McStas Exercise 1
ESS Thermal Powder Diffractometer

Peter Willendrup, DTU

This document is available as a PDF at http://2013.essworkshop.org

1 1 part 1

1.1 The ESS moderator

1. Select and prepare source:

   - Open mcgui and press the Edit/New button
   - In the editor window use Insert → Instrument template
   - Scoll down and place the cursor after the lines saying

     ```
     COMPONENT Origin = Progress_bar()
       AT (0,0,0) ABSOLUTE
     ```

   - Use Insert → Source → ESS_moderator_long to insert the ESS moderator source. Name the component instance e.g. Source. There are many optional parameter - the ones you need to use are
     - Lmin=0.1 and Lmax=5 (Produce neutrons of wavelength between 0.1 and 5 Å.
     - n_pulse=1 (Produce only one pulse)
     - focus_xw and focus_yh to 2x2cm and dist=149.9 m (Focus to a 2x2 cm rectangle at 149.9 m distance)
     - Because of a minor geometry issue with ESS moderator distributed with McStas 2.0, we will let the cold moderator play the role of the thermal moderator by using the parameters
       - T=325, tau=80e-6, tau1=400e-6, tau2=12e-6, chi2=2.5, I0=13.5e11, I2=27.6e10, branch1=0.5
     - As we will leave out the guide system as a starting point, we will further define a small moderator using size=0.02 and cyl_radius=0.02.
   - Place the Source `AT (0,0,0) RELATIVE Origin`

2. Place monitors and run simulation:

   - Place the cursor below your Source and Insert → Monitors → TOF_monitor to insert Time-of-flight monitors `AT` 0.08, 6 and 149.9 distance from the source.
   - Each of the monitor instances should have a unique `filename`

- Each of the monitor instances should have a unique instance name
- Make the TOF monitors of size 0.2 x 0.2 m
- The TOF limits on the monitors should be
  - 0-5000 μs
  - 0-10000 μs
  - 0-100000 μs

  respectively. Use nt=20 in all cases.
- Use File → Save As to define an instrument filename
- On the main McStas window, press run to compile and run the instrument.
- Use the 'simulate' mode first to see if you record TOF profiles
- Use the 'trace' mode to visualize the instrument. Are the monitors positioned correctly?
- Displaced by a small (i.e. 1mm) distance, also add TOF-lambda monitors to your instrument (Insert → Monitors → TOFLambda_monitor at the right positions in the instrument file) with parameters e.g.

```
COMPONENT TOFLsource = TOFLambda_monitor(
    tmin = 0, tmax = 5000, filename = "TOFLsample", xwidth = 0.2,
    yheight = 0.2, Lmin = 0.1, Lmax = 5)
  AT (0, 0, 0.001) RELATIVE PREVIOUS
```

- - parameters should of course be compatible with those of the plain TOF monitors and wavelengths from the source.
- Similarly Insert → Monitors → PSD_monitor's to view the cross-section of the transmitted beam.
- Optional: Try emitting long-wavelength neutrons and enabling gravity. Does gravity at all influence the thermal neutrons we set out by using?
- Optional: Try playing with the ν and τ parameters. Does this influence the intensity recorded on your monitors?

1.2 Frame overlap

- Allow two pulses to be simulated from the source by applying n_pulses=2
- Extend the TOF ranges on the monitors to observe frame overlap
- We will now emulate a frame overlap chopper by narrowing the wavelength band produced at the source. Use an Lmin setting of 0.5 Å.

1.3 Powder sample

1. Simulate a simple powder sample

- Use the one-reflection Power1 powder with these parameters:

```
COMPONENT sample = Powder1(
  radius = 0.003, yheight = 0.02, q=5 //)
      , d_phi=12)
AT (0, 0, 150) RELATIVE Source
```

- Add an EXTEND section to remove the direct/transmitted beam

```
EXTEND %{
  if(!SCATTERED) ABSORB;
%}
```

- to be placed immediately after the AT line. This is effectively the same as adding a Beamstop.

- Add an Arm at the sample position, rotated by the angle `theta`:

```
COMPONENT TOFdetArm = Arm()
  AT (0, 0, 0) RELATIVE sample
  ROTATED (0,theta,0) RELATIVE sample
```

- also add `theta` as an instrument parameter with default 60 degrees (simply write `theta=60` between the parenthesis in the top DEFINE INSTRUMENT line of your instrument code).

- Add a cylindrical TOF-PSD around your sample area:

```
COMPONENT TOF_cylPSD = TOF_cylPSD_monitor(
    nt = 100, filename = "TOF_cylPSD", nphi = 180, radius = 2,
    yheight = 0.20, tmin = 0, tmax = 10e4, restore_neutron = 1)
  AT (0, 0, 150) RELATIVE Source
```

- And add a high-resolution TOF monitor rotated by the arm:

```
COMPONENT TOFdet = TOF_monitor(
    filename = "TOFdet", xwidth = 0.01, yheight = 0.2,
    tmin=47000,tmax=52000, nt=100,
    restore_neutron = 1)
  AT (0, 0, 2.001) RELATIVE TOFdetArm
```

- Launch a long simulation and comment on the results.

- Optionally use the PowderN sample with the $Na_2Ca_3Al_2F_{14}$ sample, only changing slightly your sample paramtrization:

```
COMPONENT sample = PowderN(
d_phi=12, radius=0.003, yheight=0.02, reflections = "Na2Ca3Al2F14.laz")
AT ( 0, 0, 150) RELATIVE Source
```

2. Optionally use Monitor_nD to directly measure q and d-spacing as measured in the cylindrical geometry. (Involves instrument variables and a little c).

2 part 2

2.1 Guides

In this part you will be using the component Guide.

- You should now reset the source geometry parameters size and cyl_radius to their defaults (which should give you a 12x12cm moderator). Change the illumination (focus of the source) to match the guide entry size.
- Use geometry parameters from the general instructions for parametrizing your guide systems.
- A word of advice: The McStas guide components have their Origin / AT position at the entry plane of the guide. Hence, placing monitors and other components you should always add the length of the guide to the AT specifier of that component.
- You may optionally also use the Guide_curved, and Guide_tapering for other than the straight geometry (see the Vitess guide for this exercise)

2.2 Chopper

In this part you will be using the component Disk_chopper. Use geometry parameters from the general instructions for parametrizing disk choppers.

- A hint: For the counter-rotating chopper, omega and phi should both have negative sign.
- When no slit height (yheight) is given, the chopper assumes that the slit height is equal to the chopper radius. Furhter, the chopper always places itself with the z-axis at ”half the chopper slit height“. For this reason, you should set the yheight to a value   guide height.