SUMMER SCHOOL REPORT : MCSTAS PROJECT

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0.1 Neutron scattering theory

0.1.1 Why neutrons ?

Neutron scattering is an important tool to investigate some important features of matter. This is due to many characteristics of neutrons :

- Thermal neutrons, which are more commonly used, have a wavelength (given by de Broglie law) close to inter-atomic distances (0.5 - 10 Å), so diffraction and interference effects can be observed.
- The energy of thermal neutrons is also very similar to that of many condensed matter excitations, so the effects of elastic scattering are more observable.
- Neutrons are neutral, so they can penetrate deeply in matter without being subject to Coulomb force.
- Neutron scattering is very sensitive to isotopes and light elements, which makes it different from X-rays
- Neutrons have a magnetic moments, which makes them interact with a magnetic field

0.1.2 Scattering cross section

An important feature in studying scattering is the cross section. The cross section can be seen as the surface in which the incoming neutron should lend in order for it to interact and be scattered with the matter (so if we imagine the atoms as being disks with a certain radius, than it would be the total area of these disks). So knowing the neutron flux, the scattering cross section is : $\sigma = \frac{num\ of\ neutrons\ scattered\ per\ sec}{\Phi}$

Another related feature is often used, the differential scattering cross section, which measures the scattering in a small solid angle $d\Omega$ and is equal to $\frac{d\sigma}{d\Omega}$.

0.1.3 Wave description of neutron scattering

We start by describing scattering caused by one nucleus. We can write the incoming wave(the neutron) as :

$$\Phi_i(r) = Ae^{i\vec{k}_i.\vec{r}}$$

The scattering nucleus is in a fixed position defined with $\vec{r}_j$, and the scattered wave can be seen as a spherical wave centred in the nucleus, so the scattered wave can be written as :

$$\Phi_f(r) = \Phi_i(r_j)\frac{-b_j}{|\vec{r}-\vec{r}_j|}e^{ik_f|\vec{r}-\vec{r}_j|}$$

b_j has the dimension of a length, and is called the scattering length. To calculate the cross section, we first need to know the flux of the incoming beam.

$$\Phi_i = |A|^2 v = |A|^2\frac{p}{m_n} = |A|^2\frac{k_i\hbar}{m_n}$$

And the flux of the scattered beam is (for $r >> r_j$) :

$$\Phi_f = |\Phi_f(r)|^2 v = |Ab_j|^2\frac{k_f\hbar}{r^2 m_n}$$

And since the focus in this project is on elastic scattering (no energy transfer), then $k_f = k_i$

So given a small surface dS, the number of neutrons scattered in it is $\Phi_f dS = |Ab_j|^2\frac{k_f\hbar}{r^2 m_n}dS$. And considering that $d\Omega = \frac{dA}{r^2}$, we can now calculate $\frac{d\sigma}{d\Omega}$

$$\frac{d\sigma}{d\Omega} = \frac{num\ of\ neutrons\ scattered\ per\ sec\ in\ d\Omega}{\Phi_i d\Omega} = \frac{\Phi_f dS}{\Phi_i d\Omega} = |b_j^2|\frac{dS}{r^2 d\Omega} = |b_j^2|$$

Which gives $\sigma = |b_j^2|4\pi$

For scattering from multiple nuclei, the waves scattered from each nucleus interfere, which gives a cross section that varies according to the direction from which scattering is observed. The scattered wave function can be written as :

$$\Phi_f(r) = \sum_{j=1}^{n}\Phi_i(r_j)\frac{-b_j}{|\vec{r}-\vec{r}_j|}e^{ik_f|\vec{r}-\vec{r}_j|} = \sum_{j=1}^{n}Ae^{i\vec{k}_i.\vec{r}_j}\frac{-b_j}{|\vec{r}-\vec{r}_j|}e^{ik_f|\vec{r}-\vec{r}_j|}$$

If we consider that the nuclei are placed near each other, and near the centre, and that the observer is far from it, then $|\vec{r}-\vec{r}_j| = r$, and also :

$$|\vec{r}-\vec{r}_j| = |\vec{r}-\vec{r_{j,||}}-\vec{r_{j,\perp}}| = \sqrt{|\vec{r}-\vec{r_{j,||}}|^2+|\vec{r_{j,\perp}}|^2} = |\vec{r}-\vec{r_{j,||}}|$$

$\vec{r_{j,||}}$ and $\vec{r_{j,\perp}}$ being the parallel and perpendicular component of $\vec{r}_j$ relatively to $\vec{r}$ and the last equality is justified by the fact that |r|, and thus $|\vec{r_{j,\perp}}|$ is very small.

Now if we consider $\vec{k_f} = k_f \frac{\vec{r}}{r}$, then

$$k_f|\vec{r} - \vec{r_j}| = k_f|\vec{r} - \vec{r_{j,||}}| = \vec{k_f}(\vec{r} - \vec{r_{j,||}}) = \vec{k_f}(\vec{r} - \vec{r_j}) \ since\ the\ vectors\ are\ aligned$$

So, the scattered wave function is now

$$\Phi_f(r) = -\frac{A}{r}\sum_{j=1}^{n} b_j e^{i\vec{k_i}.\vec{r_j}} e^{i\vec{k_f}(\vec{r}-\vec{r_j})} = -\frac{A}{r} e^{i\vec{k_f}.\vec{r}} \sum_{j=1}^{n} b_j e^{i\vec{q}.\vec{r_j}}$$

$\vec{q} = \vec{k_i} - \vec{k_f}$ is the scattering vector. From here, we can calculate the differential cross section as previously done with one nucleus

$$\frac{d\sigma}{d\Omega} = |\sum_{j=1}^{n} b_j e^{i\vec{q}.\vec{r_j}}|^2$$

0.1.4 Coherent and incoherent scattering

In a given sample or material, the scattering length is not the same between the different nuclei as it varies from isotopes, and also in the same nucleus, it can fluctuate over time because of spin variations. So for a given nuclei, we can say that $b_j =< b_j > +\delta b_j$ and $< \delta b_j >= 0$. Since we're interested in the scattering from the whole sample, we can calculate $< \frac{d\sigma}{d\Omega} >$. We first have :

$$\frac{d\sigma}{d\Omega} = |\sum_{j=1}^{n} b_j e^{i\vec{q}.\vec{r_j}}|^2 = \sum_{j=1}^{n}\sum_{k=1}^{n} b_j b_k e^{i\vec{q}.(\vec{r_j}-\vec{r_k})}$$

So by taking the mean of this, and considering that $< b_j b_k >=< b_j >< b_k > \ if j\ != k\ and < b_j^2 >=< \delta b_j^2 > + < b_j^2 >$ we have :

$$< \frac{d\sigma}{d\Omega} >= \sum_{j=1}^{n} < \delta b_j^2 > + \sum_{j=1}^{n}\sum_{k=1}^{n} < b_j >< b_k > e^{i\vec{q}.(\vec{r_j}-\vec{r_k})} = \sum_{j=1}^{n} < \delta b_j^2 > + |\sum_{j=1}^{n} < b_j > e^{i\vec{q}.\vec{r_j}}|^2$$

The first part is the result of the variance of the scattering length, the incoherent part, which we can write as $\frac{\sigma_{inc}}{4\pi}$ and the second part is the coherent part, which depends on the direction of the scattering. $\frac{d\sigma}{d\Omega}|_{coh} = |\sum_{j=1}^{n} < b_j > e^{i\vec{q}.\vec{r_j}}|^2$, $\frac{d\sigma}{d\Omega}|_{inc} = \sum_{j=1}^{n} < \delta b_j^2 >$.

0.1.5 Scattering in crystals : Proof of Bragg's Law

The calculations made previously assumed that the scattering nuclei were static. In a crystal, this is not very accurate because each atom vibrates. However, it is possible to prove that, with the right approximations, the differential scattering cross section has a similar form to that found previously, with an additional factor called the Debye-Waller factor, which is a positive factor that we note e^{-2W}. So we can write (we drop the mean symbol for scattering lengths for practicality) :

$$\frac{d\sigma}{d\Omega}|_{coh} = e^{-2W}|\sum_{j=1}^{n} b_j e^{i\vec{q}.\vec{r}_j}|^2$$

Since each atom is in a unit cell, we can write it's position vector as $\vec{r}_j + \Delta_i$ with Δ_i being the position vector of the i atom in the j unit cell with a position vector of $\vec{r}_j$. So, taking the sum off all unit cells (index j) and all atoms within each unit cell (index i), we can write :

$$\frac{d\sigma}{d\Omega} = e^{-2W}|\sum_{i,j} b_i e^{i\vec{q}.(\vec{r}_j+\Delta_i)}|^2 = e^{-2W}|\sum_i b_i e^{i\vec{q}.\Delta_i}|^2|\sum_j e^{i\vec{q}.\vec{r}_j}|^2 = e^{-2W}|F_N(\vec{q})|^2|\sum_j e^{i\vec{q}.\vec{r}_j}|^2$$

where $F_N(\vec{q})$ depends only on the positions of the atoms inside the unit cell. Next we calculate the lattice sum, that is the sum over all the unit cells in the previous expression.

$$|\sum_j e^{i\vec{q}.\vec{r}_j}|^2 = \sum_{j,i} e^{i\vec{q}.(\vec{r}_j-\vec{r}_i)} = \sum_{j,i} e^{i\vec{q}.(\vec{r}_i)}$$

The last equality is true when we consider that the lattice is infinite, thus all lattice vectors (all relative numbers) are present in the sum, and thus for a fixed j, the sum over all indexes of $\vec{r}_j - \vec{r}_i$ is equal to the sum over all lattice vectors $\vec{r}_i$. And if we consider N to be the number of unit cells (which should be big considering the assumption we just made previously) we have : $|\sum_j e^{i\vec{q}.\vec{r}_j}|^2 = N\sum_j e^{i\vec{q}.(\vec{r}_j)}$ Which means $\sum_j e^{i\vec{q}.\vec{r}_j}$ is equal to 0 or N. Since the 0 solution is not physically relevant, we take a close look the condition for which $\sum_j e^{i\vec{q}.\vec{r}_j} = N$. This can only be true if each term of the sum is equal to 1, which means that for all lattice vectors $\vec{q}.\vec{r}_j$ is a multiple of 2π. Now, if we consider $(\vec{a},\vec{b},\vec{c})$ and $(\vec{a'},\vec{b'},\vec{c'})$ to be the lattice vectors and reciprocal lattice vectors, and if we write $\vec{q} = x_1\vec{a'} + x_2\vec{b'} + x_3\vec{c'}$, $(x_1,x_2,x_3) \in \mathbb{R}^3$, then $\vec{q}.\vec{r}_j = 2\pi(x_1h + x_2k + x_3l)$ is a multiple of 2π for every given triplet $(h,k,l) \in \mathbb{N}^3$. This means that $(x_1,x_2,x_3) \in \mathbb{N}^3$ and thus $\vec{q}$ is a reciprocal lattice vector. This enables us to write $\sum_j e^{i\vec{q}.\vec{r}_j} = N\sum_{\vec{\tau}} \delta_{\vec{q},\vec{\tau}}$, the sum being

over all the reciprocal lattice vectors. From here, we can express this condition as the $Laue\ condition$: $\vec{q} = \vec{\tau}$ Or, using the scattering angle, and since $q = 4\pi sin(\theta)/\lambda$:

$$\vec{q} = \vec{\tau} \implies q = \tau \ and \ \exists n \in \mathbb{N} \ \frac{\tau}{n} = \frac{2\pi}{d}$$

with d being the distance between two adjacent lattice planes perpendicular to $\vec{\tau}$ Which means that

$$q = 4\pi sin(\theta)/\lambda = \frac{2n\pi}{d}$$

Which gives $Bragg's\ Law$:

$$n\lambda = 2dsin(\theta) \ / n \in \mathbb{N}$$

0.2 Using McStas

0.2.1 Main components in an instrument

0.2.1.1 Sources

The first element of a McStas instrument is usually the neutron source. There are several types of sources embedded into the standard McStas installation, and most of them have attributes that can be set in order to determine the size of the source, the distribution of wavelengths or energy in the out-going beam, and the area in which the beam must be focused.

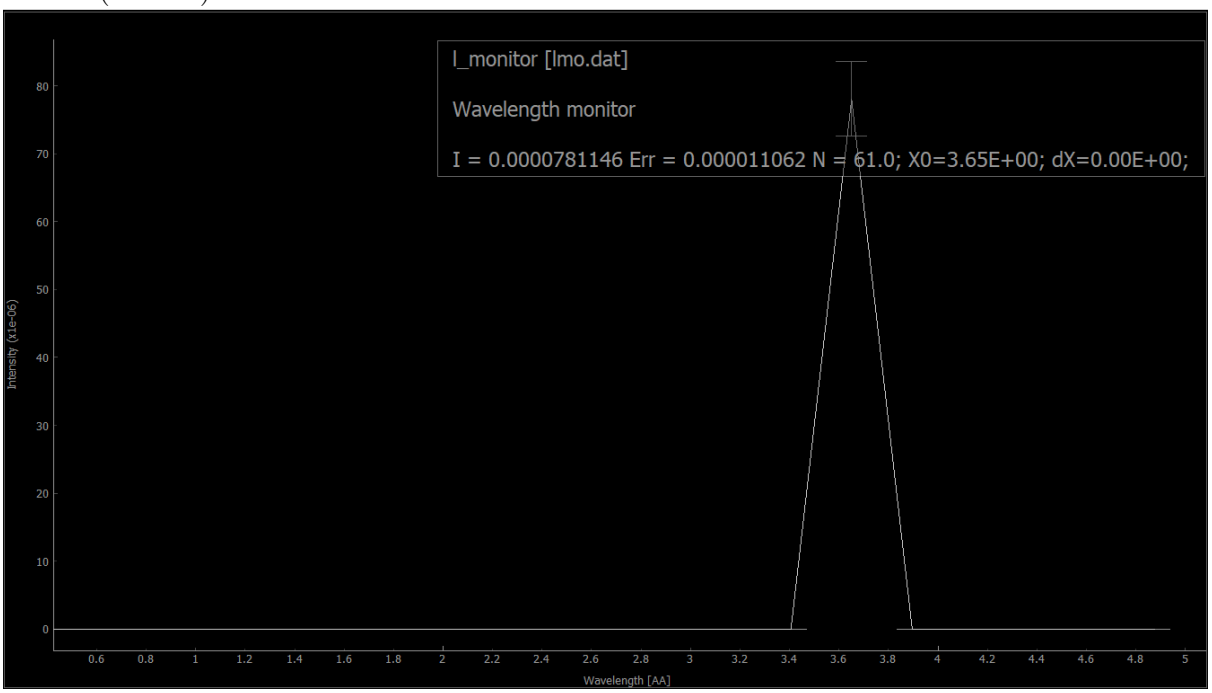
0.2.1.2 Monitors

Monitors are used to study different properties of the beam, before or after scattering for example. In McStas, all monitors are perfect, which means they do not interact with incoming neutrons, and thus can be placed one after the other without affecting the results (apart of course from the effect of the divergence of the beam which can change the results depending on where a monitor is placed). Some monitors that are often used include the PSD Monitor, which detects are records the position of the incoming neutron on the screen, the L.monitor which gives the total intensity per wavelength and Monitor.nD which is a general monitor that can be used to record various signals.

0.2.1.3 Monochoromators

Monochromators are crystals used to extract a certain wavelength from an incoming beam. For than, we use the expression : $q = 4\pi sin(\theta)/\lambda$. So for a given value of q and θ, the only scattered neutrons in θ direction are the ones with a wavelength of λ. To achieve this in McStas, a standard instrument consists of a source and a monochromator (here I use a curved one).

We set the values of q and λ that we want to examine, then we calculate θ, the angle by which the monochromator should be rotated around the y-axis : $\theta = arcsin(\frac{q\lambda}{4\pi})$ Then we place a monitor (an Lmonitor to examine the different scattered wavelenths), rotated at an angle θ from the monochromator (so the angle between the incoming beam and the scattred one recorded by the monitor is 2θ). The resulting curve from the simulation is as follows ($\lambda = 3.7$)



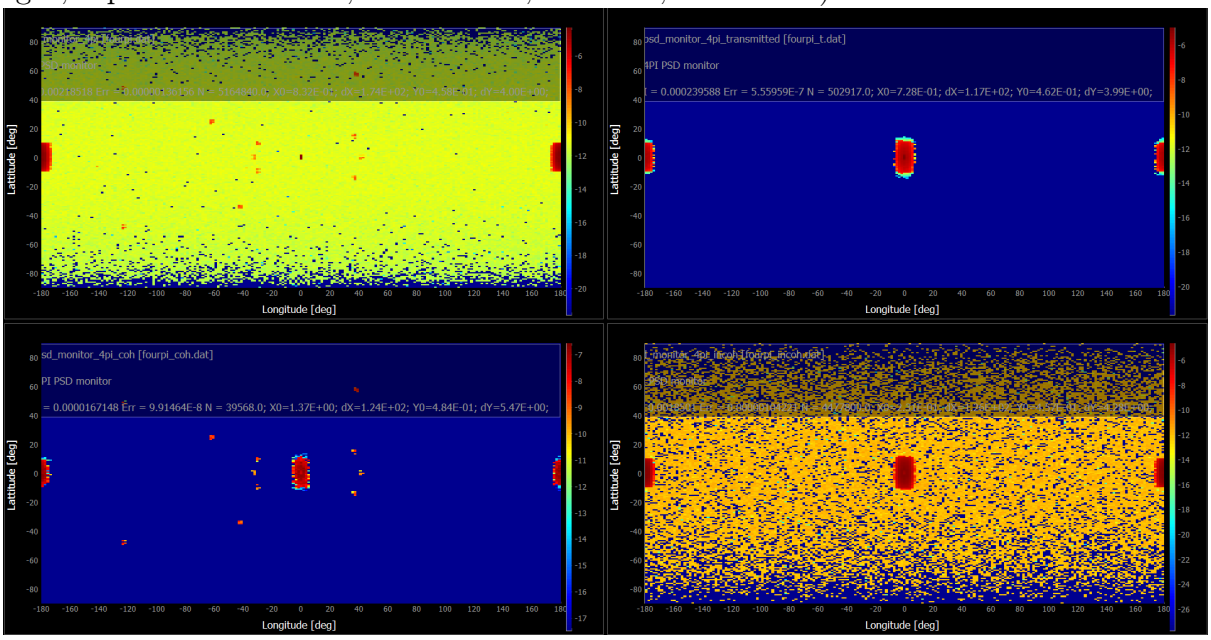
The code for the instrument can be found here.

0.2.2 Laue Camera : Detecting coherent and incoherent scattering from a single crystal

Some McStas components have output parameters that give insight on what happens when every neutron interact with it. In the case of $Single\_crystal$, there's an output parameter called hkl_info that has an attribute $type$ that contains information about

the type of scattering that happened to the incoming neutron. So using this attribute, we can set a monitor that only activates or records when this variable corresponds to the type of scattering we want.

As an example, we can use this to create a monitor that records only coherent scattering, incoherent scattering or transmitted neutrons. The picture below is of 3 monitors, each detecting a certain type of interaction, and a fourth detecting all neutrons (from left to right, top to bottom : All, transmitted, coherent, incoherent).



The code for the instrument can be found here. This approach can also be used to distinguish scattering from different components, like the sample and the sample environment.

0.2.3 Union

Union components are a way to create complicated geometries by assembling simple geometries together. When creating geometries, the user specifies mainly the material in which the volume should be made,the dimensions, and also the priority of the volume. Priority means that if two volumes overlap in a certain space, then the material of that space is the material of the volume that has the biggest priority. Naturally, no two shapes should have the same priority, even if they won't overlap. What's also different is using Union is that to use a material in a certain Union volume, the user needs first to define this material by defining all the physical processes he wants the material to have (Incoherent process, powder process...) then assembling all these processes into a single material using *Union_make_material*. Once the material is defined, it can later be

use to create either a sample with a certain geometry, or a sample environment.

0.3 Sample environments

0.3.1 What are they and why they're used

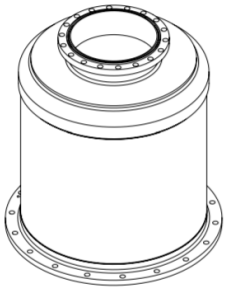
In most neutron scattering experiments, the samples need to be maintained at a certain physical or chemical state or environment, like very low temperatures (cryogenic conditioning), high temperatures, high pressure, magnetic field, or studied as a function of these parameters. The different devices used to do this are what's called sample environments (cryostats, furnaces..). Since most of these devices contain the sample, the resulting scattering is both a combination of the scattering from the sample, but also the scattering from the device, so it is important in designing such devices to keep them as neutron-neutral as possible, and also to model them in simulations to get closer-to-reality results.

0.3.2 Modelled sample environments

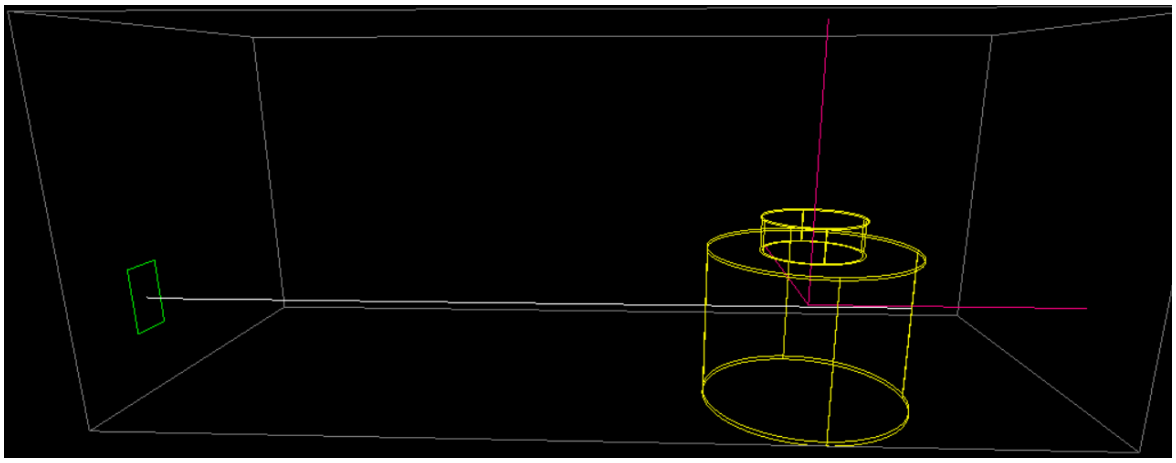
0.3.2.1 Cryostat

The specific cryostat I worked on has 5 layers, each one containing the next : Gadolinium Shield - Cryostat - Gradient screen - 77k shield - 300 K vacuum tail. In building the cryostat, I mainly used cylinders to create all the elements, and boxes to add windows for the incoming and scattered beams in some layers. All dimensions are set as parameters defined and initialised at the beginning of the file, so changing a certain dimension shouldn't require any change in the code other than changing the value of the relevant variable. The code for the instrument can be found here.

0.3.2.1.1 Calorimeter The calorimeter is a cylinder of an inner diameter of 150 mm with a thickness of 0.2 mm. At the bottom, the calorimeter is closed with a 3mm thick plate (also in aluminium).At the top, it's partly closed by an aluminium plate welded to a 24 mm vertical tube, both 2 mm thick, with a hole of 70 mm. This hole is then closed with a 1 mm thick brass plate.

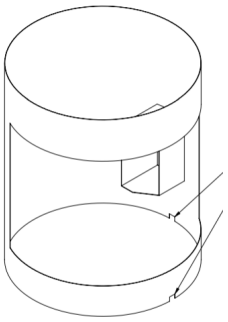


The calorimeter is not necessarily symmetrical vertically, so the total height of the cylinder is divided into two independent variables cal_top_height (the height above 0) and cal_bottom_height (the height below 0) so that the total height is their sum. This also means that the centre of the cylinder is $(cal\_top\_height - cal\_bottom\_height)/2$

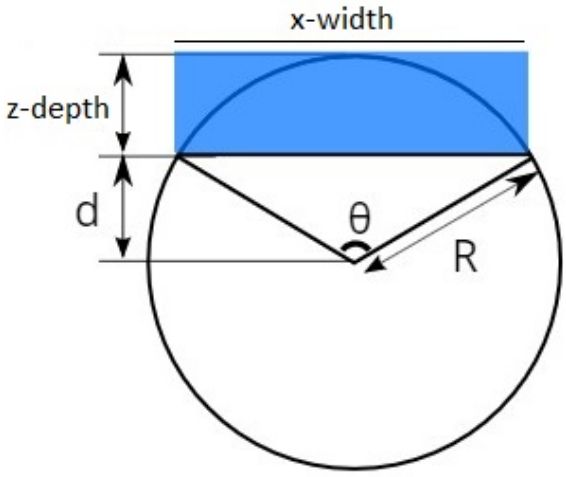


Modelled calorimeter drawn with McDisplay-webgl

0.3.2.1.2 Gadolinium shield Inside the calorimeter is a gadolinium cylinder of 130mm inner diameter and 0.25mm thickness, closed at the top and bottom with aluminium plates of the same thickness, with a hole in the top plate of the same diameter as the tube in the calorimeter. The cylinder also has vacuum windows for the incoming and scattered beam.



To model these with the existing Union geometries, I used 2 vacuum boxes (one for incoming and the other for scattered beams), of an appropriate z-depth and centre, inserted in the cylinder (which of course should have a lower priority than the two boxes). The relevant dimensions of a window are the height (according to the y-axis) and the angle coverage. So a window with the same height as the cylinder and an angle of 180°would remove half of the cylinder.



To calculate the other dimensions necessary to draw the box (x-width, z-depth, and $centre_z$, we mainly use the fact that $d = Rcos(\theta/2)$, which gives that

$$z\_depth = R - d = R(1 - cos(\theta/2))$$

$$centre_z = z\_depth/2 + d = \frac{R}{2}(1 + cos(\theta/2))$$

$$x\_width = 2Rsin(\theta/2)$$

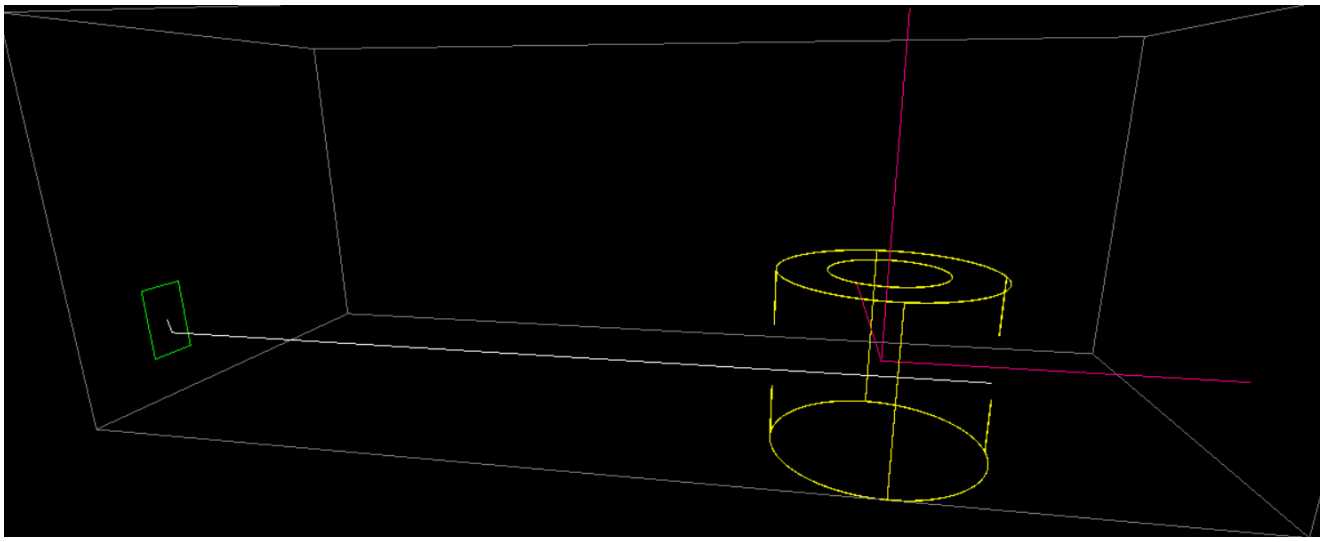


Figure 1: Gadolinium shield

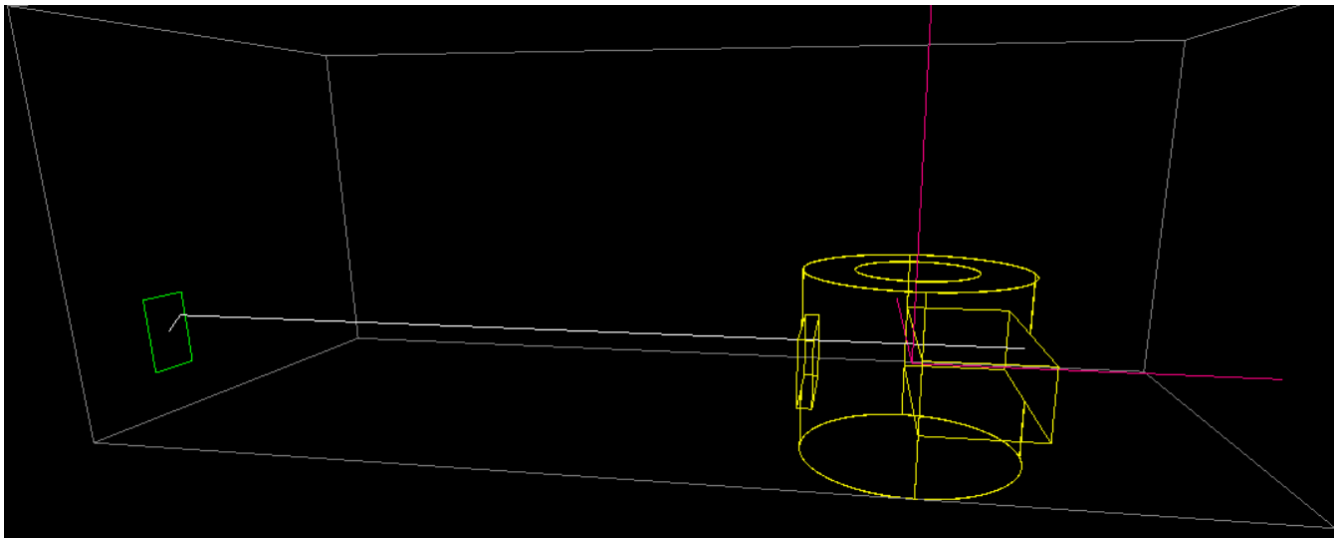


Figure 2: Gadolinium shield with boxes visualise property set to 1

0.3.2.1.3 Gradient screen Surrounding the calorimeter, the gradient screen is an 0.5 mm thick aluminium cylinder with a 190mm diameter closed at the bottom by a 1mm thick aluminium plate and at the top by a copper disk (thickness not provided so I took the same one as the bottom plate) with a similar hole in the centre. It has windows of the same dimensions as the ones in the gadolinium shield, with the difference that they're made of $50\mu m$ thick aluminium, which I modelled in McStas by two boxes for each window with a difference in z_depth parameter of $50\mu m$, the outer one of aluminium and the inner of vacuum.

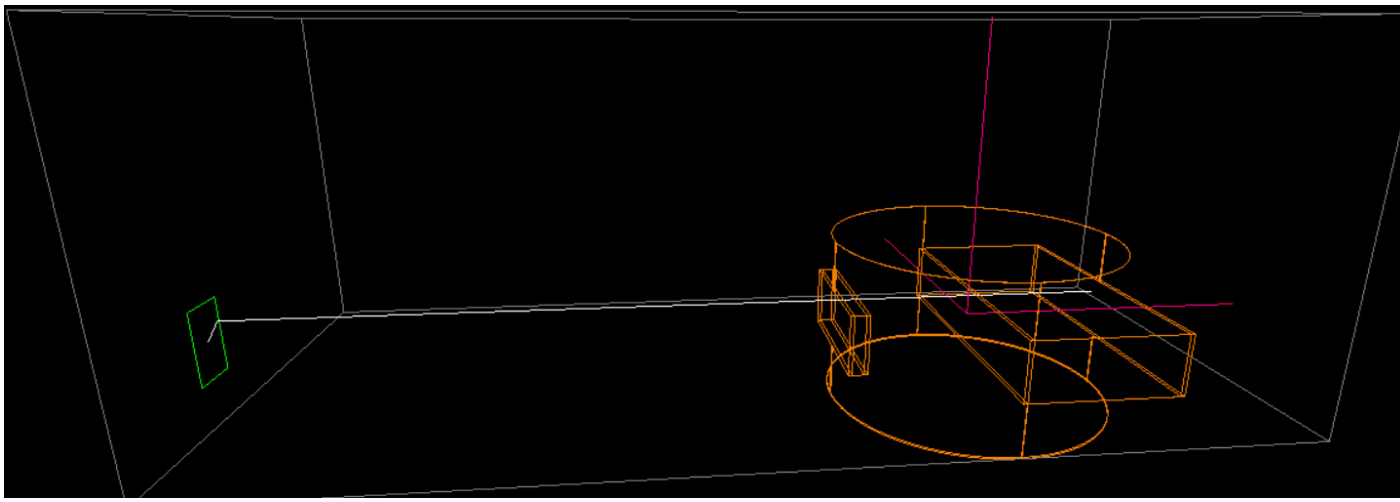
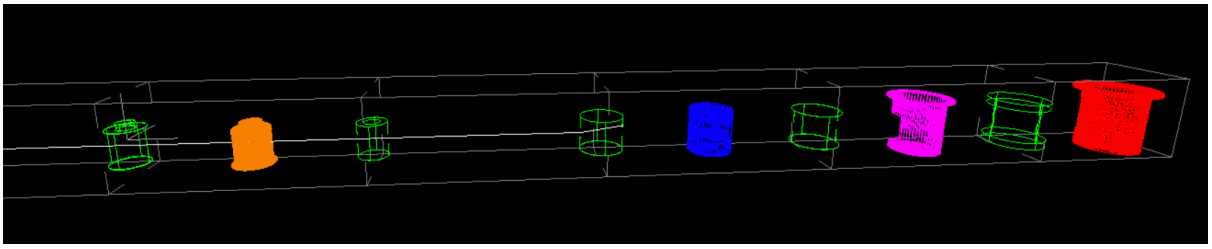


Figure 3: Gradient screen - The thickness of the aluminium screen is exaggerated in the figure for more clarity

0.3.2.1.4 77K shield This is a 1mm thick cylinder surrounding the gradient screen, it has a diameter of 210mm and 2 windows for the incoming and scattered beam that have a slightly bigger angular coverage to cope with the divergence of the beam. It is closed both at top and bottom by a 1mm thick aluminium plate.

0.3.2.1.5 300K vacuum tail It's the outer layer of the instrument, which is also in aluminium, with a thickness of 5mm and 30mm thick closing plates. The thickness is reduced to 0.5mm for the incoming beam and 0.75mm for the scattered one, which is equivalent to say that it has two windows of aluminium, which we can model in McStas in a similar way to the windows in the Gradient Screen.

The following figure shows a drawing, done in McStas, of all the 5 layers of the instrument, and the reference drawings imported to McStas as off files.
From left to right : Calorimeter - Gadolinium Shield (with no reference drawing) - Gradient Screen - 77K Shield - 300k Vacuum Tail.



References

Kim Lefmanns lecture notes on Basic scattering theory / neutron scattering
ILL neutron booklet
Article on sample environment (need to find the exact title)
ILL documents and private contact with Eddy Lelièvre-Berna