1 Abstract

Understanding the interaction of neutrons at different energies with different materials is essential while modelling nuclear reactors. The study of these characteristics is called *Neutronics*. While the primary reaction is happening in the core of the nuclear reactor, a reactor would always have components made of *non-fissionable* matter which govern crucial processes. These include something as simple as a *neutron-flux moderator*, such as Carbon-12 and H_2O or more advanced processes such as *neutron-poisoning* through Xenon-58. At a given time, there would be several thousands of these neutrons firing off at different places inside the reactor. Moreover, these interactions might be drastically different for neutrons at different energies. Statistical Mechanics provides with the tools necessary to study these processes in greater detail.

However, as it would turn out later, the equations governing *neutron-transport phenomena* turn out to be an hefty challenge to solve even for modern computers. Hence, we look at a fascinating yet unorthodox way of 'solving' this problem, that is the *Monte-Carlo Simulation*. In this project, we go over the theory of neutron-transport phenomena, the challenges associated with solving it and an introduction to Monte-Carlo simulations and its algorithm for this specific case.

2 Physical Background

Nuclear Fission reactors are based on self-sustaining chain reactions in which an actinide isotope (typically Uranium-235) splits into unstable mass-fragments and neutrons. The path a neutron would take inside the reactor can be easily approximated to being random. This is because apart from the channel through which neutrons enter the core, the structure of the fuel would alter moment-to-moment. In general, a neutron can have the following interactions with matter:

- Elastic Scattering
- Inelastic Scattering
- Capture
- Resonance
- Aborption/Fission

Out of all these, non-radiative matter does not undergo fission, hence we also term it *non-fissionable matter*. Resonance conditions are beyond the scope of this project as it's addition to the simulation is non-trivial. However, it should be noted that resonance is a characteristic of high energy (several MeVs) neutrons. Hence, we resort to leaving out the pertinent energy spectrum entirely. This leaves us with the first three entries in our list. We define something called a *Cross-Section*, which we will use define the probabilities of our interactions.

2.1 Scattering

The process in which neutrons undergo collisions with the surrounding matter (Neutron-Neutron interactions are highly *improbable*. Until and unless one is concerned with *Neutron Stars* we can ignore it) and change direction and/or energy. Since neutrons do not posses charge, they can penetrate the electron cloud easily and interact directly with the nucleus. Scattering is well-modeled as a classical collision problem. Figure 1 diagrammatically shows the process. As mentioned in [1], the only time neutron will undergo elastic scattering if the scattering angle $\theta = 0°$ in centre of mass frame. Depending on the mass of the nucleus, we can also retrieve a lower bound to the final energy a neutron would have after being scattered by it.

$$\frac{E'}{E} = \frac{A^2 + 1 + 2Acos\theta}{(A+1)^2} \tag{1}$$

where E' is the energy of the particle after collision and E is the energy of the particle before collision. θ, as mentioned before, is the impact parameter in centre of mass frame.

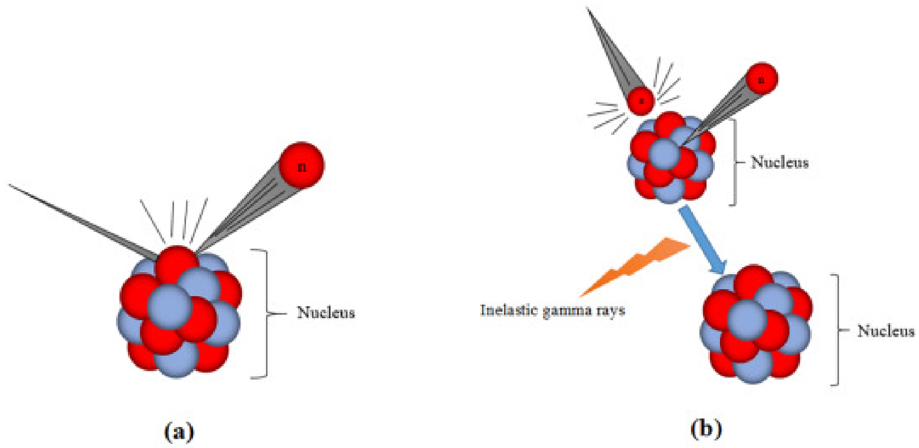

Figure 1: Elastic and Inelastic Scattering between nucleus and neutron.

2.2 Capture

In literature, the words capture and absorption are used as synonyms. However, there is a clear distinction between the two. As mentioned, capture has no classical analog and is purely quantum mechanical. The exact mechanism of absorption is not important for this paper, but typically, these are the reactions of (n, γ) type. Consider the following reaction, for instance,

$$U^{238} + n \rightarrow U^{*239} \rightarrow U^{239} + \gamma \tag{2}$$

As mentioned in [2], several other kinds of reactions also exist, which are beyond this project's scope.

3 Monte-Carlo Method to approximate neutron transport

It turns out that accounting for all the five processes (mentioned in 2) inside a reactor, the *Boltzmann Transport equation* is computationally taxing. Hence, we turn to the Monte-Carlo approach to solve the problem. The task is simple, *execute a random walk of neutrons in 3 dimensions.* This is done by keeping the system's constraints in mind: the neutron-matter interaction. Different atoms interact differently with neutrons, taking the form of *probabilities*, more specifically *cross-sections.* Each interaction has an associated cross-section for an element, which we can use in applying Monte Carlo. We analyze n times, where n is a considerable number. This allows us to approximate the energy distribution of the neutrons well enough.

3.1 Algorithmic details

The code depends on the user-given parameters for the calculation. This includes *Initial energy, mass of scatterer, number of neutrons, and associated cross-sections.* While the former two can be chosen as per the user's wish, one might refer to a chart for the cross-sections. As figure 2 suggests, the cross-sections vary with the initial energy of the neutrons. Hence care must be taken while taking inputs.
The code executes a *loop* for each neutron until it is absorbed and notes down the absorption point and the energy it had before being absorbed. The code uses the following PDFs (probability distributions) for the random walk:

- In the radial direction $= \dfrac{log(a)}{\sigma_{\text{t}}}$, where a is a randomly generated number and σ_{t} is the *total cross-section.*[1] Uniform item distribution in the angular components is noted in [1] and [2].

[1] $\dfrac{1}{\sigma}$= Mean Free Path

		Thermal neutron			Fast neutron		
		Scattering	Capture	Fission	Scattering	Capture	Fission
Moderator	H-1	20	0.2	-	4	0.00004	-
	H-2	4	0.0003	-	3	0.000007	-
	C-12	5	0.002	-	2	0.00001	-
Structural materials, others	Zr-90	5	0.006	-	5	0.006	-
	Fe-56	10	2	-	20	0.003	-
	Cr-52	3	0.5	-	3	0.002	-
	Ni-58	20	3	-	3	0.008	-
	O-16	4	0.0001	-	3	0.00000003	-
Absorber	B-10	2	200	-	2	0.4	-
	Cd-113	100	30	-	4	0.05	-
	Xe-135	400	2,000,000	-	5	0.0008	-
	In-115	2	100	-	4	0.02	-
Fuel	U-235	10	99	583	4	0.09	1
	U-238	9	2	0.00002	5	0.07	0.3
	Pu-239	8	269	748	5	0.05	2

Figure 2: Chart containing different cross-sections for materials used in nuclear reactors.

Now we convert the above quantities to Cartesian and randomly and uniformly distribute the energy between the initial and the limit given by 1. We also need to scale the absorption cross-section according to the new energies. As noted in [1], the ratio of the capture cross-section follows the following relation:

$$\frac{\sigma_{\mathrm{a}}{}^{,}}{\sigma_{\mathrm{a}}} = \sqrt{\frac{E}{E^{,}}} \tag{3}$$

where the primed quantities are the new cross-section and energy.
Also, note that,

$$Probability(Absorption) = \frac{\sigma_{\mathrm{a}}}{\sigma_{\mathrm{t}}} \tag{4}$$

which is quantified using random chance. The algorithm does this for the neutron number provided by the user, and collects and plots the data. The following sections contain the analysis of a few well-known materials whose roles in the nuclear reactor are documented.

3.2 Carbon-12

Carbon-12 is a well-known *neutron-flux moderator*. That means it is excellent at slowing down/halting neutrons at all ranges of energies. This is essential for maintaining delicate control over the fission reaction. C-12 also has a unique property where the neutrons don't scatter far away before stopping, making it viable for us to use relatively thin pieces in the *control-rods*. Figure 3 and 4 have the data analysis from our code. The following study uses $E = 10^6 MeV$.

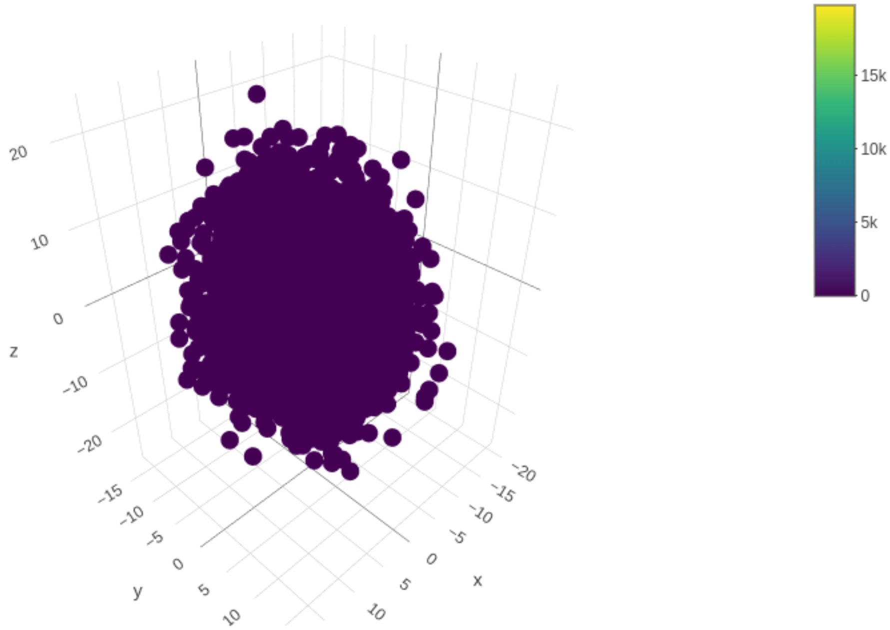

Figure 3: 3D scatter plot representing the final locations of neutrons before being absorbed. The color indicates the energy it had before absorption, as indicated by the gradient on the right.

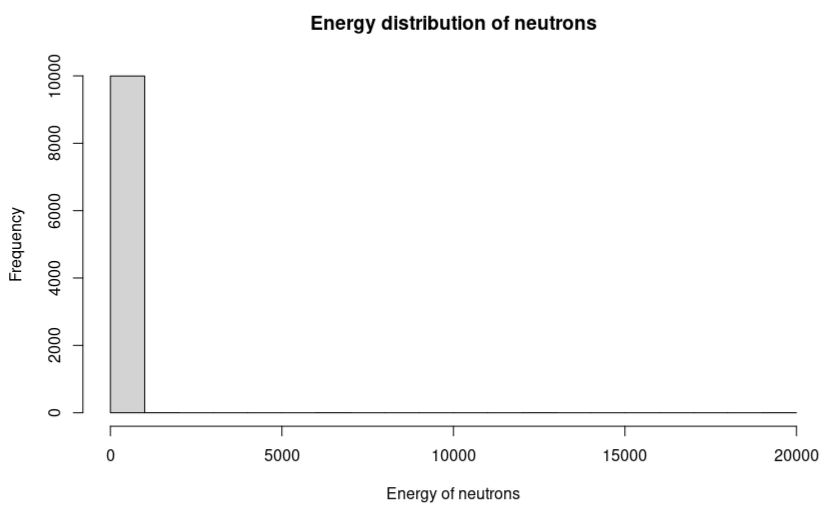

Figure 4: Energy distribution of neutrons in C-12. As expected almost all neutrons now have zero energy.

3.3 Xenon- 135

It is a well know *neutron-poison*. It can be thought of as complete opposite of a moderator. Production of Xenon-135 inside the core of the reactor is extremely dangerous. It was one of the key reasons behind the disaster in *Chernobyl*. Figure 5 and 6 depict the analysis for the target.

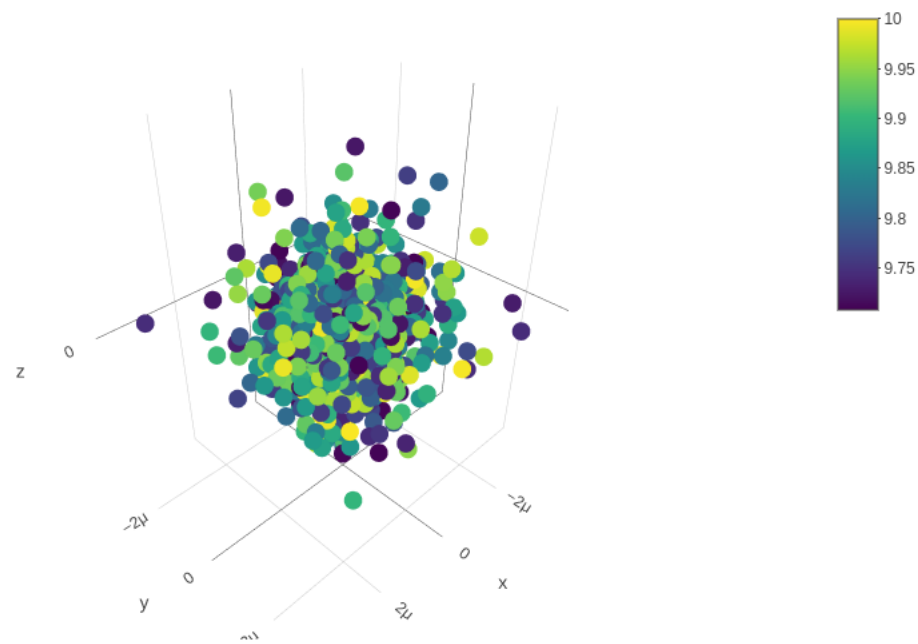

Figure 5: 3D scatter plot representing the final locations of neutrons before being absorbed. The color indicates the energy it had before absorption, as indicated by the gradient on right.

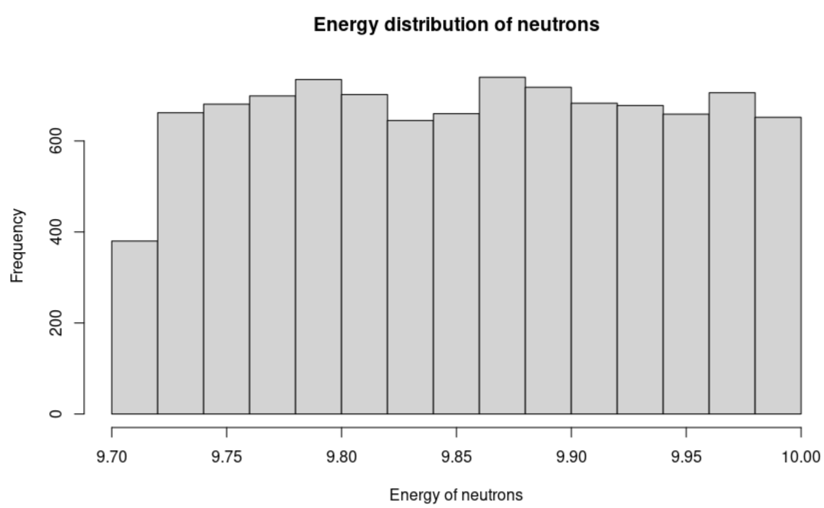

Figure 6: Energy distribution of neutrons in Xe-135. As expected high energy neutrons scatter to undesired locations, which may have devastating consequences.

4 Conclusion

We investigated the neutron-transport phenomenon and how matter interacts within the harsh environment of a nuclear reactor. We used a rather easy and yet effective technique which is used often to approximate complicated things, all it requires is random data and constraints. We verified our code named "Serpent.R" by using elements which have well-documented effects towards neutrons. The reader may wish to the same analysis for whatever elements they like.

5 Acknowledgments

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References

[1] Kenneth S. Krane. *Introductory Nuclear Physics.* Wiley India Pvt. Ltd., 2014.

[2] Jaakko Leppänen. "Development of a New Monte Carlo Reactor Physics Code". In: (2007).