Monte Carlo simulation of a fission reactor

Andreas Hadjichristou and Qi Nohr Chen
Year 2 Theory Computing Project, University of Manchester.
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The aim of the experiment is to investigate the criticality of a homogeneous fission reactor using Monte Carlo methods, by monitoring the position and energy of each individual neutron and its' subsequent interactions in each neutron generation.

1. INTRODUCTION

The ideal production of energy is one of the biggest challenges in the modern society. There are many ways energy can be sourced. One of them is the nuclear reactor whose nuclear energy has been used to generate electricity for the first time in 1951 [1]. The nuclear reactor is an apparatus that utilises neutrons to induce fission of, for example, Uranium-235 fuel. The fission may produce another neutron and create a chain reaction and cause more fission and energy release. However when constructing a nuclear reactor, the rate of fission needs to be considered which is detrimental in its' development. If the rate is too high, the nuclear reactor may overload, if the rate is too low, then it won't produce sufficient energy. The rate is highly dependent on the geometry and contents of the reactor. It would not be viable to build a nuclear reactor and trial it. Instead, computing and algorithms may be used to optimise a nuclear reactor. This investigation will use the metropolis random walk algorithm to optimise a nuclear reactor with different compositions of fuel and moderator, and a cylindrical geometry. The metropolis random walk algorithm is a computing tool that will sample out "favorable" events as well as unfavorable given certain conditions and probabilities.

2. THEORY

The probability of a neutron undergoing a process inside the fission reactor depends on the macroscopic cross section [3] Σ of the homogeneous mixture for that process defined as

$$\Sigma = \sum N_i \sigma_i, \tag{1}$$

where N_i is the number density and σ_i is the microscopic section of the component i of the mixture. The total macroscopic cross section Σ_T is defined as

$$\Sigma_T = \Sigma_f + \Sigma_s + \Sigma_c, \tag{2}$$

where Σ_f, Σ_s and Σ_c are the mixture macroscopic cross sections for fission, scattering and capture respectively. The probability distribution $P(d)$ determining the distance d that a neutron will travel before undergoing one of the three processes is defined as

$$P(d) = \frac{1}{\lambda} e^{\frac{-d}{\lambda}}, \tag{3}$$

where λ is defined to be the mean free path which is equivalent to the inverse of Σ_T. When a neutron undergoes fission, the energies of the emerging neutrons are determined by a Watt probability distribution $P(E)$ [6] defined as

$$P(E) = 0.4865 \sinh \sqrt{2E} e^{-E}, \tag{4}$$

where E is the energy of the neutron emerging. The Watt distribution is not dependent on the energy of the incoming neutron as a simplified approximation. Our model considers elastic collisions of neutrons with nuclei where the energy decrement ξ is defined as

$$\xi = 1 + \frac{(A-1)^2}{2A} \ln \frac{A-1}{A+1}, \tag{5}$$

where A is the atomic mass number of the scattering nucleus. The energy of the neutron after collision E' is then defined as

$$E' = \frac{E}{e^{\xi}} \tag{6}$$

where E is the initial energy of the neutron. The multiplicity factor k is defined as

$$k = \frac{N'}{N}, \tag{7}$$

where N' is set to be the number of neutrons of the new generation and N is set to be the number of neutrons of the old generation. As we are considering a finite homogeneous reactor, there are neutron collisions with the walls of the reactor which are approximated to be completely elastic. The directional unit vector of the neutron $\vec{v'}$ after collision is defined to be

$$\vec{v'} = \vec{v} - 2(\vec{v} \cdot \hat{n})\hat{n}, \tag{8}$$

where $\vec{v}$ is defined to be the initial directional unit vector meeting the boundary surface and $\hat{n}$ is the normal unit vector to the boundary surface at the point of impact.

3. ALGORITHM ANALYSIS

The primary algorithm used is the Monte Carlo algorithm, specifically the metropolis random walk. First, the neutrons are uniformly spawned inside the homogeneous reactor whose shape is chosen to be a cylinder. The simulation uses the Cartesian Coordinate System. Random numbers are generated for x and y positions and only the pairs resulting in a radius equal or smaller to the radius of cylinder are accepted. A similar process follows to attach a z coordinate that has to be within the range of the height of the cylinder. The initial energy of neutrons spawning is set to be 2 MeV.

An important feature of the randomly spawned neutrons is the uniformity and unbiased coordinate generation. This can be shown through a 2D confirmation plot of the coordinates of the spawned neutrons. By ignoring the z-axis of the neutron coordinates and using the plot, the uniformity can be determined by eye to roughly estimate and confirm uniform distribution.

A more quantitative way of confirming uniform distribution would be to use a histogram and plot the frequency of neutrons against the radius value from the origin. It was chosen to again ignore the z-coordinate of the neutrons for this plot again. The neutron distribution can be regarded as uniform if the histogram would show no obvious biases in position, showing a relatively straight line.

A random uniform directional unit vector is generated and accepted only if its radius in spherical coordinates is equal or less than 1. The likelihood of each interaction occurring inside the reactor depends on a cross section that is neutron-energy dependent. Experimental cross section data with corresponding neutron energy is obtained through the Janis 4.0 software [2]. In the fast neutrons region, the cross section is approximated by high order fitting polynomials. For the resonance region the algorithm matches the energy of the incoming neutron with the one that has the smallest difference with experimental data and takes its corresponding cross section.

The mean path is then calculated using the total macroscopic cross section and a random distance is drawn from the distribution following equation (3). The process occurring for the neutron is then decided by a random number γ [5] which has a range between 0 and 1.

If

$$\gamma < \frac{\Sigma_s}{\Sigma_T}, \tag{9}$$

then scattering occurs. If

$$\frac{\Sigma_s}{\Sigma_T} < \gamma < \frac{\Sigma_s + \Sigma_c}{\Sigma_T}, \tag{10}$$

then capture occurs. Otherwise if

$$\gamma > \frac{\Sigma_s + \Sigma_c}{\Sigma_T}, \tag{11}$$

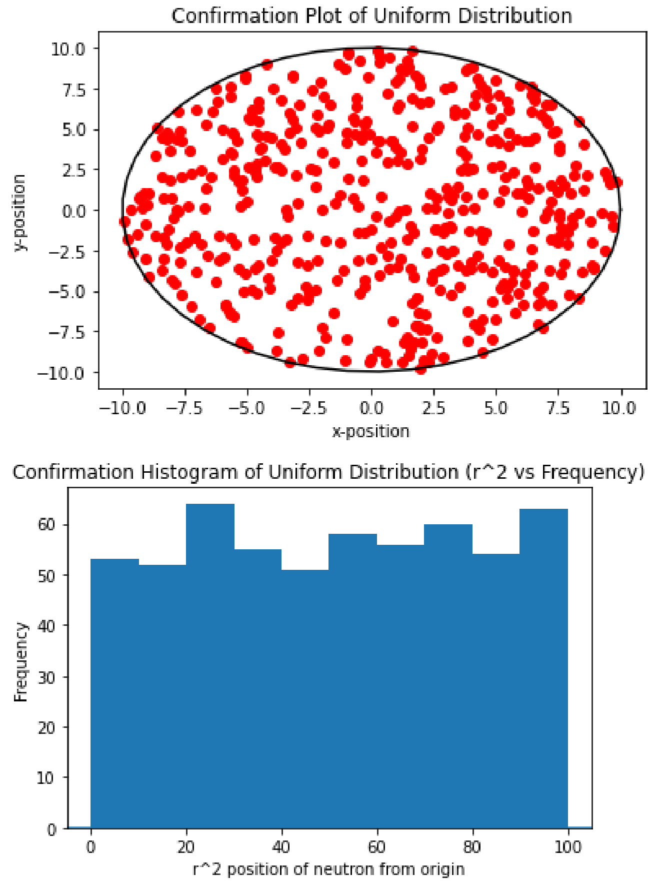

FIG. 1. A 2-D cylindrical space and its corresponding histogram plot that shows the radius of initial neutron position from the origin. Confirmation plot shows a relatively unbiased straight line. A neutron batch size of 500 was used.

fission occurs. When a neutron is absorbed by a Uranium-235 nucleus and fission occurs, the number of neutrons emerging is determined by a random integer number obtained from a discrete probability distribution of 0.1 for 1 neutron, 0.4 for 2 neutrons, and 0.5 for 3 neutrons giving an expectation value of 2.4 neutrons within the parameters of a real reactor. A random energy is then determined for the emerging neutron using the probability distribution of equation (4). Here a random energy is generated using a uniform distribution. Then a distribution value is generated between 0 and the maximum value of the normalised distribution. The random energy is only accepted if the distribution value is lower than the distribution value evaluated at the random energy. For Uranium-238 fuel the cross section for fission is negligible at the range of energies that neutrons are spawned in the simulation compared to the cross section of Uranium-235 for the specified range of energies. Thus it can be approximated to be constant and very close to 0. If the process is scattering, a random number decides by which material the neutron was scattered according to the ratio of scattering cross section of the material to total scattering cross section. It then lowers its energy using the energy decrement in equation (6).

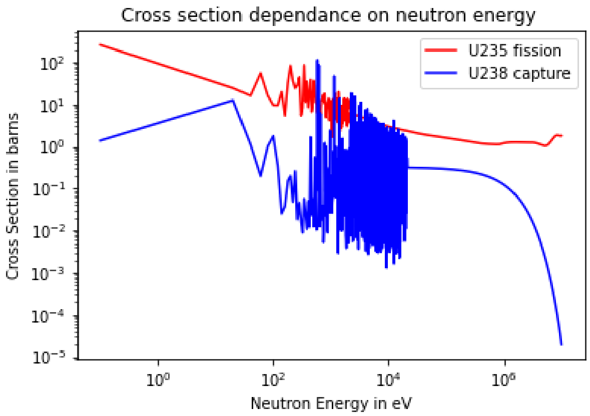

FIG. 2. The figure shows the approximated algorithm model representing cross section against neutron energy for U235-fission and U238-capture.

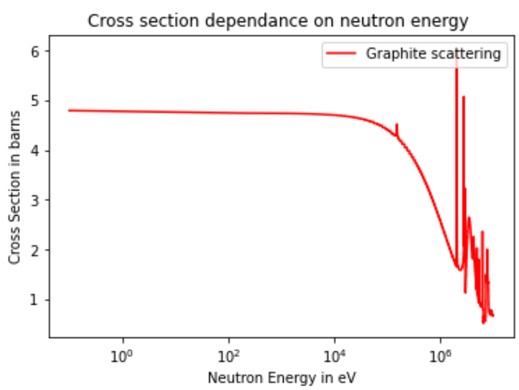

FIG. 3. The figure shows the approximated algorithm model representing cross section against neutron energy for Graphite scattering.

The algorithm then identifies the position of the neutron and checks if the neutron is found to be outside of the reactor after the distance proposed to move. The reflector material used is beryllium. A random number is generated to decide whether the neutron escapes from the reactor or reflected elastically. If its reflected, the algorithm compares the position of the neutron moved outside of the boundary surface and finds the boundary position with the shortest perpendicular distance to the outside position. However the algorithm assumes that the neutron leaving the reactor doesn't travel a great distance (approximately multiple meters), such that the distance perpendicular to the boundary position is the approximate position of where the neutron has escaped the reactor. The boundary position takes the new directional unit vector and completes the distance that it needs to travel before the next iteration.

Finally the algorithm measures the neutrons left inside the reactor, the number of fissions, scatterings and captures. Comparing the number of the old generation neutrons and the new generation neutrons the k-factor is determined.

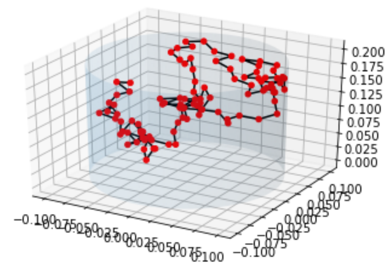

FIG. 4. The figure represents the model of a single neutron doing a random walk and scattering of the boundary surface with a constant step size. The same model is implemented in the algorithm but with multiple neutrons and energy-dependent distances, with distances following exponential distribution as in equation (3).

4. RESULTS

Reactor Density Specifications	Density (in g.cm^{-3})
U-235	18.7
U-238	18.9
Graphite	1.6
Reactor Dimension Specifications	Dimension (in m)
Height	20
Radius	10

TABLE I. The table displays the specifications of the densities of the reactor components (Moderator and Fuel) as well as the geometric specifications (height and radius of the cylinder). These specifications were used for all experiments conducted.

By investigating the relationship of cumulative energy per iteration there is a strong correlation with k multiplicity factor. For a super-critical reactor where k is greater than 1 there is an exponential rise of cumulative energy per iteration where an iteration represents a very small interval of time. For a critical reactor where k is approximately 1 the relationship tends to become linear. For the sub-critical case the relationship becomes a step-wise function.

Examining the relationship of average energy of neutron per iteration, the algorithm after 25 cycles converges to an approximately constant average energy. This number of cycles is close to the number of scatterings required to thermalize a neutron of 2 MeV to around 10 keV with graphite as the moderator material. This signifies the entry of the neutron into the resonance region.

The algorithm was tested under different material ratio parameters, to calculate the ideal moderator to fuel ratio. This was found to be approximately 20:1 (20 parts graphite moderator to 1 part fuel), with a U-238 to U-235 ratio of 0.5:0.5 for which a k multiplicity factor was calculated to be 1.005 ± 0.012. From this investigation, a super critical reactor would have a moderator to fuel ratio of 1:2 with a U-235 to U-238 ratio of 0.5:0.5, for which the algorithm has calculated

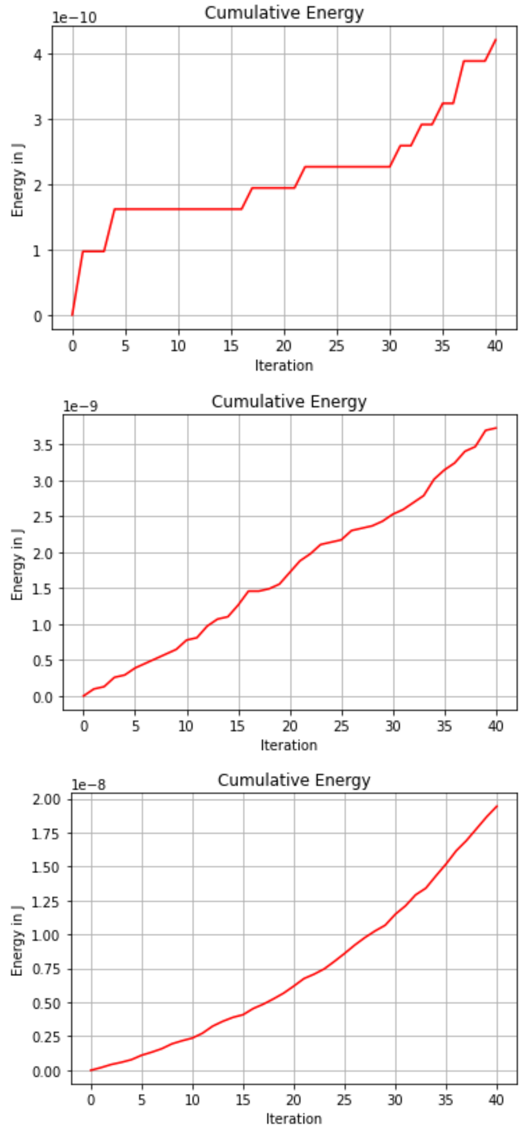

FIG. 5. The figure displays the graphs of cumulative energy in Joules, against iteration for the sub-critical,critical and super-critical case respectively. The energy comes only from fission reactions where an average of 202.79 MeV is released per fission.

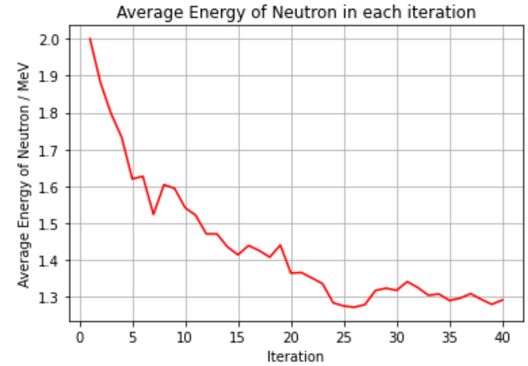

FIG. 6. The figure displays the average neutron energy per iteration. After approximately 28 cycles the average neutron energy inside the reactor is about 1.3 MeV.

Moderator to Fuel ratio	U-238 : U-235	k-factor	Uncertainty
1:1	1:1	1.034	$\pm$ 0.013
1:1	2:3	1.094	$\pm$ 0.009
1:2	1:1	1.103	$\pm$ 0.013
2:1	9:1	0.996	$\pm$ 0.017
3:1	1:1	1.047	$\pm$ 0.013
4:1	1:1	1.028	$\pm$ 0.015
5:1	1:1	1.017	$\pm$ 0.012
6:1	1:1	1.017	$\pm$ 0.012
7:1	1:1	1.012	$\pm$ 0.013
12:1	1:1	1.008	$\pm$ 0.011
20:1	1:1	1.005	$\pm$ 0.012
20:1	9:1	0.998	$\pm$ 0.017

TABLE II. This table displays the moderator (graphite) to fuel ratios and the U-235 to U-238 that were investigated and the calculated k-factor with its uncertainty.The probability of neutrons leaking outside of the reactor is set to be 3.3%. The first 15 cycles were ignored for the mean k-factors and the uncertainties due to the region of non-convergence.

k = 1.103 $\pm$ 0.013. A sub critical reactor could be reached if the ratio of U-238 to U-235 fuel was greater, as more neutrons would be absorbed rather than undergo fission.

The uncertainties of k-factor were determined by carrying three independent trials of the algorithm and taking the weighted standard deviation after ignoring the first 15 cycles.

5. DISCUSSION AND CONCLUSION

The region of resonance occurs mainly occurs due to the quantum nature of nuclear forces interacting. The energy-dependent cross section for the radioactive capture of a neutron by Uranium-238 shows strong evidence of keeping the reactor near critical state. The probability of neutron capture by resonance of U-238 fuel, found using resonance escape probability [3] with moderator to fuel ratio of 600:1 (with 1.6% Uranium enrichment) is 25.1%. The results of the simulation with the same parameters find the average resonance capture probability to be 1.1%. A possible cause of this large difference is that the model in [3] assumes absorption cross section of Uranium-238 fuel to be energy-independent and constant which is a crude approximation. The resonant peaks in the absorption cross section of Uranium-238 fuel increase the probability of a neutron being absorbed dramatically assuming that the neutron's energy falls at those peaks as it becomes thermal. The absorption probability is greatly increased due to Doppler broadening where the resonant peak becomes shorter in height and broader due to increasing temperature of target Uranium-238 nuclei(causing the resonance integral to increase).

Most neutrons in fission are released within 10^{-14}s. However, a small percentage (1%) is released after a delay. These neutrons are called "delayed neutrons" [4]. Fission fragments

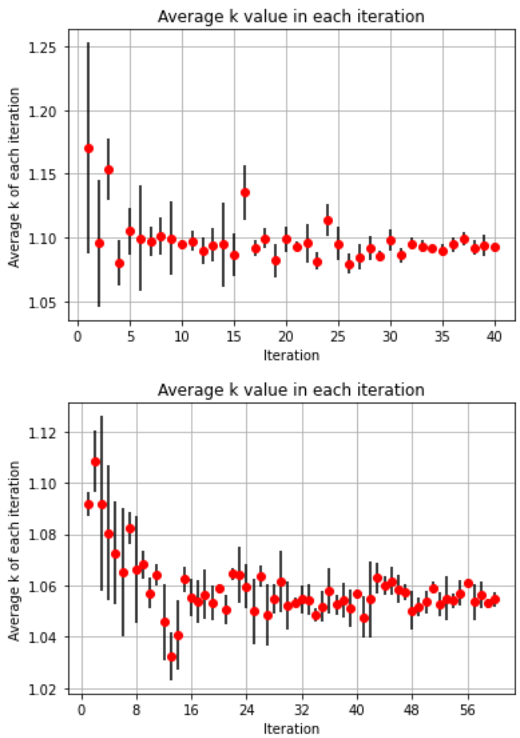

FIG. 7. The figures display the mean k-factor for each iteration for three independent trials along with uncertainties for moderator to fuel ratio of 1:1 (where 0.4:0.6 for Uranium-235 to Uranium-238). The top figure and bottom figures were carried using neutron batch size of 100 and 200 respectively.

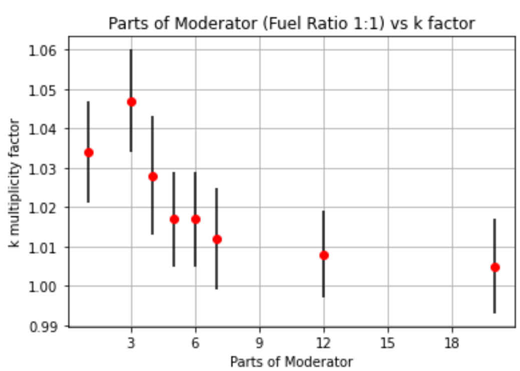

FIG. 8. The figure displays the moderator (to one fuel) parts against k factor. Data extracted from the table 2 and neglected all fuel ratios that were not 1 to 1. The figure shows a clear asymptote towards $k \approx 1$.

such as ^{87}Br which have a half life of around 56s and produces a beta minus decay for which 2% of decays account for the production of ^{86}Kr + n. Since the algorithm only considers the reactor to be prompt critical, there is a high risk of exponential rise in the number of neutrons. These delayed neutrons generally play role in reactor kinetics and maintaining a stable multiplicity factor, regulating the neutron production via the mean delay time.

Its also important to consider reactor poisoning. Reactor poisoning is due to the fragments of fission, such as xenon, with a high neutron-capture cross section. These fragments would absorb the neutrons and would cause the k multiplicity factor to decrease. This additional feature could be added to the simulation to get a more accurate result.

It should be noted that, when only considering the 1:1 fuel ratio, the k factor approaches 1 less rapidly than the increase in moderator to fuel ratio. The investigation shows that the enrichment of Uranium fuel may be the dominant factor driving the k-multiplicity factor. For example in the case of moderator to fuel ratio being 1:1 and the ratio U-238 to U-235 changing from 1:1 to 2:3 the k-factor changes by 5.8%. The convergence of the Monte Carlo algorithm for the k-factor reveals to be highly sensitive the neutron batch size chosen for the simulation. Looking at Figure 7, the 100 neutron batch appears to output a faster rate of convergence in terms of fewer neutron histories, but the mean k-factor is slightly overestimated (3.6% difference) compared to the 200 neutron batch. Using a larger neutron batch size seems to be more precise in estimating the k-factor, since by the law of large numbers the sample-averages of the k-factor converge in probability but at the expense of additional computational cost.

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