# Monte Carlo Techniques – Penetration of Neutrons through shielding

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## Abstract

The analysis of the behaviour of a neutron penetrating through shielding has been conducted. This was done by modelling the neutron as a random walk with the utilization of Monte Carlo methods. The materials that were tested included water, lead and graphite. The number densities used are , and respectively. The attenuation lengths for the materials were found to be --- respectively.

## Introduction

Monte Carlo techniques encompass a broad range of algorithms. These range from integration to weather forecasting. They excel in processes which can’t be easily solved analytically. The main idea behind those methods involves utilising random sampling to obtain a result.

One of the most common applications of Monte Carlo techniques is in random walks. A random walk is a stochastic or random process. It describes a journey of a particle which consists of randomly chosen directions. It is used to model behaviour of a particle in a liquid or a neutron passing through shielding. These two fields can be used to model the random behaviour of a particle. This is particularly useful in nuclear reactors as the geometry of the shielding can be quite intricate. It allows the accuracy to be obtained with enough computational power and its properties are statistically derivable.

## Theory

### 2.1 Inverse CFD method

The Monte Carlo method is best demonstrated by the example of an integrator. Let there be a sinusoidal curve with a very high frequency of oscillation within the range . If the frequency is of the curve is very high this means that the step size must be very small to allow for a numerical integration using trapezium method or any sized step-size method. This is evident by the Nyquist theorem. However, if we choose a step size randomly then the points statistically average out to give us the integral over many runs of the integrator. This is the spirit of the method. It allows us to approach a stochastic process and obtain reliable results over multiple runs of the simulation. This investigation is the same. It will utilize the random number generator with the help of an inverse CDF to obtain a set of vectors. These vectors will have lengths which are exponentially distributed but will also be in random directions. This allows the particle to be tracked. Its interactions with the material are then recorded. Then this single simulation is run numerous times until the average is obtained to a gratifying degree of accuracy.

If you consider an exponential distribution with the probability generating function being

|  |  |  |
| --- | --- | --- |
|  | *.* | Equation 1 |

This is known as the Beer-Lambert Law The variable indicates the depth of the particle within the material while is the mean free path [x]. The mean free path is defined as the average distance travelled between successive impacts. This probability function can be derived using the following equation:

|  |  |  |
| --- | --- | --- |
|  |  | Equation 2 |

This related the rate of absorption per unit thickness, with the intensity of the incoming radiation. This then gives us that the mean free path is

|  |  |  |
| --- | --- | --- |
|  | *.* | Equation 3 |

The distribution in Equation 1 is the exponential distribution with the cumulative probability function being

|  |  |  |
| --- | --- | --- |
|  | *.* | Equation 4 |

This allows us to obtain the inverse of the CDF.

|  |  |  |
| --- | --- | --- |
|  | *.* | Equation 5 |

If a set of random number is inputted into Equation 5 then the outcoming set will be distributed according to the exponential distribution. This equation allows for the generation of steps during the random walk. The change of variable from to is done due to the numbers being generated being within 0 and 1. Hence the range restriction allows for the variable change. If the number is multiplied by the mean free path then the step length is obtained.

### 2.2 Random number generation

The generation of random numbers is essential to the process. It is essential a set of equally distributed random numbers to ensure statistical coherence. Otherwise the bias would skew the results of the simulation. The method used in this simulation is obtained from the NumPy library and was tested against other random number generators in Section XX.

It is essential to mention that a pseudo-random generator was also tested to show the inherit flaws in utilizing. A pseudo-random generator utilizes a modulus function which distributed the numbers equally. However, it isn’t random as knowing the first number in the sequence generated allows for the discovery of the whole sequence following it. The generation occurs using

|  |  |  |
| --- | --- | --- |
|  | *.* | Equation 6 |

The variable being the modulus, being the increment, being the multiplier and being the seed. This formula allows for a generation of random numbers as long as and are prime. Also, a feature of the generator is that is divisible by 4 if is a multiple of 4. This specific pseudo generator is a Linear Congruential Generator (LCG).

### 2.3 Neutrons and shielding

The purpose of this experiment is to simulate the transmission of neutrons through shielding and calculate the specific attenuation lengths of water, graphite and lead. The particles that enter the material are distributed according to Equation 1. When a neutron hits the surface of a material it has a chance to either become absorbed or scatter. The probability of each depends on the multiple of the number density with the absorption or scattering area. The length at which the intensity of particles drops to is defined as the attenuation length.

## Method

The process that is being investigated is being modelled as a Markov Chain. This is done utilizing Monte Carlo methods. The particle is set on the surface of the material with the first step being made in the direction perpendicular to the surface. The length is obtained from Equation 5. The particle moves the step and then generates a probability. According to this probability it is either absorbed or it continues after scattering. This scattering allows it to make another step. This cycle proceeds until the particle is either absorbed, transmitted to the other end, or it reflects. The number of each of those events is counted. Then the thickness of the material is changed, and the simulation is started again. This is done until the numbers of particles at specific thickness agree between runs within a degree of error. Those numbers are then plotted and according to Equation 1 the attenuation length is found.

The object-oriented approach has been implemented due to the clear separation between random number generation and the experimental methods. This allows for the reusability of code along with the modular application of other classes like the LCG class. This also allows the experiments to be self-contained without the need for global variables. The inheritance of classes was used to ensure legibility in the code. The code doesn’t possess a user interface due to its redundancy.

Figure 1 – The table summarising the scattering constants used.

|  |  |  |  |
| --- | --- | --- | --- |
| Material name | Water | Lead | Graphite |
| Absorption area/ | 0.6652 | 0.158 | 0.0045 |
| Scattering area/ | 103 | 11.221 | 4.74 |
| Density/ | 1 | 11.35 | 1.67 |
| Number density/ |  |  |  |
| Macroscopic absorption cross area/ |  |  |  |
| Scattering cross section/ |  |  |  |
| Total mean free path/ |  |  |  |

The first part of the simulation calculates value for the attenuation length of water for thickness of . This is done to check the capabilities of the simulation as the theoretical value is . The second part deals with the complete model.

## Analysis

### 4.1 Comparison of the numerical methods

F Figure 1 shows that the Verlet methods gives the best results. This can be further confirmed by the fact that the error in energy generated over the whole runtime was . Meanwhile, the second lowest was the Euler-Cromer method which obtained for all the values tested. it is important to mention that the Improved Euler’s method provided a small error in the range of the damping coefficient passing the critical value. The inaccuracy in the Euler-Cromer method comes from the fact that its energy needs to be averaged over a complete cycle while the Verlet method doesn’t. The testing of simulations running over complete cycles wasn’t tested due to the desire to ensure fairness of the comparison method. The remaining two are not symplectic methods and it can be visually seen that they are not as accurate as the Verlet method in Figure 1 or 2. This means that the Verlet method was utilised for the rest of the investigation with modifications described in section 3.

Then the test was conducted for a damped oscillator. It consolidated that the Verlet method has the smallest error out of all the numerical integrators. As evidence by the error being barely visible on the graph. As visible in Figure 1 the error for the Verlet integrator is very close to zero for the entirety of the simulation while other integrators either increase or oscillate around the value. In Figure 2 the energy error curve is the least prominent for the Verlet method under damping as well. The time step value was chosen to be due to it being the best balance between the time taken and the accuracy of the computation. The accuracy increases with the decrease in the step size. This was more apparent for both Euler’s methods due to those two methods having the smallest degree of accuracy. It is important to note that all the methods perform very well when the value of the damping coefficient is large. Verlet’s method produced errors which were not exponential in contrast with Euler’s method. Verlet’s method was also the one that presented the error not increasing exponentially with time. This is very important for long term simulations. Even despite only a second order Taylor expansion used in Equation 18 the accuracy was much higher than anticipated.

Figure 3 – The table showing the error in the total energy for a given set of damping constants. The values are rounded to two decimal places.

### 4.2 Unforced Oscillations

A step size of *0.001 s* and a maximum time of *100 s* were used to model the unforced simple harmonic oscillator with damping terms half, double and equal to the critical damping coefficient. This was obtained from Equation 20. The value was calculated to be . The energy plots show the expected behaviour. The critically damped oscillator returned to the equilibrium position in the shortest amount of time. The heavily damped oscillator took longer while the lightly damped oscillator moved past the equilibrium point twice. This can be observed in Figure 4. The energy was calculated using Equation 6. The energy decreased the fastest for the critically damped oscillator. This can be observed in Figure 5.

All the calculations were calculated utilising the Verlet method as it was chosen to be the most accurate as explained in section 4.1. The spiral behaviour presented in Figure 5 can be attributed to the damping forces present in the system arising from the damping coefficient.

### 4.3 Instantaneously Forced Oscillations

The effects of an application of a constant force and a sinusoidal force were investigated. In the case of a constant force the time at which it was applied determined the response. All the oscillations returned to a behaviour explained in section 4.1 after a short transition period. The amplitude changed after the force was applied. When the force was applied at the equilibrium point the amplitude changed the most as can be seen in Figure 6. For the half-cycle and quarter-cycle force applications the effect was weaker, but the amplitude still decreased. Hence the plots were not included.

The sinusoidal force caused an increase in the amplitude around the frequency of the force being equal to the natural frequency of the oscillation. This can be seen in Figure 7. This increase in amplitude occurred only around the natural frequency. If at the moment of the force being applied the direction of the force was in the same direction as the velocity the amplitude increased. Furthermore, the opposite was true as well. The magnitude of the force was found to be not as dominant as expected. Towards the upper values of the force the oscillation still occurred however, reached a rest point much faster. This force had the same effect as shifting the equilibrium point. This is analogous to a suspended spring system where gravity shifts the equilibrium point.

Resonance was observed at the angular frequency calculated in section 3. It was characterised by a sharp increase in the amplitude of the oscillation at the natural frequency. A resonance curve with different damping terms is shown in Figure 8. The value of the damping term increasing caused the lowering of the resonance peak. At the heavy/critical damping the damping coefficient was too high to allow for the resonance to occur. This meant that the motion dissipated too quickly for any oscillation to occur.

## Error Analysis

The main sources of error in this simulation arose from the discretisation error, truncation error, initial conditions and the net growth in the error as the simulation progressed. The discretisation error arises from the fact that the time step at which values are evaluated isn’t infinitesimal but of a fixed value. This was mitigated by the utilisation of a very small step size. The data obtained could have been developed at higher accuracies, but the time constraints didn’t allow for this. The fact that the errors grow as the simulation progresses is since iterations utilise previous values to work out the path of the oscillator. This was mitigated by ensuring that the terms that were omitted, like in the case of a Taylor expansion, were powers of the time step allowing the convergence of the method to happen with minimal error present. The truncation error increased as the step interval decreased.

## Conclusion

The models were utilised and compared as described in section 4.1. The Verlet method was found to be the most accurate for modelling forced and unforced oscillation. The investigation into the effects of the step size onto the accuracy has been conducted. It has shown the inverse proportionality between the step size and the accuracy. This was especially apparent for the less accurate Euler’s method. It can be deduced that the smaller the size of the interval the better the prediction. It is advised to always use the smallest step size possible. However, it is apparent that the decrease of the time interval gives diminishing returns after passing the size.

The application of a constant force onto an oscillator produced a transition period after which the oscillation resumed with a shift in phase and amplitude. The sinusoidal force has been investigated with the use of a resonance plot. It was confirmed that the sharp amplitude increase occurs at the frequency close to the natural frequency of the oscillator. Lastly the Verlet method was utilised to observe the behaviour of the oscillator in the case of being heavily damped and critically damped (as described in section 4.2). It was also confirmed that resonance did not occur when the oscillator was heavily or critically damped.

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## Appendix - Code

The history of changes can be found in the GitHub repository [10].