

Virtual experiment:

templateDIFF

General purpose two-axis diffractometer



Warning: in this tutorial, most of my questions are silly, so I expect that you give me silly answers !

Abstract

This document is a tutorial about *McStas* and neutron scattering for beginners. We shall study a template diffractometer, with powder samples.

Getting started

- Run from the ILL/CS LiveDVD <<http://www.ill.eu/?id=11266>>, or get the *McStas* package at www.mcstas.org.
- Click on the *McStas* icon to start *McGUI* (see *Figure 1*)

A- Understanding the simulation model *templateDIFF.instr*

- Select menu *Neutron site/Templates* and choose the *templateDIFF.instr*
- The simulation model reflects a typical diffractometer geometry, as seen in *Figure 2*.

The *templateDIFF* model is representative of most neutron diffractometers. Optionally, you may have a look at the *templateDIFF* description by clicking on the *Edit/New* button (top right side of *McGUI*). It consists in a list of components positioned in space, with intercalated C code. Close the editor window afterwards.

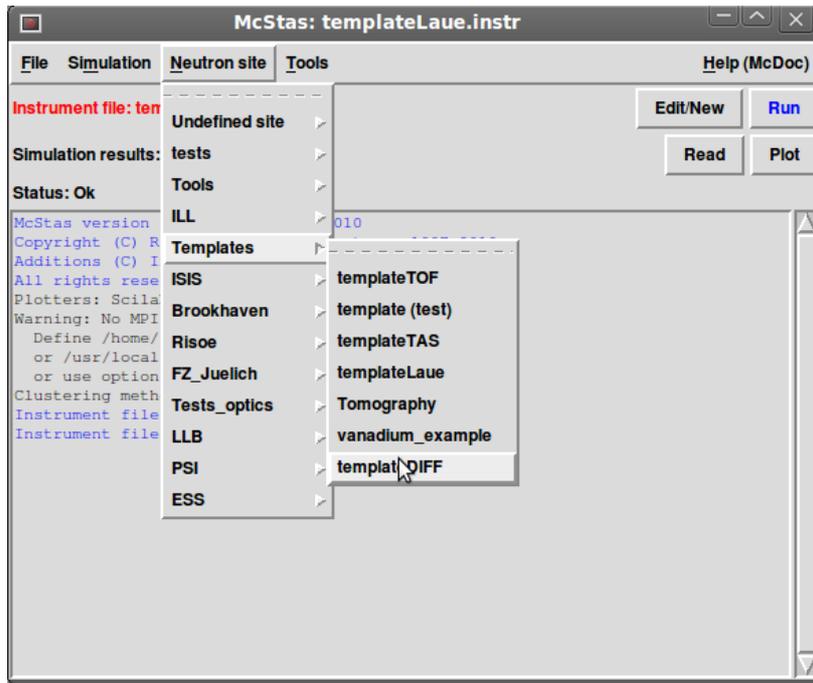
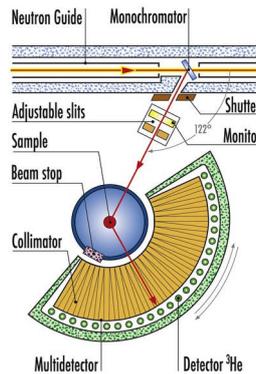


Figure 1: The McGUI main McStas window (mcgui)



Figures 2: top view of the D1A instrument. D1B and D20 are other thermal diffractometers at the ILL

- Click on the **Run** button (on the top right side). The instrument description is assembled into a running programme.
- The 'Run simulation' dialog opens (Figure 3). Instrument parameters are shown with their default values. Contextual help exists when moving the mouse over each parameter name. Additional help can be obtained when selecting the top-right **HTML docs** button.

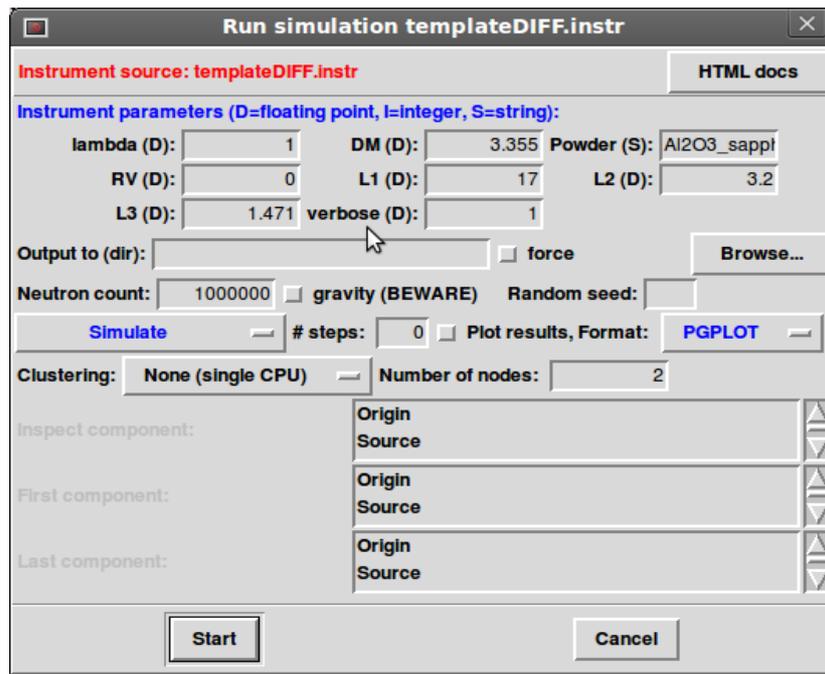


Figure 3: The McGUI/Run window.

B- 3D view of the instrument (virtual reality)

- Set 'neutron counts' to 1.
- Change the *plot results format* from PGPLOT to HTML/VRML
- Start the simulation in *Trace 3D* mode with VRML viewer.
- A 3D view of the instrument appears
- In the 3D view you can walk and visualise the instrument geometry.
- Question 1: Identify the monochromator, the sample, and the detector

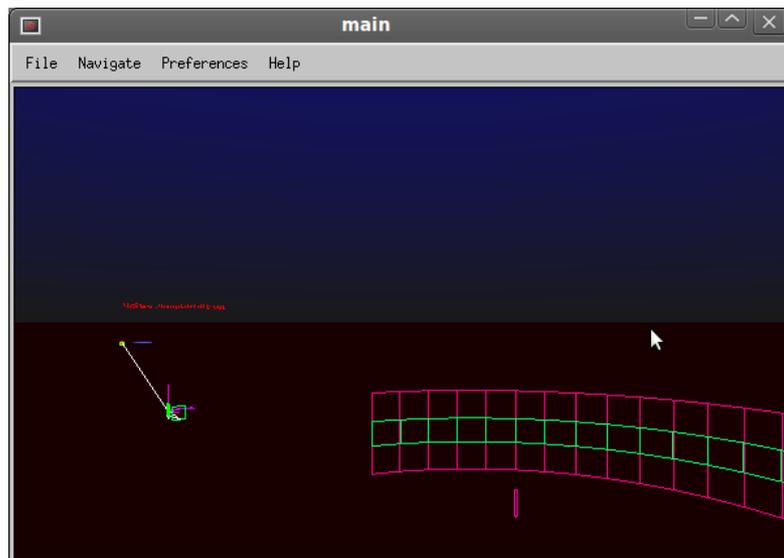


Figure 4: A 3D view of *templateDIFF* with VRML view.
Use mouse and left/right buttons in Walk mode to wander around.

Once completed, close the 3D view and return to the McGUI main window.

C- Diffractometer configurations

We shall now start to perform simulations with diffractometer. For this purpose, we have defined as input parameters:

- the measurement wavelength λ [Å].
- the monochromator lattice spacing (distance between atoms, in Angstrom= 10^{-10} m). The default is 'Graphite 002' (DM=3.355 Å).
- the monochromator curvature RV
- the sample definition. The default sample is a Sapphire (Al₂O₃) powder.

The so-called *take-off* angle is the one that neutrons are deflected by at the monochromator position. Usually, this angle is set to fixed predefined values on most diffractometers. It is possible to rotate the monochromator in order to select the crystal reflection to use, which each correspond to a given neutron wavelength. Monochromators are crystals that scatter neutrons by the *mighty power* of the Bragg's law:

$$n\lambda = 2d \sin(\theta)$$

where λ , d and θ are the neutron wavelength [Å], the lattice spacing [Å] and the scattering angle [radians, beam *half* deviation angle] respectively.

Question 2: Compute the take-off angle at the monochromator, for $\lambda = 1$ Angs. You may use the *Applications/Accessories/Calculator*, or *Applications/Science/QtOctave (Matlab clone)*.

Repeat this procedure for some possible monochromator lattice spacings, and report your results in the following Table 1.

Monochromator, $\lambda = 1$ Angs.	Take-off [deg] 2θ
PG 002 d=3.355 Å	
PG 004 d=1.607 Å	
Si 111 d=3.135 Å	
Ge 117 d=0.7946 Å	
Ge 335 d=0.8655 Å	
Ge 115 d=1.0925 Å	
Ge 113 d=1.712 Å	
Cu 220 d=1.278 Å	
Cu 002 d=1.807 Å	

Table 1: diffractometer configurations

The Bragg's law can be used for basically all samples measured in diffraction. Knowing that best diffractometer resolution will be reached for e.g. take-off angles 2θ between 60 and 130 deg, select a reasonable monochromator to use.

The monochromator is set as flat (RV=0) as default. Make a scan of the curvature

- Set 'neutron counts' to 1e6. Set the #steps=10 and RV=1,4 (from 1 to 4 in 10 steps).
- Use *Simulation* mode and *PGPLOT* plot results format.
- Specify a directory where to store results 'Output to (dir)' as for instance *curvature*.

Simulation will take a few minutes. Take your time, and get a coffee meanwhile. To speed-up

computation, select the MPI clustering method (on Linux and MacOSX systems). Click on the McGUI **Plot** button and search for the maximum flux. Now select the automatic curvature with RV=-1 and launch a simulation with **#steps** to 1 and output directory to *curvature_auto*. The optical curvature is indicated in the simulation log. **Do they match ?**

D- Scattering on quartz

We shall now study the two phases of quartz, α and β . Many other samples exist in the McStas database. This data base can be accessed from the McGUI Help menu in the **Component Library index**.

Click on the Run button (top right side of McGUI)

- The sample should be set as **Powder=SiO2_quartza.laz**
- Set '*neutron counts*' to 1e6. Set the **#steps** to 1.
- Use *Simulation* mode and *PGPLOT plot results format*.
- Specify a directory where to store results '*Output to (dir)*' as for instance '*quartza*'.
- Press the **Start** button and wait until the simulation ends (*e.g.* less than 30 seconds).
- Click on the **Plot** button to display results from each monitor/detector in the simulation.

We shall now take a look at all these plots.

The name of detectors in the simulation have been defined 'reasonably', and appear in the order from the source to the end of the instrument.

1. Estimate the monochromaticity from the wavelength spread ratio $d\lambda/\lambda$ (3rd plot). Is the simulation wavelength range +/- 1 % from the source sufficient (look at the instrument description code) ?
2. From the 4th plot, determine the atomic distance of the first intense peak at small angle in Quartz α (use the Bragg law).
3. The last plot is the same as the 4th one, but with a vertical position sensitive detection as well. Why are there arcs ?

Repeat these steps with the **Powder=SiO2_quartzb.laz**

Comparing the two simulations, what is the origin of the change you see ?

Silica has many different phases depending on temperature. The Quartz α exists for ambient temperatures (normal sand on the beach), whereas the β phase appears when heating, from 573°C at P=1 bar. For very high temperatures (more than 1650 C), silica melts.

There are only small changes of the atomic distances and arrangement between the two solid phases. **Compute from Bragg's law angles where main peaks should appear:**

Quartz α : atomic distances at 4.2452 and 3.3371 Å

Quartz β : atomic distances at 5.4543 and 2.7272 Å

Liquids appear as a broad oscillating signal, usually without sharp peaks.

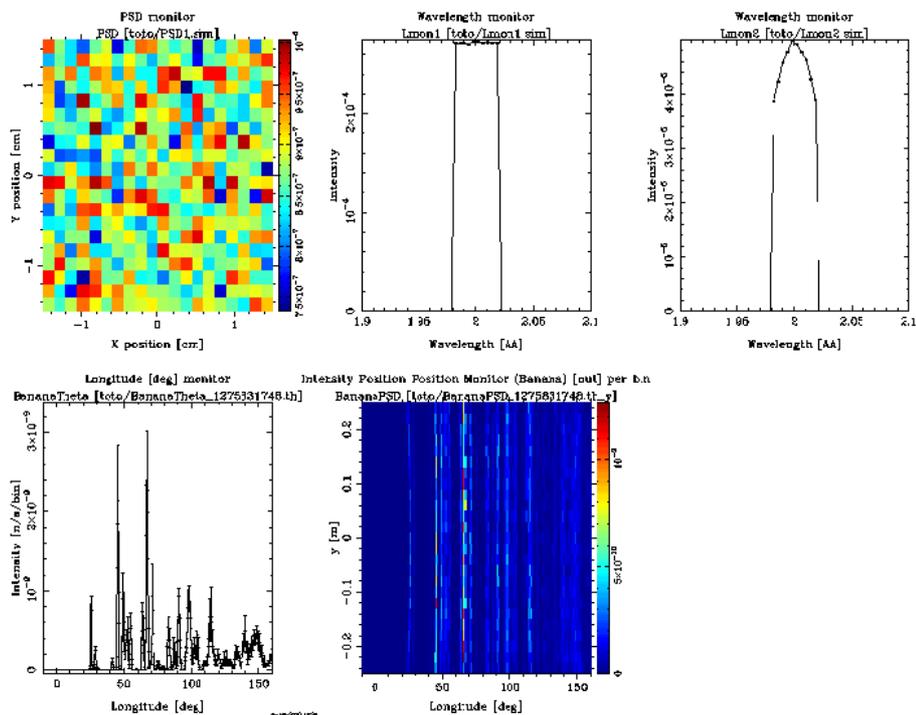


Figure 5: results from the diffractometer simulation with a Quartz sample. Press the 'L' key on the window to toggle log-scale mode. Click on sub-plots to enlarge them. Statistics are given above each enlarged plot (total flux I, centers X0 and Y0, gaussian half width dX and dY). Press 'Q' to exit.

By changing the monochromator take-off angle, we may select a smaller or longer wavelength.

Question: What will be the effect of choosing a longer wavelength (such as $\lambda=2 \text{ \AA}$) ? (use the Bragg law to estimate the 'd' value corresponding to a 90 deg detection angle)

To verify your guess, set **lambda=2** and output directory to '*colder*', and restart simulation for Quartz β . Compare the peak positions for the two results.



The peak resolution of a neutron instrument depends much on the scattering angle and the neutron energy.

Looking in detail on the diffractograms for the two last simulations (lambda=1 and 2), can you qualitatively see a variation of peak resolution (width) along the angular detection range (low angle, around 90 and above – locate broadest/thinnest peaks) ?