VITESS Exercise Day 1
ESS Thermal Powder Diffractometer

Here are some detailed instructions on how to simulate the instrument components used in the exercise. Parts in blue are optional in case you have time: they are added just in the VITESS description because they are either Vitess specific or "just one click away" in Vitess.

1 Exercise 1

1.1 The ESS moderator

1. Select and prepare source:
   - Select the ESS source: `source` →`source_ESS_2012`
   - click on *"moderator description file"*, read explanation in log-window
   - Select the ESS thermal moderator: `Browse` →`FILES/moderators/ESS` →`EssLPThermal.mod`
   - click `Edit` and look at the parameters; close without changing
   - check *source power* (5 MW),*pulse repetition rate* (14 Hz) *proton pulse length* (2.857 ms)
   - choose *database*: 2013_Schoenfeldt (optional: read documentation `Help` →`Modules R-Z` →`source_ESS_2012`)
   - choose *number of trajectories* to be simulated
   - choose wavelength range, time range (one pulse), divergence range
   - read explanation of *direction defined*. Set *direction defined* (virtual window) and coordinates of last monitor as window coordinates (149.9m, moderator size)
2. Place monitors and run simulation
   - select a ToF monitor: `visualize data` → and either `mon1_time` or `monitor1D` with time as parameter. Look at parameters and give necessary ones.
   - select two more ToF monitors. Give parameters again OR use `Edit` →`Copy Module Parameters` on first one and `Edit` →`Paste Module Parameters` on second and third. Take care to give output files different names.
   - put `space` modules in between (found under `spacewindow`)
   - press `Check` button to see if your instrument description is ok
   - press `Start` to run simulation

- adjust time window in monitors if necessary
- take a look at the log file: are you loosing trajectories and intensity somewhere?
- take a look at the `instrument.inf` file created by the simulation in the directory you are running VITESS in: are the monitors at the right distance from the source?
- add ToF-λ monitors: `mon2_tofwl` or `monitor2D`
- optional: gravity: change simulated wavelength band to >10 Å; compare beam position at 6m for *direction defined* by virt window / by divergence with gravity on/off; go back to first settings

3. Pulse time structure and flux
   - insert a `capture_flux` module (found under `evaluation`), run with both settings and write down result / save log file.
   - tip: you can un-check the *AutoPlot* option in monitor modules if you don't want plots to pop up

1.2 Frame overlap

- adjust the simulated/plotted time in source and monitors to observe frame overlap
- restrict simulated waveband such that no frame overlap occurs. Set lower limit to 0.5Å

1.3 Powder sample

1. simulate sample
   - place a powder sample component `sample` →`sample_powder` at 150 m
   - use *sample file* NAC_0.pow, edit to set sample extensions (cyl. of 6 mm diameter, 3 cm height)
   - look at the two-dimensional divergence for one wavelength (`monitor2D` or `mon2_div` with wavelength filter)
   - place a cylindrical `detector` in "monitor only" *usage*. Set *distance* to 2 m, *height* to 20 cm, *width* to 10 cm as well as *number of rows*, *columns* and *layers* to 200, 100 and 1. Center it at 60° scattering angle.
   - place tof-divergence monitor behind
2. analyze
   - Observe measured scattering angle, q or d-spacing with `evaluation` →`eval_elast` (don't forget to choose *time of flight* option and give total *flight path* from source to detector)
   - optional: set detector usage to normal, simulate a 1 cm thick layer of ^{3}He detector at room temperature with 10 bar, compare

2 part 2

2.1 Guides

- take number of trajectories and neutron intensity from the logfile, spectrum at sample position from monitor
- find slits in `spacewindow` →`slit`
- select `guide` module with constant shape, set entry and exit width and height to 12 cm, piece length to total length and number of pieces to 1.
- create reflectivity files with `Tools` →`Generate Mirror Files`, use quadr. Swiss Neutronics description ("yes") and give desired coating and output filename
- give name of generated mirror file as *Reflectivity files*
- optional: Replace linear by **parabolic guide**, compare focusing. Where is the focal point? How large is the beam spot at the sample position? - for a parabolic (or elliptic, or curved) guide shape, you need more than one piece. The focal point calculated from entrance and exit width/height is given in the logfile.
- the logfile also tells you where the neutrons are lost: already in the guide, or at the slit
- optional: Bend the so far straight part of the guide horizontally to avoid direct line of sight (with a width of 12 cm and a length of 142.9 m, you need a radius of $R = L^2/(8w)$ =21.271 km). Confirm that this curvature avoids direct line of sight by counting the number of reflections. What is the uncertainty of this test? - for a **curved guide**, set the curvature radius and don't forget to use more than one pice (not too many). Observe increase of simulation time if more shorter pieces are used for a more accurate shape. Count number of reflections in curved guide part by setting *add to color* to 1, plot color with `monitor1D`. You also see the different colors in the logfile, so to test line of sight, you can alternatively set the initial color to 1 in the source moderator file (since color 0 is not shown in the logfile) and see from the logfile that the minimal color after the curved guide is 2. Note that the sample changes the color value! Look at the instrument.inf file to see the total horizontal shift.

2.2 Chopper

- Select `chopper` →`chopper_disc` and edit chopper file. For a chopper below the guide, put a negative offset *window position* combined with positive *rounds / min.*. Set position of axle to radius-window_height/2 (see drawing in helper file)
- Confirm the given offset with the tool `Compute Chopper Phases` (use the smallest wavelength and the pulse length as time delay)

- look at logfile: are neutrons passing by outside the chopper? If so, adjust window height and axle position to account for edge effects (a cicular window opening a rectangular guide).