

Sometimes data from time-of-flight (TOF) neutron scattering instruments automatically output data in a GSAS formatted manner. While GSAS [1, 2] is wonderful refinement software, it was not written to work with propagation vectors (\mathbf{k}) for describing magnetic structures with representational analysis. In those cases, it is clearly advantageous to work with FullProf [3] and/or SARA*h* [4] for performing a representational analysis of the magnetic scattering. To bring multi-bank TOF data into FullProf is not difficult, albeit slightly tedious. This short tutorial is written in a way that should be approachable for those already familiar with FullProf.

The procedure has three parts:

1. Exporting data from GSAS
2. Formatting the data files
3. Editing the FullProf input file

1 Exporting data from GSAS

1. Create an experiment file in GSAS (`*.exp`)
2. Load in the GSAS formatted data using the correct instrument parameter file (`*.iparm`, `*.prm`, etc). This part is essential, as the instrument scientist carefully measures these values with known standards and GSAS is capable of easily converting the measured intensity into a normalized intensity for analysis.
3. Open LIVEPLOT, and under the options menu of EXPGUI, set the X-units to time (as collected) and the Y-units to normalized.
4. In LIVEPLOT, under the file menu, export the plot as a `.csv` file.
5. In your favorite column delimiting text editor (MS Excel or OpenOffice calc), open the `*.csv` file and copy out the first two columns, which read as time and observed intensity.
6. Paste the two columns into an empty text file. IMPORTANT note: Excel typically gets the end-of-line delimiter incorrect (carriage return). These need to all be replaced by hard returns. Notepad++ (Windows) or vi (Linux/Mac) are useful for accomplishing this.
7. Save the data file as something memorable, i.e. “`sample1-bank1-HIPD.dat`” and place it in the same directory as your `*.pcr` file.
8. You just exported the data for one detector bank. This must be repeated for each histogram (detector bank) in your data set. For experiments performed at Los Alamos, data from HIPD should end up with 8 `*.dat` files, data from NPDF yields 4 files.

2 Formatting the data files

In your favorite simple text editor, add the following lines to the beginning of each data file:

```
XYDATA BaFe2Se3 5K  
HIPD 5747  
bank 1
```

```
INTER 1000 100 0 0
```

TEMP 5

5.00204992 0.402605683

5.00454998 0.400449097

The lines are described as follows:

1. Describes the format (XYDATA) and contains a comment (BaFe2Se3 5K).
2. Comment stating the instrument name and run number.
3. Comment describing the bank number.
4. Blank.
5. Tells Fullprof to multiply the x column of data by 1000, which converts milliseconds to microseconds. The 100 is an arbitrary scaling factor for the y column of data.
6. Tells FullProf the temperature at which the data were collected.
7. Data, for the next many lines.
8. After the data, make sure to leave a blank line

These steps must be repeated for each detector bank.

3 Editing the FullProf input file

3.1 Editing the diffractometer constants

In FullProf, each data file corresponding to each detector bank needs to be added as a new pattern. This does become rather cumbersome, but allows simultaneous refinement of all banks, allowing an accurate analysis of both the nuclear (high Q) and magnetic (low Q) scattering. I will not outline the exact procedure on how to accomplish this, but the FullProf manual outlines this and the GUI EDPCR makes this fairly straightforward.

After the *.pcr file has been told to add several TOF patterns, you will notice several lines in your *.pcr file like the lines below:

```
!   Zero   Code   Dtt1   Code   Dtt2   Code   2ThetaBank  -> Patt# 1
    2.861   0.00  5040.984   0.00   -1.601   0.00   153.000
!
!   Zero   Code   Dtt1   Code   Dtt2   Code   2ThetaBank  -> Patt# 2
    4.071   0.00  3579.626   0.00   -1.300   0.00   90.000
```

Here, I show the diffractometer constants for two detector banks, supplied by the instrument scientist, formatted for FullProf. Within EXPGUI, it is very easy to read of these values for each bank in the HISTOGRAM tab. To translate from GSAS into FullProf:

FullProf	GSAS
Dtt1	DIFC
Dtt2	DIFA
Zero	Zero
2ThetaBank	Angle of the bank

3.2 Editing the profile terms

You will also have to edit the profile terms. An example from a functional FullProf *.pcr file is shown here:

```
! Sig-2    Sig-1    Sig-0    Xt        Yt        Z1        Z0        Size-Model
0.000    76.603    0.000    0.019    0.000    0.000    0.000    0
0.00    0.00    0.00    0.00    0.00    0.00    0.00
!   Gam-2    Gam-1    Gam-0    LStr      LSiz
0.000    0.000    0.000    0.000    0.000
0.00    0.00    0.00    0.00    0.00
!   a        b        c        alpha    beta     gamma    #Cell Info
11.887030 5.416300 9.143000 90.000000 90.000000 90.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
!   Pref1    Pref2    alph0    beta0    alph1    beta1
0.000000 0.000000 0.000000 0.031690 0.608000 0.000100
0.00    0.00    0.00    0.00    0.00    0.00
```

The conversions are roughly as follows:

FullProf	GSAS
Sig-1	sig-1
beta0	bet-0
alph1	alp
beta1	bet-1

These must also be replaced for each detector bank and will depend on which peak profile you opt to use.

Happy refining!

References

- [1] A. C. Larson and R. B. Von Dreele. General Structure Analysis System (GSAS). *Los Alamos National Laboratory Report LAUR*, pages 86–748, 2000.
- [2] B. H. Toby. *EXPGUI*, a graphical user interface for *GSAS*. *J. Appl. Crystallogr.*, 34:210–213, 2001.
- [3] J. Rodriguez-Carvajal. Recent advances in magnetic structure determination by neutron powder diffraction. *Physica B*, 192:55–69, 1993.
- [4] A. S. Wills. Symmetry and magnetic structure determination: Developments in refinement techniques and examples. *Appl. Phys. A*, 74:S856–S858, 2002.