

How to reduce NOMAD data

10/12/2012

IDL files you will need for data reduction

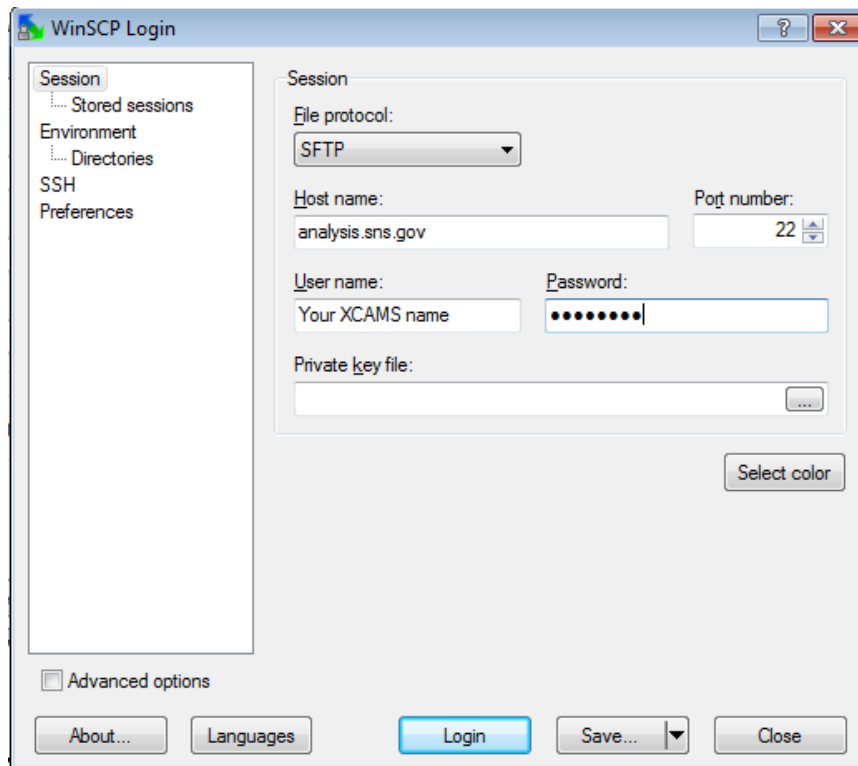
- **bin9999.bat** is the template file for reduction of a single raw data file
- **dosome.bat** is the macro which reduces several data files
- **idlstart.pro** is the IDL program needed to initialize the IDL
- **nomad.calfile** is the NOMAD calibration file, created during your experiment
- **normdatapdf.dat** is the Vanadium normalization file
- **backpdf** is the background file

The help is available for most programs by typing its name followed by **,/help**

To recover from an error type **retall** or **close,/all**

Remotely access your data

1. Go to <http://analysis.sns.gov/> and chose connection option appropriate for you OS (NX Client for Windows machines)
2. Go to <http://winscp.net/eng/download.php> and download the “**Installation package**” of WinSCP version for you OS
3. Install and run the program
4. Use your XCAMS account credentials to set it up



4. Make sure that NX machine client is running and then log in
5. Use WinSCP help file to guide your trough the interface

1. Start NX machine and open the Terminal



2. Go to your user directory you created during the experiment (SNS/NOM/IPTS-XXX/shared by default)

3. Make sure you have all six files by typing **ls** to display the content of the folder

4. Type **xterm -e idl idlstart.pro &** in command line. A separate terminal should open

A screenshot of an IDL terminal window. The window title is "idl". The terminal output shows:

```
IDL Version 7.1.1 (linux x86_64 m64). (c) 2009, ITT Visual Information Solutions
Installation number: 212462.
Licensed for use by: Oak Ridge National Laboratory

% Compiled module: FTEQS.
% Compiled module: JO.
% Compiled module: FTEQS.
% Compiled module: JO.
IDL>
```

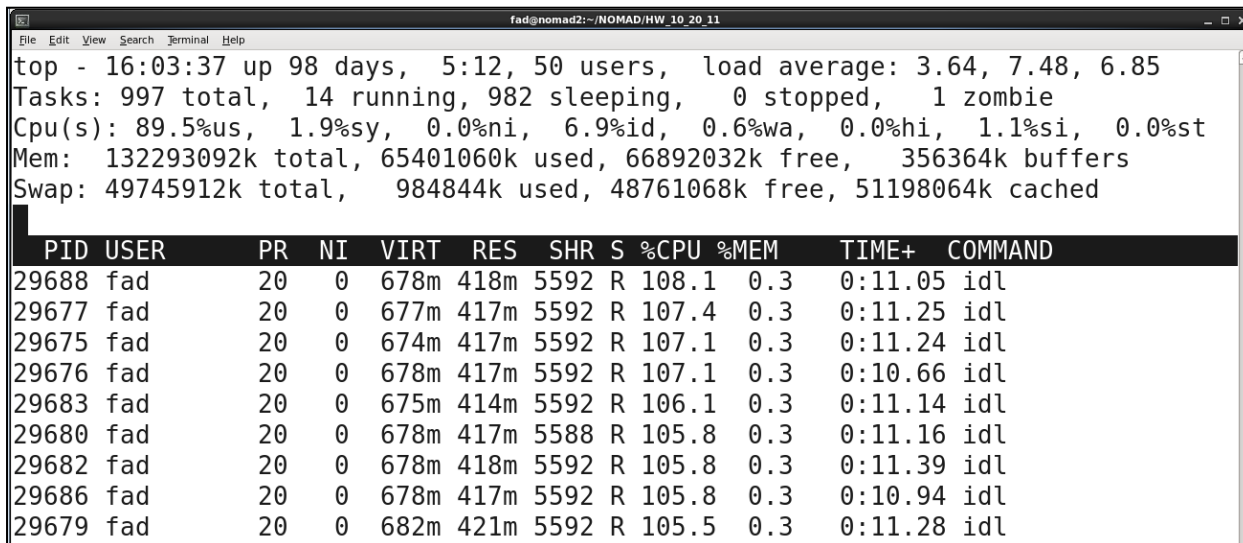
5. To generate a logbook for your experiment type **readtitles**. Enter your IPTS number, first and last run numbers (to see the actual numbers type **\$ls ../0** from shared folder)

6. To start with data reduction type **makebin,3138**, where 3138 is the run number you want to reduce. If you need to reduce several files type **makebin** and hit 'Return', then provide minimum and maximum run numbers

7. Go back to the first terminal and type **source dosome.bat** and hit 'Return'
Something like this will show up

```
[fad@nomad2 HW_10_20_11]$ source dosome.bat
[fad@nomad2 HW_10_20_11]$ IDL Version 7.1.1 (linux x86_64 m64). (c) 2009, ITT Visual Information Solutions
IDL Version 7.1.1 (linux x86_64 m64). (c) 2009, ITT Visual Information Solutions
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IDL Version 7.1.1 (linux x86_64 m64). (c) 2009, ITT Visual Information Solutions
```

8. Now you should wait until IDL is done. Check the status by typing **top** in the command line
(press Ctrl-C to cancel)



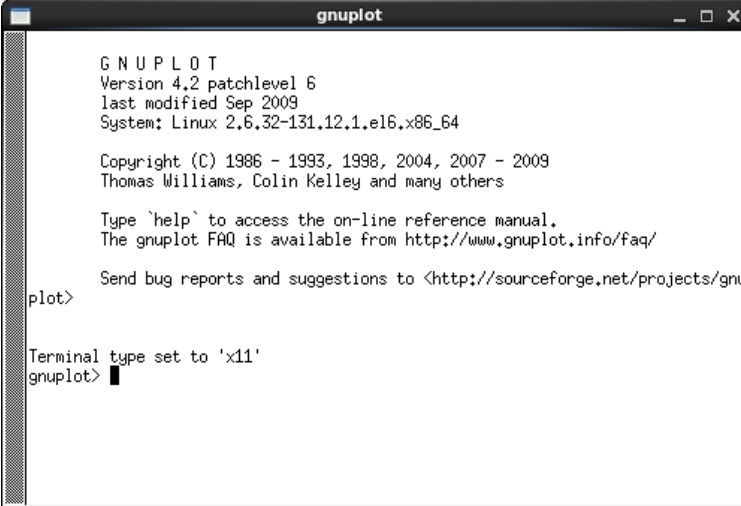
```
fad@nomad2:~/NOMAD/HW_10_20_11
top - 16:03:37 up 98 days, 5:12, 50 users, load average: 3.64, 7.48, 6.85
Tasks: 997 total, 14 running, 982 sleeping, 0 stopped, 1 zombie
Cpu(s): 89.5%us, 1.9%sy, 0.0%ni, 6.9%id, 0.6%wa, 0.0%hi, 1.1%si, 0.0%st
Mem: 132293092k total, 65401060k used, 66892032k free, 356364k buffers
Swap: 49745912k total, 984844k used, 48761068k free, 51198064k cached

  PID USER      PR  NI  VIRT  RES  SHR  S  %CPU  %MEM    TIME+  COMMAND
 29688 fad        20   0   678m 418m 5592 R 108.1  0.3   0:11.05 idl
 29677 fad        20   0   677m 417m 5592 R 107.4  0.3   0:11.25 idl
 29675 fad        20   0   674m 417m 5592 R 107.1  0.3   0:11.24 idl
 29676 fad        20   0   678m 417m 5592 R 107.1  0.3   0:10.66 idl
 29683 fad        20   0   675m 414m 5592 R 106.1  0.3   0:11.14 idl
 29680 fad        20   0   678m 417m 5588 R 105.8  0.3   0:11.16 idl
 29682 fad        20   0   678m 418m 5592 R 105.8  0.3   0:11.39 idl
 29686 fad        20   0   678m 417m 5592 R 105.8  0.3   0:10.94 idl
 29679 fad        20   0   682m 421m 5592 R 105.5  0.3   0:11.28 idl
```

On the left hand side it shows your XCAMS ID, on the right hand side it shows how many IDL processes you run and for how long. When no IDL processes are visible, you're done.

9. To plot reduced data you can use any software you like. Here, we give an example how to look at your data with *gnuplot*

10. In terminal type **xterm -e gnuplot &**. The window will appear:



```
gnuplot
GNU PLOT
Version 4.2 patchlevel 6
last modified Sep 2009
System: Linux 2.6.32-131.12.1.el6.x86_64

Copyright (C) 1986 - 1993, 1998, 2004, 2007 - 2009
Thomas Williams, Colin Kelley and many others

Type 'help' to access the on-line reference manual.
The gnuplot FAQ is available from http://www.gnuplot.info/faq/

Send bug reports and suggestions to <http://sourceforge.net/projects/gnu
plot>

Terminal type set to 'x11'
gnuplot> █
```

11. To plot your data type **plot 'file name'**. Use comma to separate datasets (*w/l* means line plot)

```
gnuplot> plot 'NOM_5175SQ.dat' w l, 'NOM_5197SQ.dat' w l, 'NOM_5191SQ.dat' w l █
```

12. To zoom in, hold left mouse button to draw a rectangular. To auto scale type **set au** and re-plot the data again.

13. Refer to gnuplot help file online to learn how to change font size, save figure and etc.

How to change parameters in $g(r)$ function

First, you should use **makebin** routine to histogram the raw data and obtain **allxxxx.dat** files

In IDL window type **restore,'all3138.dat**. Type or copy from corresponding bin3138.bat file the following

```
creategr,a3138,b3138,back='back3062.dat',norm='normpdf2503.dat',hydro=0,qmin=30,qmaxft=30,sc=3138,maxr=50,inter=0
```

Now you can change background (back) and normalization (norm) files, as well as Q_{\max} (qmaxft). Inter=1 shows what corrections are being made.

For full explanation of each parameter type **creategr,/help** in IDL window

Once the command is executed six files will be created:

NOM_3138SQ.dat is $S(Q)-1$

NOM_3138ftf.dat is $g(r)$

NOM_3138ftnat.dat is $g(r)$ with steps in r equivalent to resolution π/Q_{\max}

NOM_3138ftl.dat is $g(r)$ with the envelope (Lorch) function applied

NOM_3138ftfrgr.gr is $G(r)=r*g(r)$

NOM_3138ftlgr.gr is $G(r)$ with the envelope (Lorch) function applied

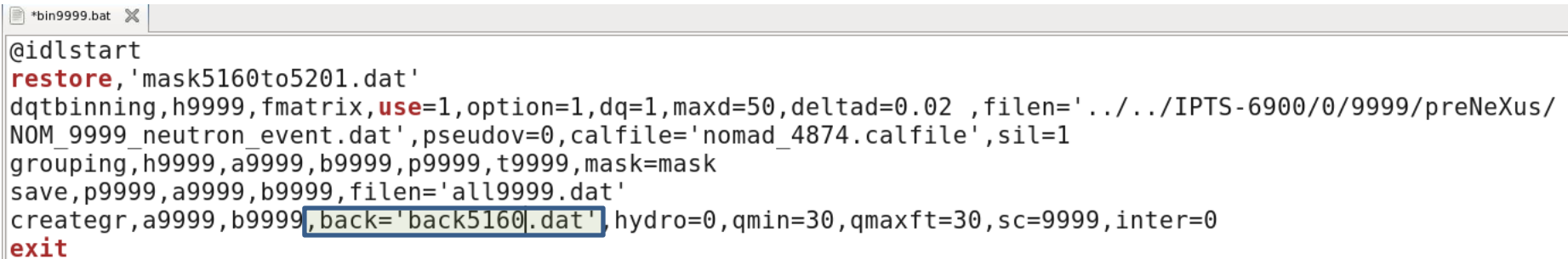
How to make a background file

Bin the background file using **makebin** (in example below it is file 5160).

In IDL window type the following commands

```
IDL> restore, 'all5160.dat'
IDL> makeback, a5160, b5160, file='back5160.dat'
% Compiled module: MAKEBACK.
% Compiled module: VAR_DEFINED.
```

Use different file name for different types of background. Do not forget to include the background file into **bin9999.bat** template



```
*bin9999.bat X
@idlstart
restore, 'mask5160to5201.dat'
dqtbinning, h9999, fmatrix, use=1, option=1, dq=1, maxd=50, deltad=0.02, file='../.. / IPTS-6900/0/9999/preNeXus/
NOM_9999_neutron_event.dat', pseudov=0, calfile='nomad_4874.calfile', sil=1
grouping, h9999, a9999, b9999, p9999, t9999, mask=mask
save, p9999, a9999, b9999, file='all9999.dat'
creategr, a9999, b9999, back='back5160.dat', hydro=0, qmin=30, qmaxft=30, sc=9999, inter=0
exit
```

How to make a normalization file

Bin the vanadium run using **makebin** (in example below it is file 5260).

In IDL window type the following commands

```
>restore,'all5260.dat
```

```
>createnorm,b5260,b5261,gsas=1,norm='norm5260.dat'
```

where, b5261 is the vanadium background, gsas=1 is the switch to make normalization file in gsas (1) or PDF (0) formats, norm='norm5260.dat' is the name of normalization file. Don't forget to change **bin9999.bat** template after new normalization file is created. Use gsas=2, dspace=dspace, to make file with give d-space binning.

How to make a GSAS-type file

In order to generate gsas file, the raw data has to be re-binned in d-space. In order to do it use template file '**bin_GSAS.bat**' in IDL window

```
>makebin,[x1,x2...],bin='bin_GSAS.bat'
```

where, x1,x2... are the run numbers of the files you want to reduce in GSAS format. This will generate list of bat files, which can be executed with source dosome.bat

Important! make sure you re-bin background and normalization files in GSAS format first

How to make a PDFgetN-type file

It is done in the same way with '**bin_PDFgetN.bat**' template