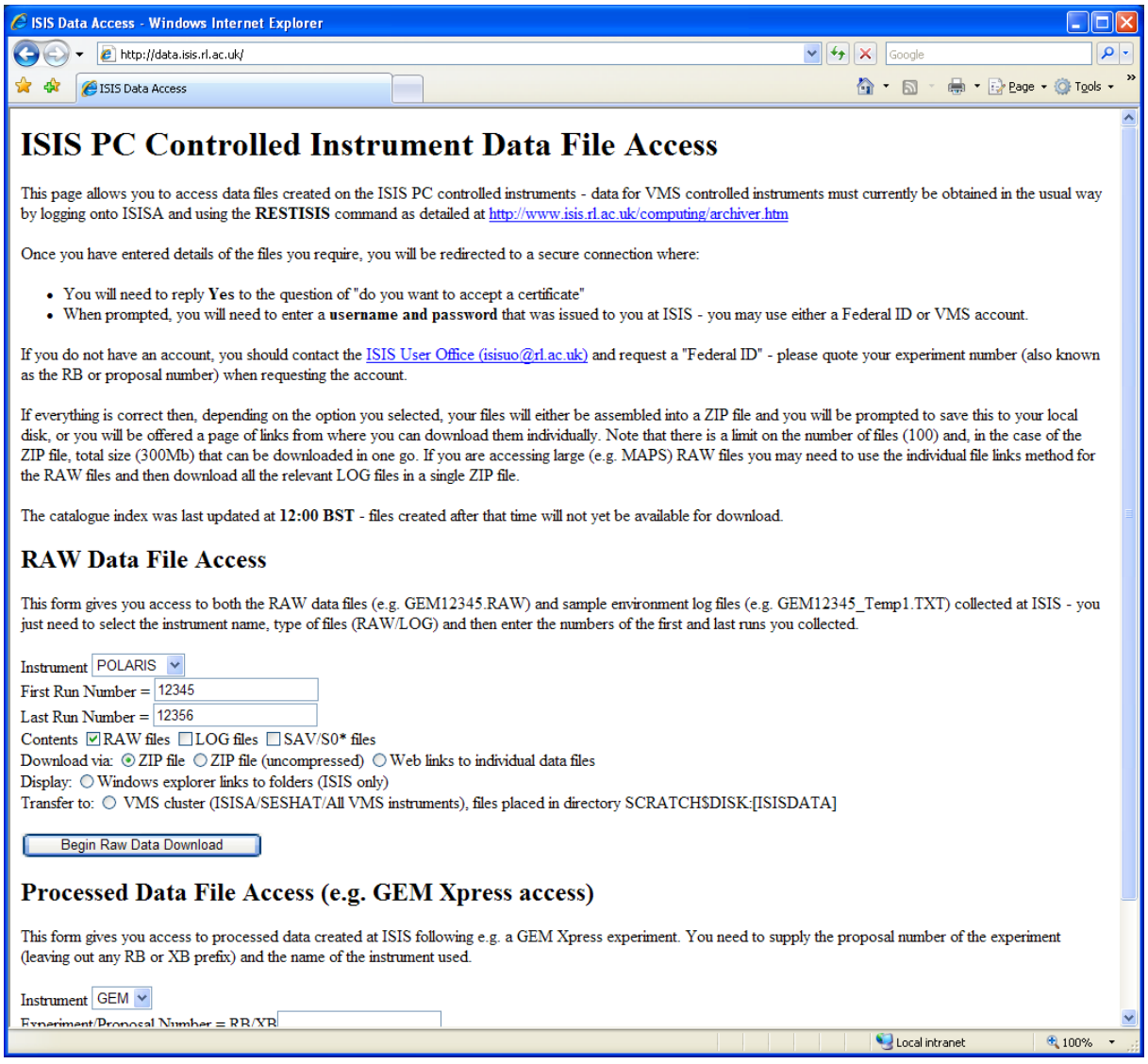
5. Download your Polaris RAW data files

In order to access your RAW data files you will need a valid user id (called a *Federal id*) and password which will have been issued to you by the STFC FBU IT group. If you do not have a Federal id, or have forgotten it, please contact either the ISIS User Office or a Polaris Instrument Scientist.

Using a web browser go to http://data.isis.rl.ac.uk

Half way down the page you'll see a section labelled "RAW Data File Access" (below).

- From the Instrument pull-down menu select "Polaris"
- Enter the first and last run numbers required in the appropriate fields
- If you only want RAW files, remove the tick from the "LOG files" check box.
- Select your preferred download route by pressing the appropriate "Download via:" radio button.
- Finally, press the "Begin Raw Data Download" button to start the process.



A dialogue box will open telling you that the process may take a few minutes (press OK), and depending on what browser you are using you may get a security certificate warning - chose whatever option is needed to enable you to continue to the web site to download the files.

A second dialogue box should then open where you will be prompted for a username and password. This is where you need to enter your Federal id and password.

At this point you may get an error message saying that the site is not available (Internet Explorer 7), but if you click OK to this message the new web page displayed contains a hyperlink to the zipped folder containing your RAW data files. Clicking on this hyperlink should allow you to download the zipped folder to your own computer, from where you can extract the RAW files to the location you chose in step 3, above. If you have any problems contact a Polaris Instrument Scientist - we may be able to get the files to you some other way, e.g. *via* the ISIS ftp site.

One last thing: a copy of the relevant pages from the Polaris User Manual (the green folder in the Polaris cabin) which tells you how to use some of the commands...

OpenGENIE Commands To Inspect Polaris Data:

Data normalisation (focusing):

```
>>  <wksp> = cfocus(run_number)        (or afocus, bfocus, efocus)
```

where *<wksp>* is a user-defined name for the workspace and *run_number* is the run number. If *run_number* is omitted, the user will be prompted for the number.

On the Polaris instrument control computer *ndxpolaris* ONLY (the right hand screen displaying the remote desktop session), use *run_number* = 0 to specify the current run:

```
>>  <wksp> = cfocus(0)                 (or afocus, bfocus, efocus)
```

To display the workspace use the *display* command:

```
>>  display <wksp>                    (may be abbreviated to  >>  d <wksp>)
```

An alternative command ALLFOCUS will normalise all 4 detector banks into consecutive entries in the workspace array *w[ ]*. The workspace array *w* is dimensioned to 100 entries - once this number has been filled the array index reverts back to 1.

```
>>  allfocus run_number
```

To display the diffraction data use the *display* command :

```
>>  display w[n]                       where n is an integer between 1 and 100
```

Note: the ALLFOCUS command will not work if a variable or workspace with the name *w* has already been created, as OpenGENIE will not be able to determine if the variable/workspace or the array is being referenced.

To add together several consecutive runs into a single data set (e.g. if data collection from a sample has been split into a series of shorter runs, such as in a time resolved study) use the ADDRUNS command:

```
>>  <wksp> = addruns:a(first_run_number,last_run_number)
```

will add together data collected in the Polaris A bank detectors for the series of runs from *first_run_number* to *last_run_number*. Use :B, :C or :E qualifiers to process data from the B, C and E detector banks respectively. Use the qualifier :P for data collected from samples contained in the Paris Edinburgh pressure cell (this will apply a correction to account for attenuation of the beam by the WC anvils and TiZr gasket, and omit the instrument background subtraction).

Absorption correction of data in OpenGENIE:

The CORRECT routine is available to carry out an absorption correction for cylindrical sample geometry:

```
>>  <wout> = correct(<win>)
```

where *<win>* is the name of the OpenGENIE workspace containing the normalised data. The corrected data are written to the workspace *<wout>*.

To calculate quantities required, such as number of scattering units per unit volume and the total scattering and attenuation cross sections, use the utility *SETUP_CORRECT*.

```
>>  setup_correct
```

(*SETUP_CORRECT* also has an optional */AUTO* qualifier which will write the quantities required for the absorption correction to a global variable *correct_global* to enable a single attenuation correction to be applied to a sequence of runs from the same sample, e.g. a temperature scan in a furnace or cryostat - the procedure for this is described below.)

OpenGENIE Commands to write data files:

The PROCESS routine is available to automate the writing of data files in GSAS, FULLPROF or CCSL formats:

```
>>  process/a first_run_number  last_run_number
```

will generate GSAS format files for data collected in the Polaris A bank detectors for the series of runs from *first_run_number* to *last_run_number*. Use /B, /C or /E qualifiers to process data from the B, C and E detector banks respectively. Files are written to the current OpenGENIE default directory with filename *Xnnnnn.gsa* (where *X* is the detector bank letter and *nnnnn* is the 5 digit run number).

Note: if the first and last run numbers are omitted, the routine will prompt the user for them.

To generate FULLPROF (Ins = 10) format data files add the /F qualifier:

```
>>  process/c/f first_run_number  last_run_number
```

will generate both FULLPROF *and* GSAS format files for data collected in the Polaris C detector bank. The FULLPROF format files have filename *Xnnnnn.dat* (where *X* is the detector bank letter and *nnnnn* is the 5 digit run number).

To generate CCSL format data files add the /T qualifier:

```
>>  process/e/t first_run_number  last_run_number
```

will generate both CCSL *and* GSAS format files for data collected in the Polaris E detector bank. The CCSL format files have filename *Xnnnnn.xye* (where *X* is the detector bank letter and *nnnnn* is the 5 digit run number).

Absorption Correction During Processing of Multiple Data Sets

To apply the ***same*** absorption correction to a large number of normalised data sets (e.g. following temperature scans in a furnace or cryostat) before writing GSAS, etc. format files add the /ATT qualifier to the PROCESS command:

```
>>  process/c/att first_run_number  last_run_number
```

will first launch the *SETUP_CORRECT* routine to acquire the necessary sample information before normalising, correcting and writing the data files automatically using the routines described above. The parameters required in the absorption correction are written to named fields in the global variable *correct_global* and are copied to the .correct field in the workspace storing the normalised diffraction pattern.

To generate data files in GSAS, FULLPROF or CCSL format from normalised diffraction patterns in an OpenGENIE workspace use the commands:

```
>>  GSASGEN(<wksp>)
>>  FULLPROFGEN(<wksp>)
>>  CCSLGEN(<wksp>)
```

where *<wksp>* is the name of the OpenGENIE workspace containing the normalised data. This will generate data files with the same file name construction and default time-of-flight limits as generated using the PROCESS command, above.

To force these routines to prompt for file names, time-of-flight limits, etc. add the `/NODEFAULT` qualifier:

```
>>  GSASGEN/NODEFAULT(<wksp>)
>>  FULLPROFGEN/NODEFAULT (<wksp>)
>>  CCSLGEN/NODEFAULT (<wksp>)
```

Miscellaneous OpenGENIE Commands:

To change the current default directory use the `cd` command in OpenGENIE:

```
>>  cd "c:\\_userdata\\user"
>>  cd "..\\newuser"
```

To check the current default directory use the `pwd` command in OpenGENIE:

```
>>  pwd
```

Appendix - Using user-specified background and vanadium files to normalise data

During normalisation of Polaris data using the AFOCUS, etc. commands OpenGENIE will use default instrument calibration files, which contain the standard background (empty instrument) and vanadium data sets. These files are called `aback.dat` and `avan.dat` (and `bback.dat`, `bvan.dat`, etc. for the other detector banks) and are stored in the `_calibration` folder. Generally, these files will be appropriate to the most recent ISIS running cycle at the time of

downloading the files from the ISIS ftp site. In most cases, using calibration files from the "wrong" cycle will make negligible difference to the normalisation of your data.
Nevertheless, the `_calibration` folder also contains data files from previous cycles: these are easily identified as their file names include a run number, e.g. `cb53876.dat` is a background data set from the Polaris C bank; `ev55556.dat` is a vanadium data set from the E bank.

To normalise RAW data files using specified background and/or vanadium calibration files use the POLFOCUS routine:

```
>>  <wksp> = POLFOCUS:A(nrun=55970,back=54974,van=54975)
```

this will normalise Polaris A bank data from run number 55970 using the background file created from run number 54974 and the vanadium file created from run number 54975.

```
>>  <wksp> = POLFOCUS:C(nrun=52978,
            bfile="c:\\polopengenie\\_calibration\\cb52980.dat",
            vfile="c:\\polopengenie\\_calibration\\cv52931-46.dat")
```

this will normalise Polaris C bank data from run number 52978 using the background file "`cb52980.dat`" and the vanadium file "`cv52931-46.dat`".

(the same background file could have been specified by using the option `back=52980`; however, because the vanadium file name does not conform to the standard Polaris naming convention, use of the `vfile=` option allowed its full name to be specified. Note also the requirement to use double backslash characters ("`\\`") in the file name specifications.)

The data in the workspace may then be corrected for absorption, and GSAS, Fullprof, etc. format data files written, using the `correct`, `gsasgen`, `fullprofgen`, etc. commands described above.

Alternatively, instead of using the POLFOCUS command to use specific background and vanadium runs, simply rename the run number-specific files you wish to use (these are all in the _calibration folder) to `aback.dat` and `avan.dat` etc. and use the AFOCUS, etc. commands as described above (it's probably a good idea to make a copy of the files first and then rename them).