A Monte-Carlo simulation of neutron transmission through water, graphite, and lead

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Abstract

Using scattering and absorption cross sections for water, graphite, and lead (and other established values such as their densities), the transmission of neutrons through a given thickness was investigated. Scattering was modelled isotropically, with an exponentially distributed step length, and absorption was modelled using a ratio of the cross sections.

It was found that for 1,000,000 neutrons (over 20 loops to find the mean and the standard deviation, which is equal to the error of the program), the percentages of neutrons reflected (R), absorbed (A), and transmitted (T) in 10.0 cm of water, graphite, and lead, were:

	Water			Graphite			Lead		
	R	A	T	R	A	T	R	A	T
Value	84.71	15.07	0.22	78.10	0.79	21.10	71.39	9.87	18.72
Error	0.03	0.03	0.01	0.03	0.01	0.03	0.05	0.03	0.05
$\sigma_{scattering}$	103.0			4.74			11.221		
$\sigma_{absorption}$	0.6652			0.0045			0.158		

Table 1: All percentages have been rounded to two decimal places, which is fewer than the number of decimal places in the given cross section data - asides from water's scattering cross section which has one decimal place. Cross sections are given in barns.

Further to this, the variation of these percentages with thickness of materials, in 0.25 cm intervals, was found. By using the linear of a logarithmic graph of the number of neutrons transmitted against distance, characteristic attenuation were found to be:

	Water	Graphite	Lead
Characteristic attenuation length/cm	2.04	35.97	13.01
Error/cm	0.01	0.36	0.01
Reduced χ^2	42,350	221	180

Table 2: Again, percentages have been rounded to two decimal places. The large values of reduced χ^2 indicate that the errors on the points is too small – suggesting more loops should be run to determine the standard deviation more accurately.

Introduction

The principle mathematical tool used for this program is the use of random numbers - they determine how far a neutron will scatter, in what direction, and whether it is absorbed on not on a collision. The use of random numbers is commonly referred to as the "Monte Carlo" method. A simple example of this is in the calculation of pi: a pair of (non-antithetic) random numbers between zero and one can be generated, and if the distance of this point is less than one unit it can be added to a counter of included points. The number of these points divided by the total number of points (and multiplied by four) can give a relatively accurate value for pi with a large number of points, though due to the random nature of the points this value will vary with each simulation. The general term for the exclusion of points outside a boundary is "rejection sampling".[1]

An important application of this method is to nuclear reactors. Neutrons are heavily involved with fission reactors – they can induce a fission reaction, and multiple neutrons can be produced by this reaction. To prevent a chain reaction, the number of these neutrons must be controlled, and they must be moderated to approach the energy of a "thermal neutron", where the absorption cross section for uranium is highest.[2] By creating a simple model of scattering and absorption processes of a neutron transmitting through a material, an indication of the effect of the material's dimensions on transmission can be found. Improving on this model and using more computational power (to generate more data, similarly as can be done in simulating pi to improve accuracy) will increase confidence in the resulting data.

Despite uncertainties in nuclear power in the United Kingdom (due to commercial viability, at least), this type of simulation is still applicable elsewhere Code such as MCNP, "Monte Carlo N-Particle Transport Code", can be used to aid reactor design, though it can also be used for medical physics purposes, such as radiography.[3] [4]

Theory

Most of the theory used for the simulation will be explained in context, and references be pointed to where detailed explanations are required. An important starting point for the model is considering the attenuation of intensity (number of neutrons) with thickness of material, which leads to the following pair equations:

$$I(x) = \exp\left(-\frac{x}{\lambda}\right) \quad , \qquad 1$$

where I is the intensity, x is the displacement, and λ is the mean free path which relates to the macroscopic and microscopic cross sections thusly:

$$\lambda = \frac{1}{\sum} = \frac{1}{n\sigma} \quad , \qquad 2$$

where n is the number density, σ is the microscopic cross section, and $\sum$ is the macroscopic cross section. To calculate the mean free path for both absorption and scattering processes, the total macroscopic cross section is simply the sum of these two macroscopic cross sections.

As has already been said, the standard deviation of the resulting percentages is equal to the error in the simulation. For a large number of simulated neutrons, the central limit theorem can be used to obtain an estimate of how this error varies with the number of neutrons transmitted – it should be inversely proportional to the square root of the number of neutrons transmitted.[5]

Exponentially distributed steps

To assign a scattering event an exponentially distributed path length, a set of uniformly distributed random numbers had their natural logarithm taken, and then they were multiplied by a negative mean free path. This procedure was found by integrating an exponentially decreasing curve (probability density function) to find its cumulative distribution function, then taking the inverse of this.[6] The main part of the program uses a mean free path calculated from the total cross sectional area, however the success of this process can be demonstrated with figures 1 to 4, which use a mean free path due to absorption only (~45 cm).

Figure 1 shows that randomly generated points seem to be uniformly distributed. Taking logs and multiplying by the negative mean free path gives the histogram shown in figure 2.

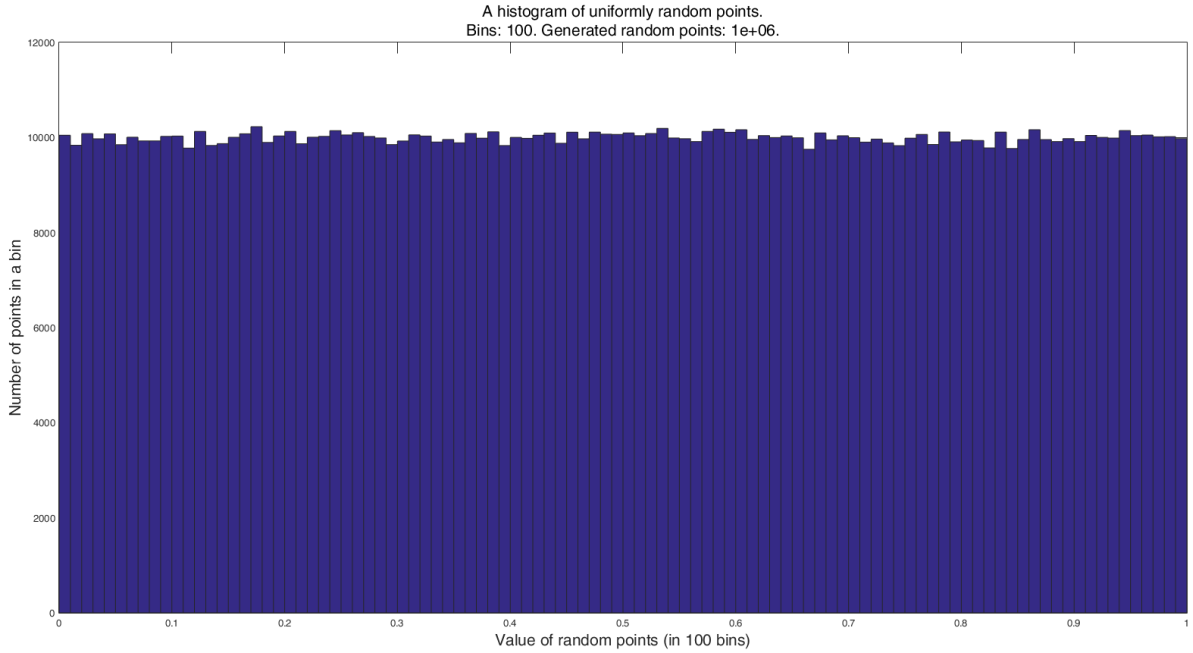

Figure 1: This figure shows that the number of points varies about a mean, which is equal to the number of points divided by the number of bins. The standard deviation (standard error) from this mean should be, on average, close to the square root of this mean.

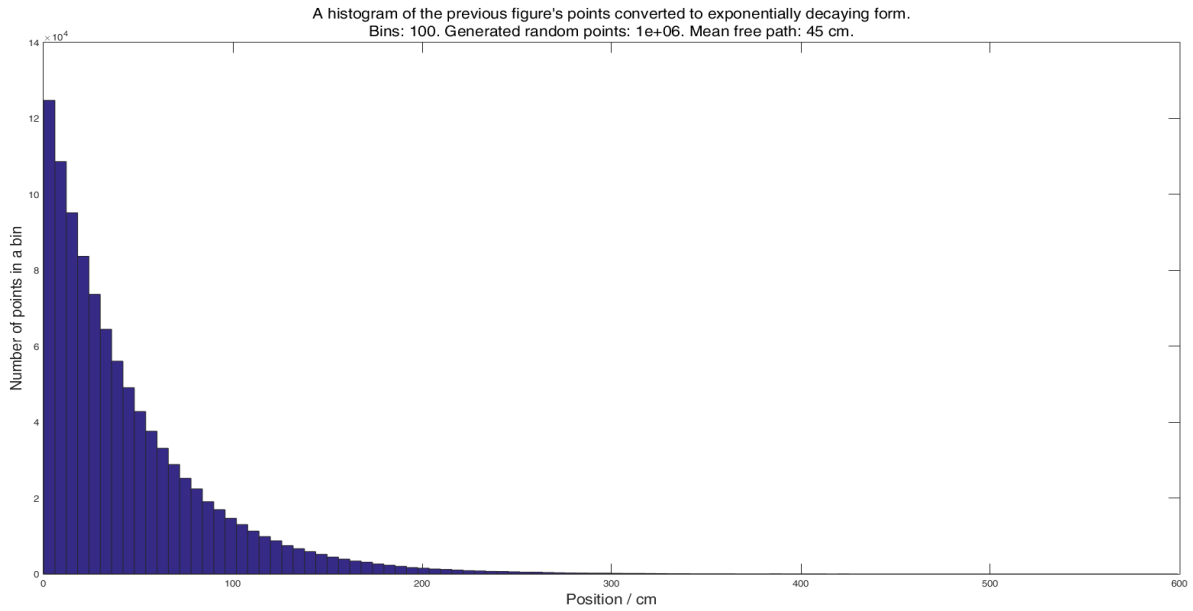

Figure 2: This figure shows that using the outlined method of taking the natural logarithm and multiplying by the negative mean free path produces figure 1, an exponentially decaying curve.

Taking the mean positions of the bins, and the number of points in a bin converts the histogram (figure 2) into a plot of points, with the same exponential form. To linearise this, the natural log of the points can be taken, as is shown in figure 3 alongside the line of best fit which was fitted to all the points - apart from those which were neglected due to the log of zero being negative infinity.

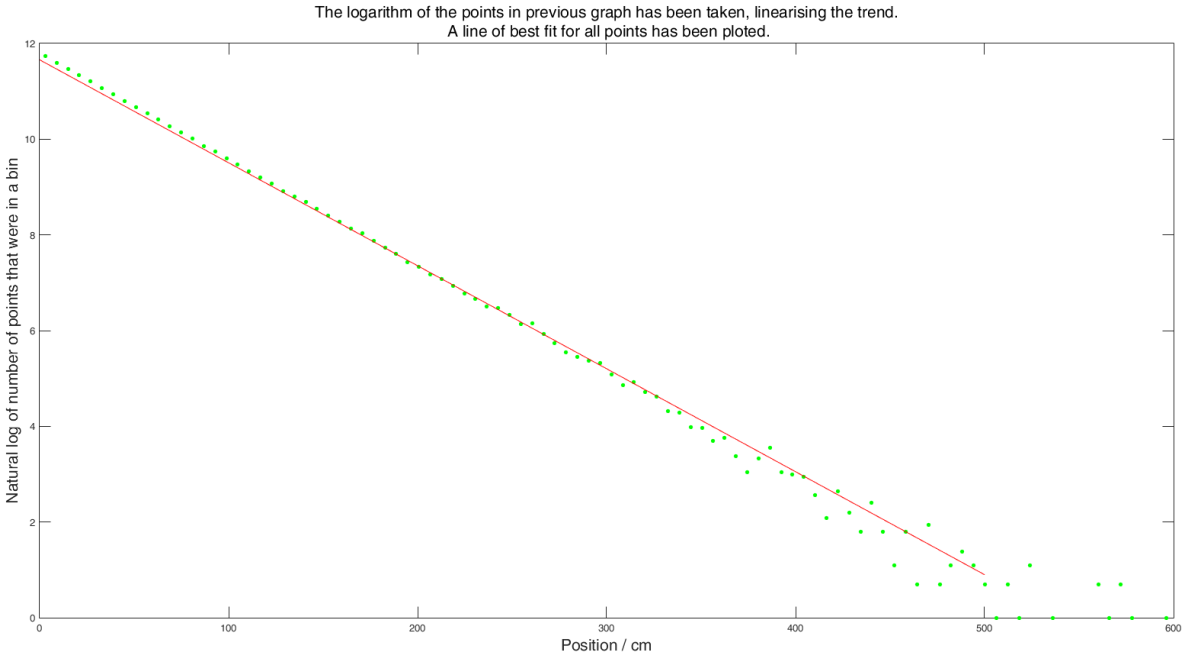

Figure 3: This plot shows that bins with a low number of points in them are able to skew the line of best fit quite heavily. In an extreme case, bins with zero points in turned to negative infinity, so they were removed. By ignoring the bins which had zero points in the mean free path changes - the particles appear to travel further, on average, before decaying.

Repeating this procedure (and taking the negative inverse of the gradient to obtain the output mean free path) 10,000 times gave, for an input mean free path of 45 cm, an output mean free path of 46.9412 ± 1.1272.

Isotropic directions

It is necessary to find a way to make a neutron move in a random direction when it collides with a molecule and scatters. It seems plausible to generate two polar coordinates, theta and phi, and to convert these to Cartesian coordinates, x, y, and z - however the probability density of a point being on a sphere's surface isn't uniform (as the elemental surface area of a sphere depends on one of the coordinates - leading to a higher concentration of points at the poles). Thus, a conversion factor has to be used to remove this dependency. A formal argument is made by Cook in his "…Production of a Spherically Symmetric Probability Distribution".[7]

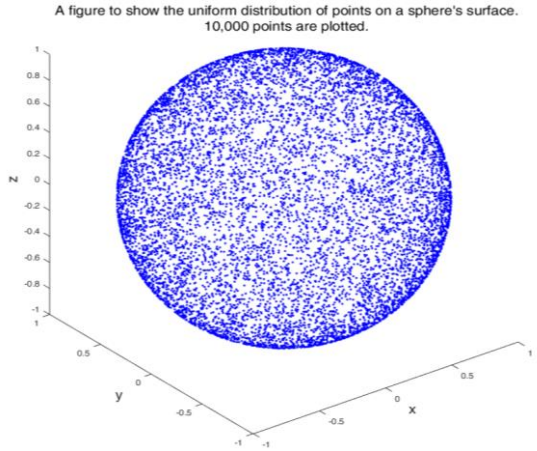

Figure 4: This figure shows that, by eye, there is no bunching of points at the poles using the referenced method for picking points on a sphere.

Combining the methods used for producing a random direction and a randomly generated step length of exponential form, a random walk can be produced - shown in figures 5 and 6. The only differences between these examples and the random walks for neutrons in water, graphite, and lead, is the mean free paths differ in these materials, and in these materials the neutron histories end under certain events.

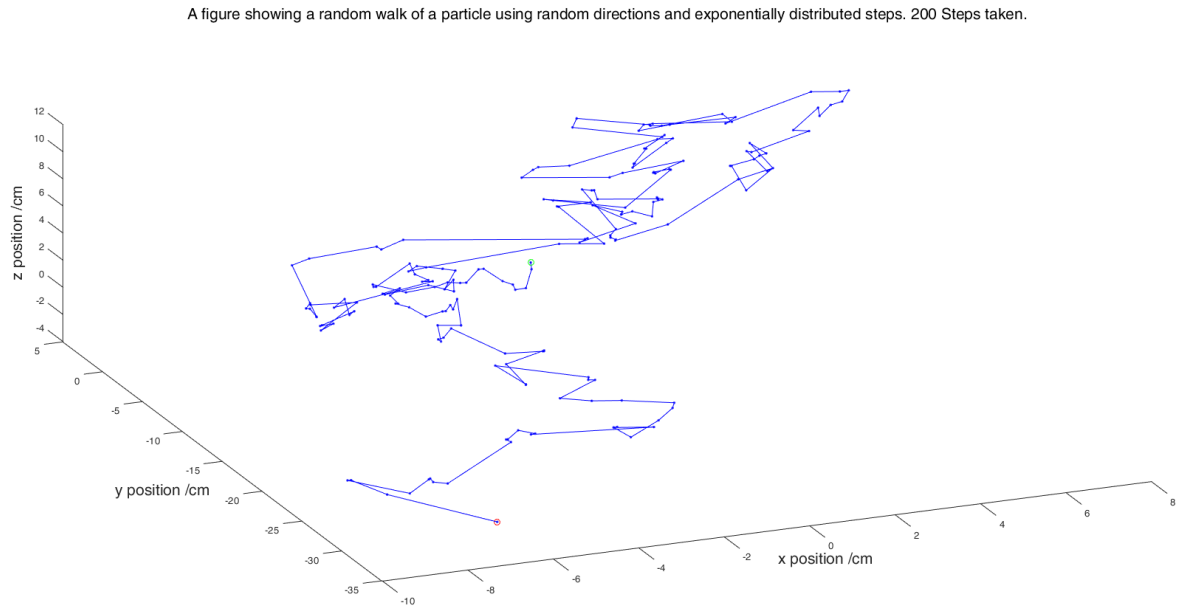

Figure 5: For this random walk, the mean free path was set to be 1 cm for simplicity. This distance between the lines connecting the dots varies, and the direction does too. Across all 200 steps, the mean step distance in the x, y, and z directions tended to be around zero, and the mean path length tended to be around one.

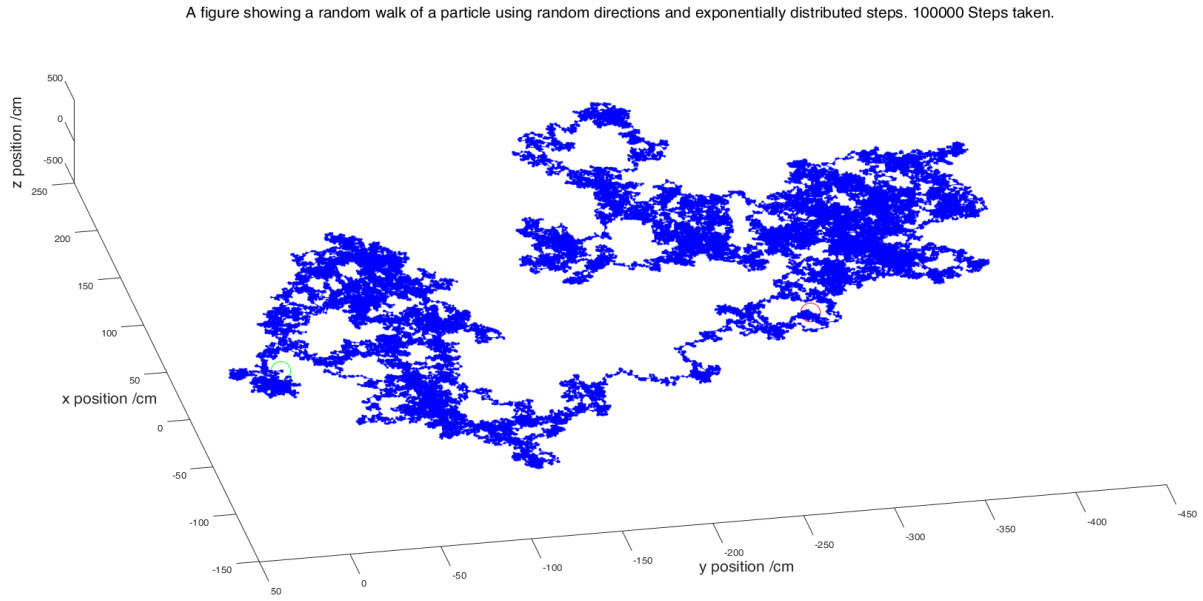

Figure 6: The setup for this plot is the same as for figure 5, however many more steps have been taken. The starting (far left) and ending (lower right) points have become separated, suggesting that the exponential distribution of steps means that the random path for a large number of steps does not tend towards zero displacement (at least not until a much larger number of steps is taken).

Absorption or scattering

All neutrons are fired from $x = y = z = 0\ cm$, and the first step is in the positive x direction only. On colliding with a molecule, at the end of a step, they can either be scattered or absorbed. Scattering will occur until the particle is absorbed, or until the particle exits the medium – if its position is less than 0 cm, it has been reflected, and if it is greater than the thickness of the medium, it has been transmitted. If a random number between zero and one, u_i , is less than or equal to the following ratio

$$u_i \leq \frac{\sigma_{absorption}}{\sigma_{absorption} + \sigma_{scattering}} \quad , \quad 3$$

where σ are microscopic cross sections, then the neutron is absorbed and a count can be added to the number of neutrons that have been absorbed. If u_i is greater than this ratio, the neutron scatters and moves until it collides again. Similarly, when a neutron is either reflected or transmitted, counters for those increase. When these counters increase, the history of the neutron ends and a new incident neutron is simulated.

By repeating this process for different materials and different thicknesses of them, their effect on the reflection, absorption, and transmission of neutrons can be found. By repeating these calculations, means and standard deviations (errors in the simulation) can be calculated.

Results

Using mean free paths calculated from the total cross sectional area for each material, the following plots of neutrons scattering through to transmission were obtained for thicknesses where the percentage of transmitted neutrons was low.

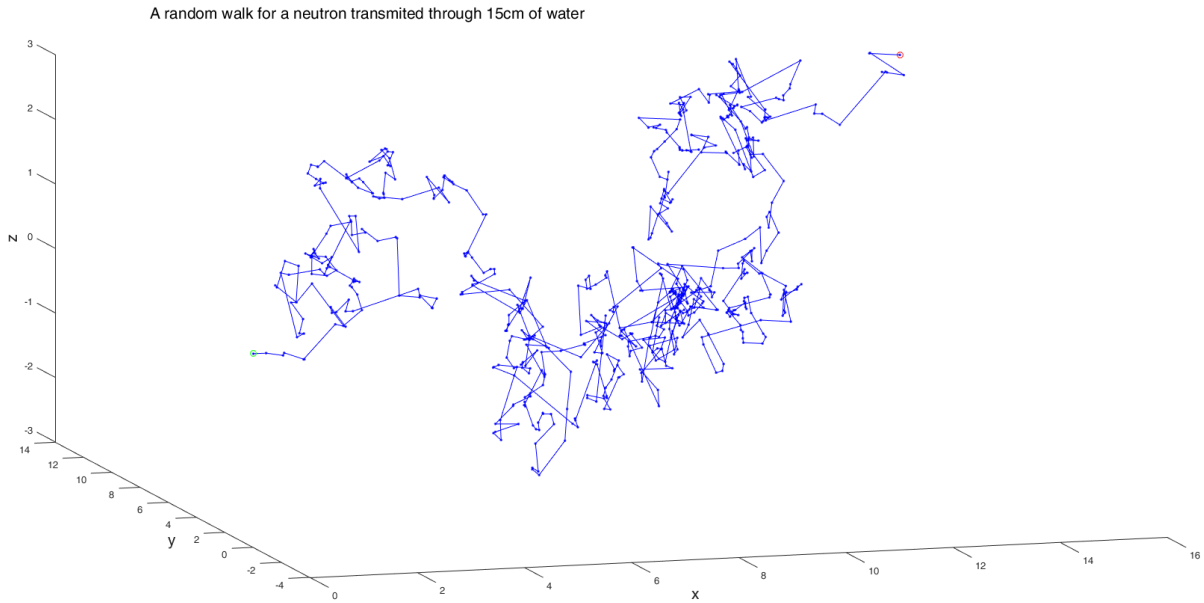

Figure 7: As table 1 suggests, the probability of a neutron transmitting through 15cm of water is very small – however a large number of neutrons can be simulated, hence it's not difficult to produce a similar plot. As can be seen, the neutron history ends when $x = 15\ cm$. The transmission condition has no dependency on the y and z coordinates.

A comparison of figures 7, 8, and 9 suggests that the characteristic attenuation length for water will be the lowest of the three materials, and the characteristic attenuation length for graphite will be the largest.

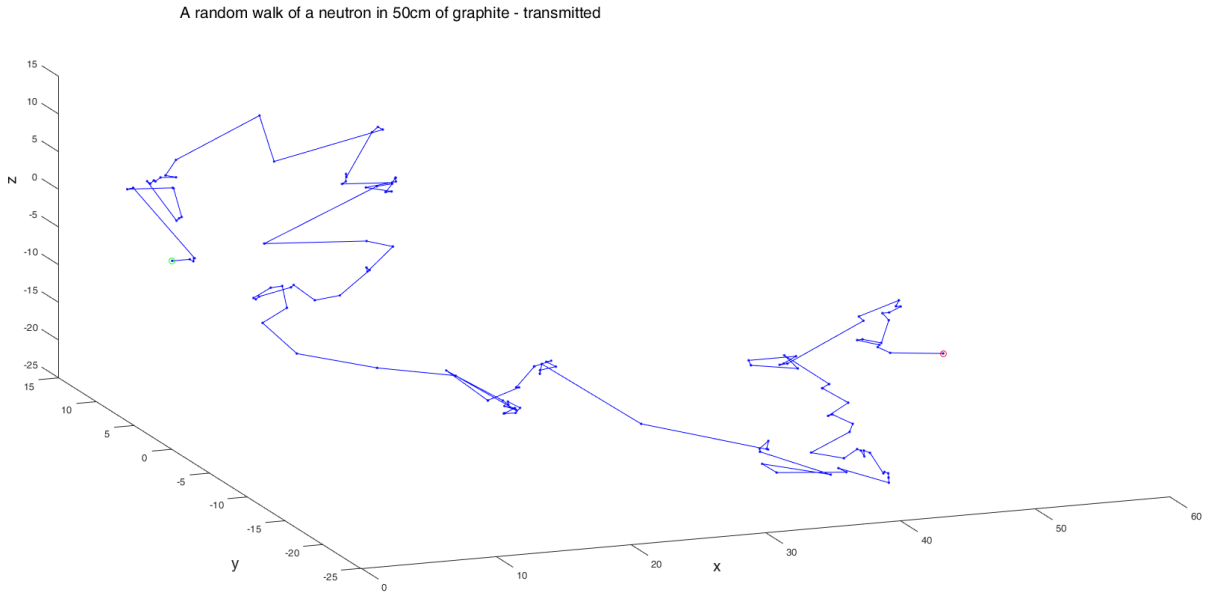

Figure 8: A path for a neutron transmitting through graphite. As well as making less collisions on the way to transmission, this particle's position varied more than water in the y and z coordinates.

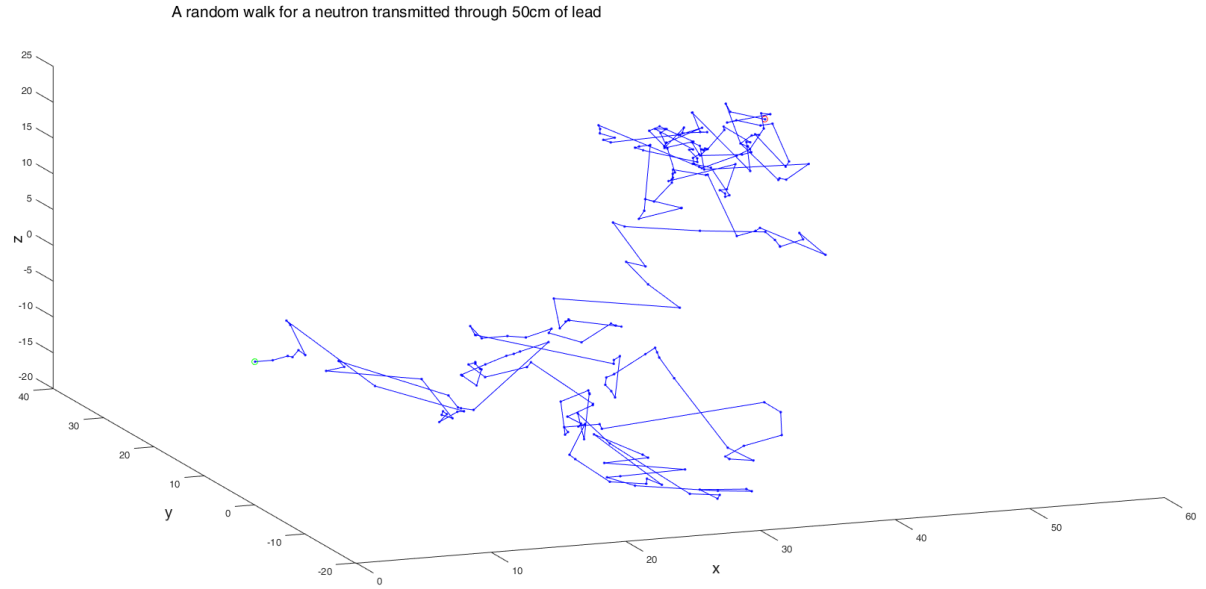

Figure 9: A path for a neutron transmitting through lead. Especially near the end, it seems clear that the characteristic attenuation length of lead should be lower than that of graphite.

Due to the percentage of neutrons transmitted being low at large thicknesses, the fractional error is largest for these thicknesses - hence these values were compared to see the effect on the error of using a larger number of neutrons. Table 3 shows that, for 10,000 neutrons (and 10 loops), the simulation does not seem reliable - the percentage of transmitted neutrons fluctuates between 10.25 and 10.75 cm, and the fractional errors are much larger than is desirable. Conversely, when using 20 loops of 1,000,000 neutrons (100 times as many), the fractional error becomes about ten times smaller. This strongly suggests that

(p.t.o).

$$\sigma_{error} \propto \frac{1}{\sqrt{N}} \quad , \quad 2$$

where N is the number of neutrons in the simulation. In theory, this means desired accuracy could be obtained if enough time and computational power were available, but due to these being constrained the accuracy of data is limited.

Percent transmitted	Error	Thickness	Number of neutrons
0.203	0.045	10.00 cm	10,000 (10 loops)
0.168	0.038	10.25 cm	10,000 (10 loops)
0.152	0.045	10.50 cm	10,000 (10 loops)
0.162	0.051	10.75 cm	10,000 (10 loops)
0.21617	0.00448	10.00 cm	1,000,000 (20 loops)

Table 3: A comparison of the percentage of neutrons transmitted for similar thicknesses of water, which clearly shows the benefit of using more neutrons in the simulation.

When finding the effect of thickness on reflection, absorption, and transmission, intervals of 0.25cm seemed to give an acceptable smoothness to the curves produced in figures ten to thirteen (using 100,000 neutrons over 10 loops).

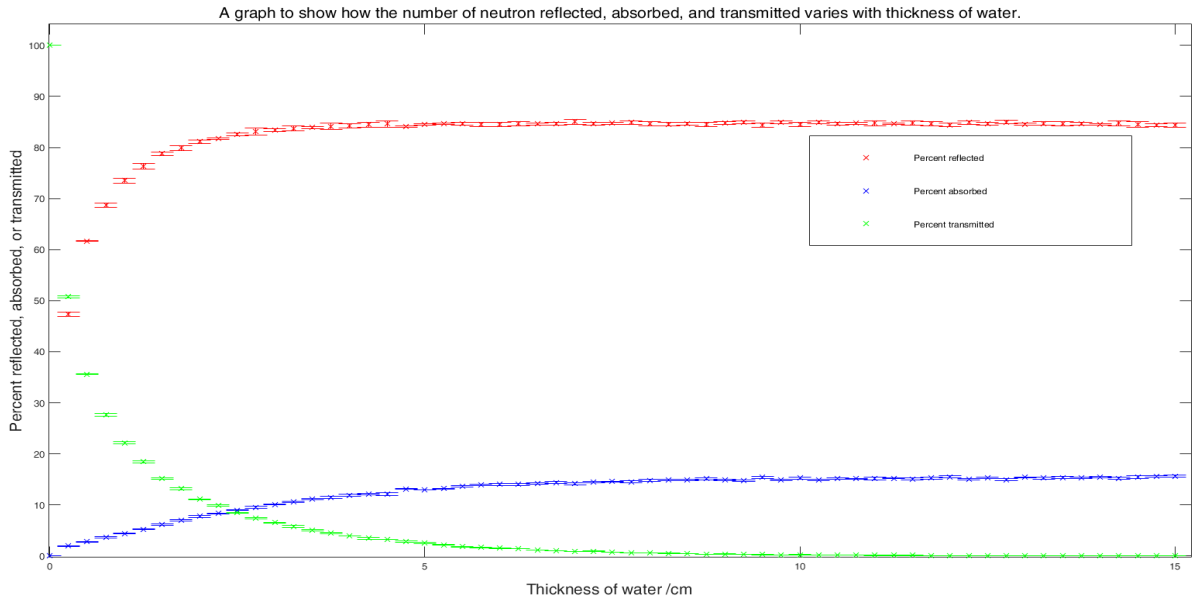

Figure 10: Due to simulating over a smaller range of thicknesses for water than with graphite and lead, it would be appropriate to use a smaller thickness increment for this plot. A noticeable discontinuity is around 5cm for the percentage absorbed.

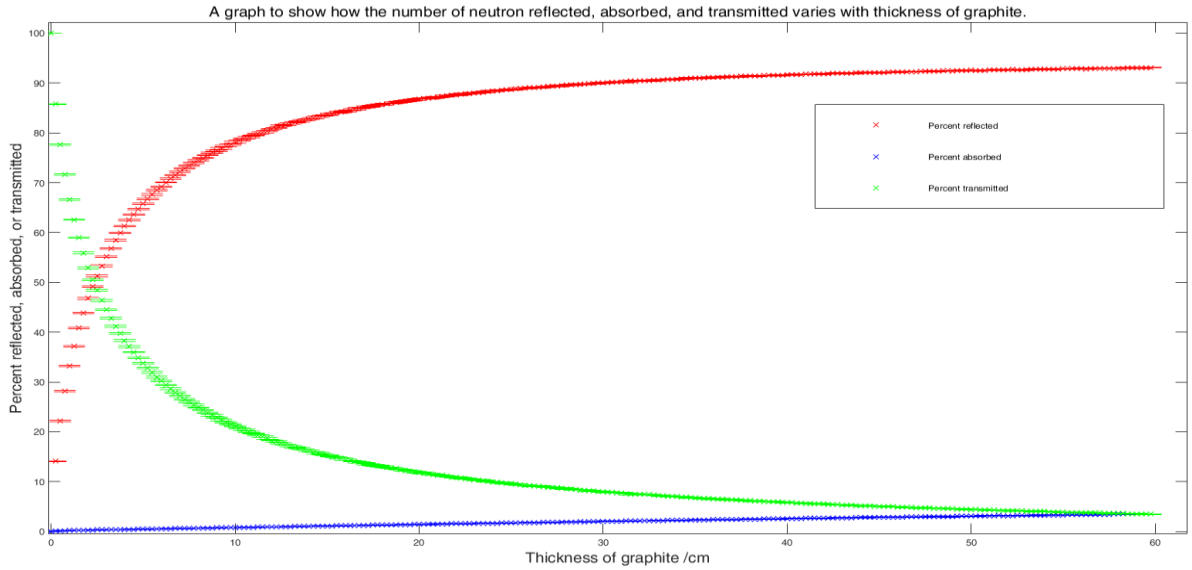

Figure 11: Due to the range of thicknesses expanding, the curve for this figure and figure 12 appears smoother than that for figure 10. The percentage of neutrons absorbed appears to be linear with thickness for graphite.

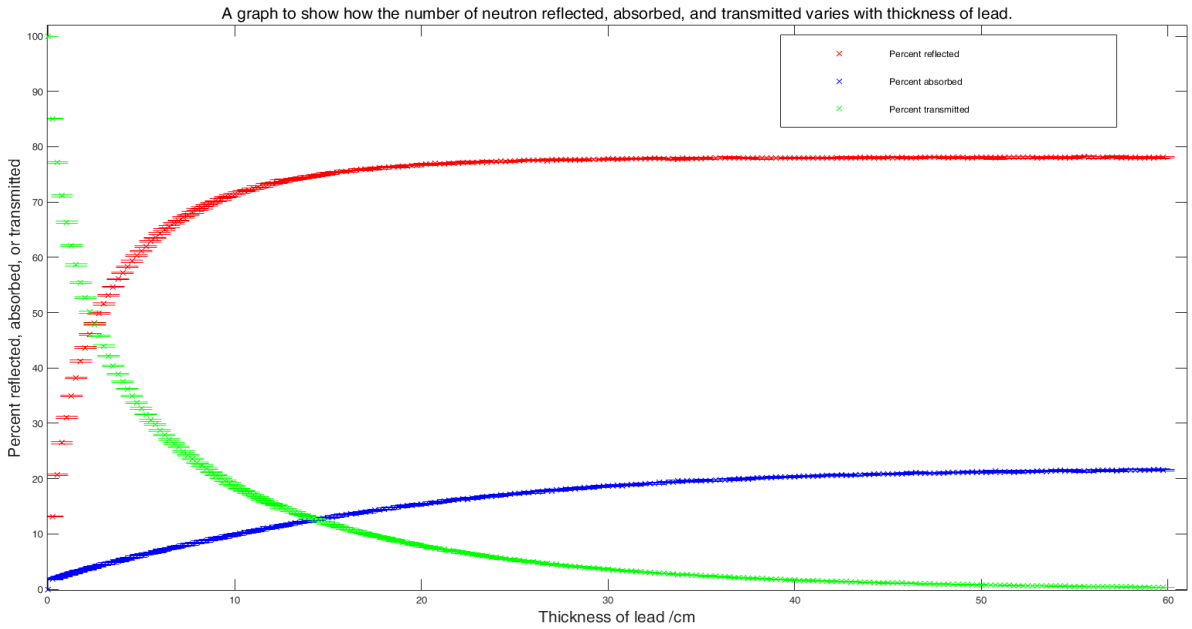

Figure 12: Compared to figure 11, this figure suggests (by the sharper rise in percentage of neutrons absorbed) that the absorption cross section of lead is larger than that of graphite – in agreement with established data.

Figures 11 and 13 show how the number of neutrons and the number of loops used in the simulation affect errors. For a large number of neutrons, the number of loops shouldn't need to be large as the error in the resulting values should be low (though more loops does reduce uncertainty in the error).

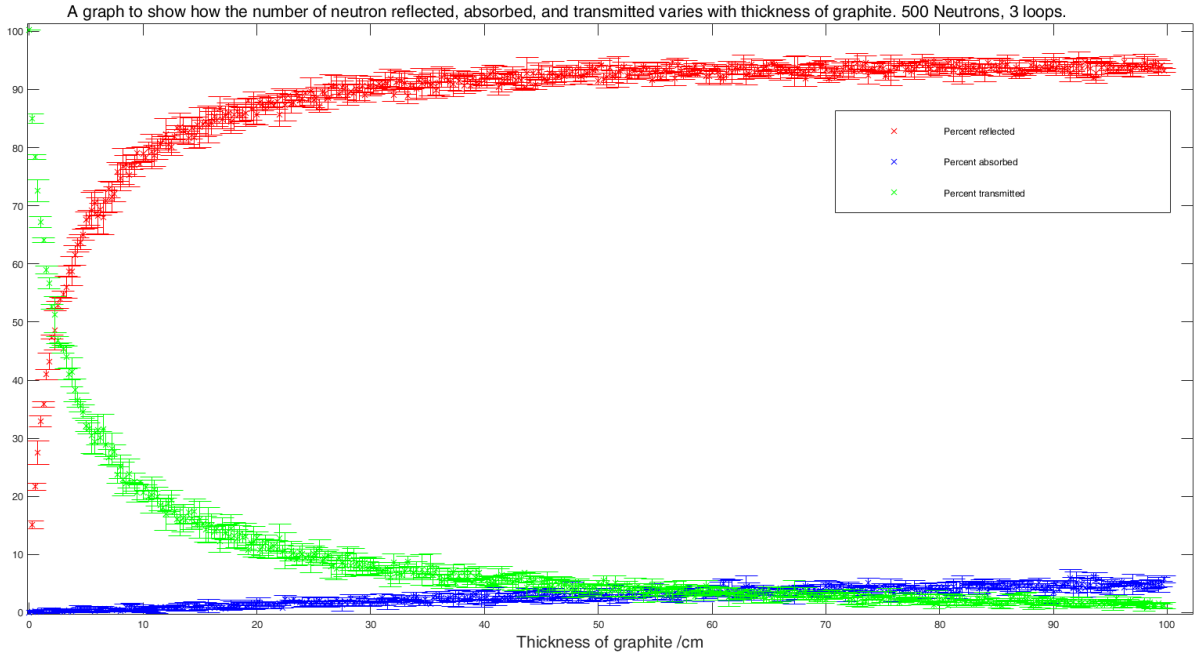

Figure 13: This figure is to verify visually that using a larger number of neutrons in the simulation is necessary to keep the error in the simulation small.

Figures 10 to 13 show that the percentage of neutrons transmitted falls exponentially, and even small thicknesses of material (a few centimetres) can reflect most of the incident neutrons in all cases. Due to having the largest scattering cross section, water can reflect the most of the neutrons at small thicknesses. For all materials, after a certain distance the increase in the number of neutrons reflected became negligible, and the decrease in transmitted neutrons was primarily due to the increased absorption of neutrons.

By taking the natural logarithm of the number of neutrons transmitted and dividing errors in N (for a given thickness, the error in the number of neutrons transmitted) by N, the characteristic attenuation length of each material could be calculated similarly as with figure 3 (take the negative inverse gradient) – however, as figure 14 shows, the linear part of the curve has to be isolated first. Figures similar to figure 14 can be obtained for water and graphite, and they have not been shown due to the similarity. The main difference is that the linear parts of the graphs occur in different regions: For water, this was between 2 cm and 11 cm, for graphite it was between 30 cm and 60 cm, and for lead it was between 15 cm and 60 cm.

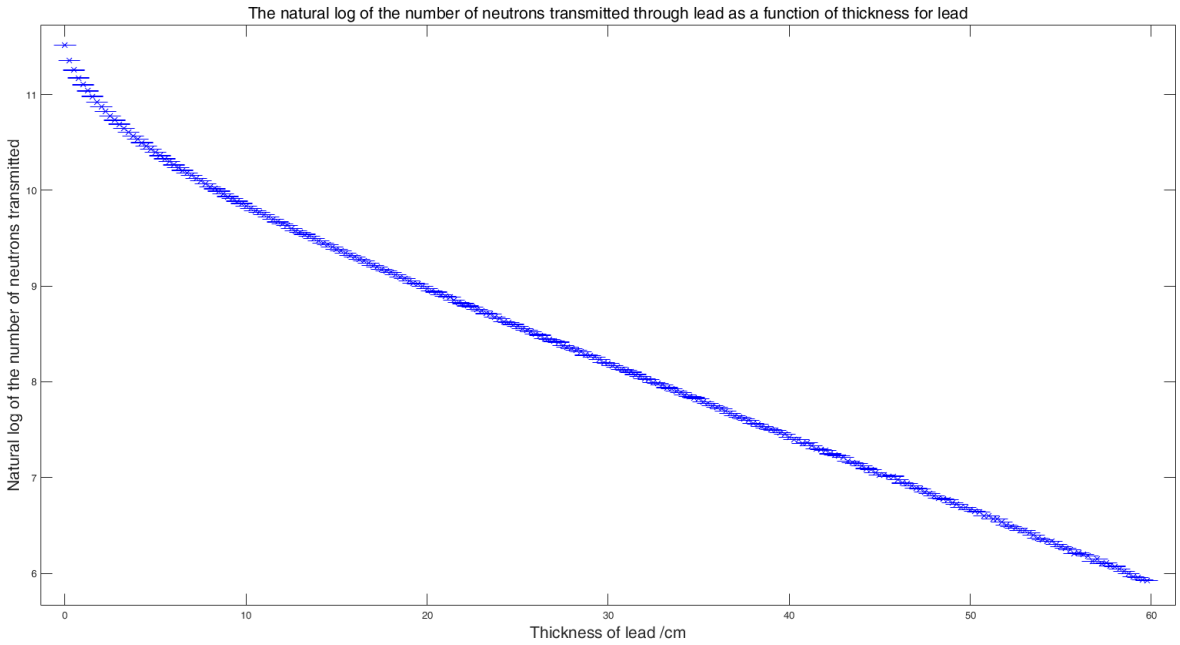

Figure 14: The curve appears to become linear after thicknesses of around 5cm, however the range 15cm to 60cm was used to avoid the non-linear part of the curve.

To find the characteristic attenuation length, its error, and χ^2 values, the data in the mentioned linear regions was analysed by using **MATLAB**'s polyfit command and manipulating the output arrays.

Discussion

Although figures of random walks have been provided, achieving a sense of depth and direction with them is difficult without being able to rotate the image. This could be overcome by using thickness or colour to represent distance.

A useful thing to verify would be the uniformity of points on the sphere's surface, shown in figure 4 – obviously, even a slight bias to movement in one direction would have a large effect on the data. For example, if points were concentrated at the z-poles the neutrons would tend to travel in the x-direction less, hence less neutrons would transmit through a given thickness.

The effect of the exponentially distributed step function on the input mean free path could be verified by ignoring all bins after and including the first bin with zero items in. It seems likely that this would bring the output mean free path closer to the input mean free path, indicating the function works in practise as well as theory.

Water has the largest total cross section by far, hence it's expected it has the smallest characteristic attenuation length. For 10 cm of material, despite its small absorption cross section water has the largest number of neutrons absorbed – this is because the chance of collision is much higher, so there are many more chances for the neutrons to be absorbed. Lead absorbed more neutrons than graphite both due to the larger total cross sectional and its larger absorption cross section. A comparison of tables 1 and 2 indicates that, in general, the characteristic attenuation length is decreases with an increase total cross sectional area.

Conclusion:

By applying Monte Carlo methods to a simple model of a neutron colliding with molecules, the number of neutrons transmitted through 10 cm of material was found, as shown in table 1. It was found that the fractional error of the simulation was proportional to the inverse square root of the number of neutrons used, as is indicated in table 3. Table 2 shows the calculated characteristic attenuation lengths of each material, and an attempt at describing the modulus of these is made by considering the absorption and scattering cross sections in the discussion. Figures 10 to 13 show that the desired exponential decay of intensity (number of neutrons) with thickness, which was described in the theory section, has been met – hence the model and the methods used are in agreement with theoretical expectation.

References:

[1] Dupree, S. A., Fraley, S. K. *A Monte Carlo Primer, Volume 2,* United States of America, Springer, 2004.

[2] Freedman, R., Young, H. *University Physics, 13th Edition*, United States of America, Pearson Education Limited, 2013.

[3] Vukmanovic, O. *UK nuclear build requires taxpayer rescue – Citi*. [Online]. [08/05/2015]. Available from: http://uk.reuters.com/article/2012/05/08/uk-nuclear-britain-edf-idUKBRE8470XC20120508

[4] *A General Monte Carlo N-Particle (MCNP) Transport Code.* [Online]. [08/05/2015]. Available from: https://laws.lanl.gov/

[5] Woodbury, G. *An Introduction to Statistics*, Canada, Thomson, 2002.

[6] Gentle, J. E. *Computational Statistics*, United States of America, Springer, 2009

[7] Cook, J. M. *Technical Notes and Short Papers: Rational Formulae for the Production of a Spherically Symmetric Probability Distribution*. 1957.