MATH6103 - PROJECT

Monte-Carlo Methods in Neutron Transport Codes

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1 INTRODUCTION

On July 16, 1945, the scientists working at Los Alamos on the Manhatten Project bore witness to the culmination of years of research and innovation – the successful execution of the Trinity test. The discovery that bombarding a nucleus with neutrons could result in an atom being split into smaller atoms, and in the process release a substantial amount of energy, was a significant moment in the history of mankind. The subsequent realisation that such a process could result in a “knock-on” effect, triggering more atoms to be split, releasing even more energy, was the next significant moment. These simple ideas have themselves provided us with so much death, destruction and fear, while simultaneously giving us power and crucial research insights that in the sweet irony that only life can provide, also help save lives, in fields such as medical imaging. One of the many research areas that was borne from the Manhatten Project was neutron transport codes (due to their direct relation to the mechanism by which a fission reaction occurs), and the associated Monte Carlo methods used to numerically solve it.

1.1 PROJECT GOALS

This project is about creating a toy box through which to demonstrate the physics the scientists at Los Alamos sought to exploit in their development of the first atomic bomb. Though we should note that, while a nuclear detonation device is the original inspiration for the work they did (and thus this project), the utility of the work is not limited to just that. Through simple tweaking of the code one could use it as a diffusion simulation, for example, to see how neutrons disperse through a water medium. But we digress.

In this project we will implement a particle simulation for neutrons in a constrained medium, and track the behaviour of this population as they interact with their surroundings. As we will discuss, neutrons are what drive fission reactions in fissile materials - so it stands to reason that to have more neutrons would be to have more chance of having a fission reaction occur, and thus more chance of a, to be scientific, “large boom”. However, merely having neutrons present is not sufficient for ensuring that a sustained fission reaction occurs - after all, neutrons are always ’present’ around us, and yet Uranium doesn’t seem to spontaneously combust in nature (or so the German’s would have us believe). So the question becomes: what do we need to do to ensure that it does?

In the spirit of keeping with the Los Alamos designs, we will assume a perfectly spherical geometry for our medium. To simplify our work, we will also assume our “bomb” is entirely composed of a single isotope mass of particles, which we will take to either be Uranium-235 or Plutonium-239 (for their fissile nature, which is to say, their willingness to undergo a fission reaction under certain conditions, which we will discuss). For our neutrons, we will assume that our population of particles are travelling with the same energy, and that they are not travelling so fast as to require relativistic adjustments (though this actually plays into our favour due to quantum effects which affect the fissile efficacy of materials when bombarded with neutrons travelling at such high speeds). All these assumptions we for now state without explanation, though will describe later in this report.

The results we seek are to see that, adjusted for computational limitations, there is a density (unique to each isotope) which acts as a boundary separating whether a fission reaction will be sustained or not. We will compare our results to expected trends, and discuss what our simulations suggest for the materials.

1.2 Source Code

The code for this project is open sourced on GitHub, along with the source code for this report, and relevant papers / resources. The reader may choose to correlate the findings in this project with the source code for a more in-depth understanding of the simulation. See [6] for a link to the source. The code for the particle simulation on its own is in "src/ParticleSimulation.jl", and the code for running an experiment where multiple simulations are run is in "src/ParticleSimulationComparisons.jl".

2 BACKGROUND

2.1 WHAT IS THE PURPOSE OF NEUTRON TRANSPORT CODES?

As we alluded to in the introduction, neutrons play a crucial role in engineering problems relating to nuclear energy production and control. Neutrons are the driving force in fission reactions (technical justification for which will be covered in the theory section), and so it is important to understand the dynamics of a population of neutrons within a fissile material. This is where neutron transport comes into play. Neutron transport studies concern the behaviour of neutrons within some medium, highlighting the number of neutrons present, their movement, and their interaction with the medium.

This knowledge isn't solely limited to nuclear fission however, nor is it constrained to weapons development. We'll highlight a couple particularly interesting (and relevant) applications for neutron transport codes, though should emphasise that this list is by no means exhaustive.

Nuclear Weapons

As highlighted in the introduction, the development of nuclear weapons during World War Two was a significant motivating factor for early study of neutron behaviour, and their relation to nuclear chain reactions [8]. It was only as a result of development at Los Alamos that neutron codes came into the forefront of academia, and their application is seen directly. The most obvious use case for neutron transport codes in nuclear weapons development (and what we seek to observe in this project) is using them to determine the conditions required for a chain reaction to be super-critical - that is, for the reaction to be self-sustaining in a way that grows to consume all available fissile material, otherwise known as an explosion.

Nuclear Fission Reactors

The natural lead on question from "can we exploit the energy released in a fission reaction to build a bomb", is "can we exploit the energy released in a fission reaction to power our homes"? A bit more wholesome a question, the answer as we know is of course yes. Neutron transport codes (and more generally readiation transport codes, which are just more abstract particle transport codes) are used in a similar manner to how they are in nuclear weapons development, though with a different aim. Whereas for nuclear weapons we want to see our chain reaction reach super-critical state, we do not want this for our reactors - it would be counterproductive to spend much time building a reactor, only for it to suddenly not exist. Thus we use transport codes here to determine what conditions are required to keep chained fission reactions at a controllable level (i.e., sub-critical), while still being able to harness energy from it.

Radiation Shielding

Being inherently a particle simulation that considers radioactive materials and their interactions with their environment, neutron transport codes see a direct application in providing consult on how best to design reactors to safeguard us from its effects as well. For example, one can show that water is an excellent radiation protection mechanism by running a simulation which describes a region of water surrounding a fissile material that interacts with a population of neutrons. You can measure the (simulated) radiation levels outside the water region. This kind of simulation is more commonly known as a neutron diffusion, and is a simplificatoin of neutron transport.

Particle Accelerator Design

Particle accelerators have been using transport codes to simulate the dynamics of interactions between nuclei and sub-atomic particles [1].

Fusion Reactor Design

Radiation transport codes are used to determine radiation amounts, and general particle interactions, inside a fusion reactor [9]. These help inform design decisions, and provide a way to test components of a reactor without the expensive and time consuming process of constructing one (see for evidence, ITER).

2.2 What work has been done in the field?

Since the 1940s, neutron transport codes have seen wide reaching applications, as we've highlighted above. However this came about only after years of intensive research in both physics and mathematics, and has itself been the generator of new concepts in both fields. Here we'll provide a briefly highlight the outcomes of neutron transport research in the past, and in the modern day.

Historical Work

We have already covered much of the historical work done and what led to interest being developed in neutron transport codes, and so will not repeat ourselves here. However, we will make note on one other core idea which emerged from the nuclear weapons development at Los Alamos shortly after World War Two, which is the work done by John von Neumann and Stanislaw Ulam in developing Monte Carlo methods. In fact, the work they did was directly borne from a wish to study neutron chain reactions. The term “Monte Carlo Method” can be used to describe a broad class of solutions to problems, but in large they all share the characteristic that they depend on some stochastic process for their simulation. In the theory section we will cover specifically what a Monte Carlo Method means to us, and how we will use them, but for now we will just note their significance. The discovery of Monte Carlo methods came at a time where computers were beginning to become both more powerful and available, which helped propell them to academic stardom, as they became the subject of intense research. Since then, much work has been done on developing lead on processes and applying them to various fields, where today the study of Monte Carlo methods can be considered its own sub-field of statistics, with its own class of problems and applications – and only a memory of its beginnings as a tool for nuclear weapons development [3].

Modern Work

More modern research largely concerns numerical methods for computing properties around neutron transport for increasingly complex geometries and chemical compositions – essentially a problem of quantity and efficiency. Somewhat understandably however, much of the work done in this field is either classified or commercial in confidence, which is to say source code for industry standard simulations is next to impossible to find, and even getting access to software for running your own simulations requires permission from the owners and a large sum of money. Nevertheless, one such well respected code is the “Monte Carlo N-Particle Transport Code” (MCNP). It is capable of very general simulations, and is used in simulations for nuclear reactors, among other things. Perhaps expectedly, it is developed by Los Alamos

[5].

Where in this project we simplify our problem considerably to be for a uniform neutron energy, spherical geometry, discretised time neutron particle simulation that is capable of handling only a few thousand particles, the MCMP code is much more robust. It is able to handle neutrons that have a specifies energy distribution, can run the simulation for a prescribed geometry (i.e., is not confined to that of a sphere), and can handle many orders larger than a few thousand neutrons. Additionally, it provides a wealth of diagnostics information and features for simulating scenarios. For example, it is able to handle the existence of neutron shields – something we propose as an extension to this project in our conclusions. It is also malleable enough to not just be useful for neutron particle simulations, but can also handle electron transport as well. To refrain from fawning over a piece of technology further, it is a highly capable industry standard code for neutron transport, and this project we have completed here could itself be viewed as a toy version of MCNP.

3 Theory

3.1 Assumptions

We will somewhat unconventionally begin by stating what our assumptions are in our model, as we will use this to guide the theory that we develop by making specific reference to them. We will assume:

- All neutrons have the same kinetic energy
- Our medium will be a single isotope solid that is isotropic in density. This material will be either Uranium-235 or Plutonium-239
- Our medium's geometry will be perfectly spherical
- All neutrons after moving will have an event occur, which will be either an elastic collision, a capture collision, or a fission reaction. Notably, we are ignoring the case of in-elastic collisions
- We only consider $(n,2n)$ fission reactions
- There is a single point neutron source at the centre of the sphere which only emits neutrons at the start of the simulation

What each of these means we will touch on as we come across them, though for now take them for granted. After introducing the theory for them, we will discuss the implications of making these assumptions.

3.2 Nuclear Fission

While nuclear fission can occur without the aid of neutron bombardment (via a process known as "spontaneous fission"), here we will concern ourselves exclusively with the case of a fissile material being subject to a population of energetic neutrons.

3.2.1 Fission Process

When an energised neutron collides with a fissile material such as Uranium-235 or Plutonium-239,

$$n + {}^{235}U \rightarrow {}^{236}U^* \rightarrow {}^{134}Xe + {}^{100}Sr + 2n$$
$$n + {}^{239}Pu \rightarrow {}^{240}Pu^* \rightarrow {}^{134}Xe + {}^{103}Zr + 3n$$

The neutron is initially absorbed by the Uranium / Plutonium nucleus, however, both of these elements become unstable with the extra mass. One of the potential outcomes of this instability is that the atom splits into two, and in the process of doing so, extra neutrons are emitted at high energy. Alongside this a large quantity of energy is released, which is what is harnessed in nuclear reactors (and provides that explosive power in a bomb).

Criticality
Criticality with respect to nuclear fission reactions describes whether or not a system is self-sustaining in its reaction. There are a couple of associated terms:
Super-critical: This is the state of a self-sustaining fission reaction which continues to grow in strength
Sub-critical: This is a fission reaction which has failed to reach a state of being self-sustaining, and will eventually (if unaided) fizzle out Often when dealing with nuclear transport codes, one wishes to answer the question of whether a system will be super- or sub-critical. This is, in large, the question we also seek to answer for some given initial conditions.

3.2.2 Neutron Transport

We will build up the neutron transport code, describe its components, and then relate them to our project. We will largely follow the derivation given in [2]. Where we come across a part of the derivation that relates to an assumption we make in our model, we will have an aside *in italics* to emphasise the discrepancies between the standard neutron transport model and ours.

At the heart of neutron transport is a wish to describe how neutrons are distributed in some system. Let $N(\vec{r},t)$ describe the density of neutrons in some medium, where $\vec{r} \in \mathbb{R}^3$ describes a position and $t \in \mathbb{R}$ a time. If we let $\vec{v}$ describe neutron velocity,

To identify the particle density $N(\vec{r},t)$, we need to take into account the particle velocities, $\vec{v}$, in the medium we're considering. We can describe the distribution of particles by the density function $n(\vec{r},\vec{v},t)$. The particle density can then be described

$$N(\vec{r},t) = \int n(\vec{r},\vec{v},t)\mathrm{d}^3 v$$

Normally we don't talk about particle velocities when dealing on atomic scales - instead we talk about orientation, and energy. If we let $\vec{\Omega} = \vec{v}/\|\vec{v}\|$ be the unit vector which describes direction, then we can use the familiar $E = \frac{1}{2}mv^2$ to determine the particle's energy. Note then that the quantity

$$n(\vec{r},E,\vec{\Omega},t)\mathrm{d}^3\vec{r}\mathrm{d}E\mathrm{d}\vec{\Omega}$$

describes the number of particles in the volume $\mathrm{d}^3\vec{r}$ around the position $\vec{r}$ that have energy E within $\mathrm{d}E$, moving in direction $\vec{\Omega}$ within a direction change of $\mathrm{d}\vec{\Omega}$. Note that we can describe the small differentials above in spherical coordinates, as we can reason that

$$\begin{aligned}
\mathrm{d}\vec{\Omega} &= \sin\theta\mathrm{d}\theta\mathrm{d}\varphi \\
\mathrm{d}^3\vec{v} &= v^2\mathrm{d}v\sin\theta\mathrm{d}\theta\mathrm{d}\varphi \\
\mathrm{d}E &= mv\mathrm{d}v
\end{aligned}$$

If we take the energy version of our density function and make substitutions for above, we then get the relation

$$n(\vec{r},E,\vec{\Omega},t) = \frac{v}{m}n(\vec{r},\vec{v},t)$$

This relation will come in handy in a minute. *Note here that this is a function of energy and angle. Recall from our model's assumptions that we specified our neutrons will be monoenergetic, and that we have an isotropic source. Thus, here, our value for E won't be a variable, and similarly our direction vector will be distributed in an expected manner.*

Stepping aside, we'll consider what can affect the number of neutrons we have in our medium. The most obvious one is that there is some source of neutrons - we'll call this rate $q(\vec{r}, \vec{v}, t)$ (*Recall we said we're assuming a single source of neutrons, which scatters isotropically, and only emits at the start of the simulation.*). Next, we know our neutrons can collide with the fissile material with some probability - we've already considered the possibility of fission reactions occurring, which is an example of the outcome of such a collision. This will require some expanding on, so for now we can just call this term $\left(\frac{\partial n}{\partial t}\right)_{\text{coll}}$. Then we know that neutron change can be described:

$$\frac{\mathrm{d}n(\vec{r}, \vec{v}, t)}{\mathrm{d}t} = \left(\frac{\partial n}{\partial t}\right)_{\text{coll}} + q(\vec{r}, \vec{v}, t)$$

where

$$\begin{aligned}\frac{\mathrm{d}n}{\mathrm{d}t} &= \frac{\partial n}{\partial t} + \frac{\partial \vec{r}}{\partial t}\frac{\partial n}{\partial \vec{r}} + \frac{\partial \vec{v}}{\partial t}\frac{\partial n}{\partial \vec{v}} \\ &= \frac{\partial n}{\partial t} + \vec{v}\nabla n + \frac{\vec{F}}{m}\frac{\partial n}{\partial \vec{v}}\end{aligned}$$

and in the last line there we've used the familiar $F = ma = m\frac{\partial \vec{v}}{\partial t}$. Thus, our neutron transport equation in its current state is:

$$\frac{\partial n}{\partial t} + \vec{v}\nabla n + \frac{\vec{F}}{m}\frac{\partial n}{\partial \vec{v}} = \left(\frac{\partial n}{\partial t}\right)_{\text{coll}} + q(\vec{r}, \vec{v}, t)$$

Note that the term $\frac{\vec{F}}{m}\frac{\partial n}{\partial \vec{v}}$ is most often ignored when it comes to neutron transport as its effects are negligible. So that slight simplification gives us:

$$\frac{\partial n}{\partial t} + \vec{v}\nabla n = \left(\frac{\partial n}{\partial t}\right)_{\text{coll}} + q(\vec{r}, \vec{v}, t)$$

Where equality is taken in the physicist's sense. The next obvious step is to try and explain how collisions affect the neutron change. To do this, we need to talk about nuclear cross sections and collision kernels.

Cross Sections

When we talk about nuclear cross sections, we are talking about the number of interactions that occur for a particle in a given "area". Think you are driving a car through the streets of your home town. At any given point in time as you travel, there are any number of events happening around you - maybe a pedestrian is crossing the road, or a bird flies past, or maybe you hit another car while looking for things to notice. In some parts of town, say in the main street, it is more likely there will be things going on than if you were on the outskirts of town. Or maybe there is an event on in one area that makes it harder to focus on driving. A crude analogy, but in heart is comparable to what a cross section represents. The cross section,

$\Sigma(\vec{r}, \vec{v})$, describes the average number of "interactions" that will occur for a particle if it is at position $\vec{r}$ (the location in town) travelling at speed $\vec{v}$ (however fast your are hooning).

The dual to talking about a cross section is to talk about a particles "mean free path" instead. This is more intuitive, and effectively describes the average distance a particle would expect to travel before it has an "event" occur with another particle (i.e., a collision takes place).

Note that one of our assumptions was that, when we come to do our simulation, all neutrons will have an event occur after moving. This is somewhat a lie as an assumption, and somewhat not. In reality we will effectively be drawing a randomly sampled distance travelled (that is informed by the material's nuclear cross section describing mean-free path), and assuming that a neutron has a collision after that distance. Our assumption would more accurately be represented as some form of time independence - whereby in a single pass of our simulation we may process a series of collisions simultaneously, though we would not necessarily expect these to actually occur simultaneously in a real life reaction, because of these varied distances travelled (among other reasons)

Scattering Probability

Next, when an event does occur, i.e. a neutron collides with another particle, we need to describe how the two particles react to this. This is done using a "scattering probability function", which is an energy distribution function for the particle that is subject to the collision from the neutron. Let, then, $f(\vec{r}, \vec{v'} \rightarrow \vec{v})$ describe the probability that the secondary particle will be emitted with velocity $\vec{v}$, after the atom is struck by a neutron with velocity $\vec{v'}$ at position $\vec{r}$.

In the neutron code, this distributino will be different for elastic and in-elastic scattering, and is, of course, a distribution. In our model however, we 1. are not considering in-elastic scattering, but 2. are also assuming a simple uniform distribution, as is used in [4]

Secondary Particle Count

This one is easy to explain - when a collision event occurs (e.g. a fission reaction), what is the average number of secondary particles emitted by the collision event? Let $c(\vec{r}, \vec{v})$ describe such an average for a causal neutron of velocity $\vec{v}$, where the collision occurs at $\vec{r}$. This would describe, for example, the number of neutrons which come out of a fission reaction, and is what ties the speed of a colliding neutron with the energy going into the reaction. Intuitively we might expect an atom to react to a collision a bit differently if it a neutron is smashed into it as opposed to receiving a small bump (where "small" and "smashed into" are taken to be their more scientific, scale-appropriate counterpart adjectives).

By convention we set this to 1 for collisions which do not generate any secondary particles, such as absorption.

We stated in our assumptions that we would only consider $(n, 2n)$ *fission reactions for simplicity. Thus, this is actually just a piecewise function for us, there it is* 2 *if we have a fission reaction, and otherwise is* 1.

Collision Kernel

The collision kernel is what ties all the above together. It describes the average number of secondary particles of velocity $\vec{v}$ that are produced for every unit of distance travelled by a neutron with velocity $\vec{v'}$, at position $\vec{r}$. Then, combining what we've just reasoned about above, the collision kernel is given:

$$\Sigma(\vec{r}, \vec{v}' \to \vec{v}) = \Sigma(\vec{r}, \vec{v}')c(\vec{r}, \vec{v}')f(\vec{r}, \vec{v}' \to \vec{v})$$

Perhaps we can use a boxer as an analogy. Imagine you are standing in a boxing ring, but you have many opponents. Let this be a nightmare, and lets say you can't fight back against any punches you receive. How many punches might you expect to receive, as a function of where you are in the ring, and how fast will the teeth fly out of your mouth based on those punches? We might expect that if there are more opponents in the ring with you that you will lose more teeth (i.e., the number of secondary neutrons increases). Similarly, if some of these boxers are good at their job, then maybe the punches they throw will have a lot of energy. One might not wish to be hit by a punch with more energy, but perhaps in the process of contemplating whether it is something you enjoy or not you would notice that your teeth fly out of your mouth faster when you receive harder punches (i.e., neutrons which collide with an atom at higher speed will result in secondary neutrons being ejected at higher speeds). The information the collision kernel captures is analogous to the number of teeth that fly from your mouth given a hard hitting punch from one of these ferocious foes, based on where you're standing in the ring. Though one does wonder if it is easier just to read the equation...

When we come to our simulation we will essentially skip this as a necessity, and instead emulate the collisions themselves by random choices (the Monte Carlo method creeping in), and can handwave a lot of the complexity that a collision kernel seeks to represent away due to our assumptions of isotropic scattering and monoenergetic neutrons

Now that we can describe the behaviour of our particles when a collision occurs, we can describe the collision term. For a neutron with velocity $\vec{v}$, its collision frequency can be described by $\|\vec{v}\|\Sigma(\vec{r}, \vec{v})$. Thus, for a population of neutrons with velocity $\vec{v}$ in a unit volume, the rate at which reactions occur is given by

$$\|\vec{v}\|\Sigma(\vec{r}, \vec{v})n(\vec{r}, \vec{v}, t)$$

We are assuming that the particle that collides with the atom is "lost" (in reality it isn't lost, but is ejected again for example in the case of a fission reaction), and so for every collision with a particle v the systme will lose $v\Sigma(\vec{r}, \vec{v})n(\vec{r}\vec{v}, t)$ particles, but the system will gain however many particles come out of the collision event. Thus, the collision term can be summarised:

$$\left(\frac{\partial n}{\partial t}\right)_{\text{coll}} = \overbrace{\int v'\Sigma(\vec{r}, \vec{v}' \to \vec{v})n(\vec{r}, \vec{v}', t)\mathrm{d}^3 v'}^{\text{Neutrons gained from all possible collision events}} - \overbrace{v\Sigma(\vec{r}, \vec{v})n(\vec{r}, \vec{v}, t)}^{\text{Neutrons which participate in a collision}}$$

Substituting this back into our transport equation:

$$\frac{\partial n}{\partial t} + \vec{v}\nabla n = \left(\frac{\partial n}{\partial t}\right)_{\text{coll}} + q(\vec{r}, \vec{v}, t)$$

$$\frac{\partial n}{\partial t} + \vec{v}\nabla n + v\Sigma(\vec{r}, \vec{v})n(\vec{r}, \vec{v}, t) = \int v'\Sigma(\vec{r}, \vec{v}' \to \vec{v})n(\vec{r}, \vec{v}', t)\mathrm{d}^3 v' + q(\vec{r}, \vec{v}, t)$$

And were done! This is (a) general neutron transport equation. In deriving this we've highlighted a few key points, as in our simulations, we don't actually seek to implement this equation directly. Instead, we implement components that were used to build the equation up. Next we'll discuss what we will simulate, and how our assumptions tie into modifications to the above.

Energy Representations

Notably, in the above derivation, we've kept everything in terms of velocity. However, as we noted at the start of the derivation, it is possible to instead express those same quantities in terms of a direction vector $\vec{\Omega}$, and particle energy, E. In that spirit, we can express our functions in terms of these similarly:

$$\Sigma(\vec{r}, \vec{v}' \to \vec{v}) \iff \Sigma(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega})$$
$$f(\vec{r}, \vec{v}' \to \vec{v}) \iff f(\vec{r}, E' \to E, \vec{\Omega}' \to \vec{\Omega})$$

3.3 Methodology

In our experiment, we don't wish to directly solve the neutron transport code we've just derived. Instead, we seek to model components of it, and run a Monte Carlo style simulation of it. We are implementing a particle simulation, and so will start by defining the properties of our system. We will have a sphere of varying radius, though will be approximately on the order of 10^{-10}cm. The reason for this is explained in the limitations section.

Our simulation process is described below. For every simulation cycle:

1. For every neutron present in the simulation:
   a) If this neutron is outside the medium, or it has been absorbed, skip processing it
   b) Randomly sample this neutron's next travel direction and distance
   c) Determine its new (x, y, z) position
   d) Check if the neutron has moved to be outside the medium. If it has, mark it as having escaped and return to (1)
   e) Randomly choose an event to occur, with weight to optinos given by nuclear cross section data:
      - Elastic scattering collision. Then continue (neutron will be "scatterred" at start of next simulation cycle).
      - Capture collision. Mark the neutron as absorbed, and continue.
      - Fission collision. Generate a new neutron at this position, and continue.
2. Collect data about neutrons present, generated, escaped, and captured

The reason this can be referred to as a "Monte Carlo Method" is seen when we consider the stochastic behaviour that we introduce into the system. When we decide a neutron's next direction to move in, we randomly sample its direction and distance (with experimental data to inform this sampling). Similarly, using data, we determine

Let (L, θ, ϕ) describe a neutron's next direction to move and the length of that movement, and let ξ denote a uniformly sampled random variable. In our assumptions, we stated that we are assuming isotropic scattering - thus, $\phi = 2\pi\xi$ (this being the off axis scattering angle). For the scattering angle in the plane of collision, however, we cannot simply assume a uniform distribution. Often we take a distribution such that $\mu = \sin\theta = -1+2\xi$ [2]. Thus, to determine θ, we have $\theta = \text{asin}(-1+2\xi)$. Normally this angle would affect the energy loss, however because we are assuming that all our neutrons have the same energy (and no in-elastic collisions occur), this energy calculation is something we ignore (this is what we refer to when we say we're breaking the laws of thermodynamics in our limitations section). We then know which direction our scattered neutron will travel - next we need to know how far it will move.

As was described in the previous section, the nuclear cross section describes, roughly, how often we would expect a specific collision event to occur. Its dual statement is concerns "mean-free paths", as we have also described. In our simulation, we can randomly sample this mean-free path value to determine how far our neutron may travel. We will justify the relation we get, however, and draw this conclusion from [4]. First, let $P(L)$ describe the probability that a particle will move L units of distance without making a collision. Then

$$P(L) = \frac{\text{number of particles that move to depth of L}}{\text{number of trials}} = e^{-\Sigma_t(E)L}$$

where $\Sigma_t(E)$ describes the total nuclear cross section (the sum of individual cross sections) for a particle of energy E. Recall again that this is a constant for us, as we assume monoenergetic neutrons. This is a fairly standard probability distribution function, and so then we can describe the probability of a neutron travelling some path up to L long as the CDF of this:

$$F(L) = 1 - P(L) = 1 - N_0 e^{-\Sigma_t(E)L}$$

where N_0 is the number of trials. If we wish to sample the length L to first collision (as we do in our simulation, note), then letting this be ξ again, we have $F(L) = \xi$, and so:

$$\begin{aligned}
\xi = F(L) &= 1 - e^{-\Sigma_t(D)L} \\
1 - \xi &= e^{-\Sigma_t(E)L} \\
\iff L &= -\frac{1}{\Sigma_t(E)} \ln(1-\xi)
\end{aligned}$$

But noting that ξ is uniformly distributed, $1-\xi$ is equivalent to ξ, so we can just write

$$L = -\frac{1}{\Sigma_t(E)} \ln(\xi)$$

Then we only hvae to reason about this strange $-\frac{1}{\Sigma_t(E)}$ term we have. We have a relation between mean-free path and collision kernels, hwich states that

$$\lambda = (n\sigma)^{-1}$$

where λ is an expected path distance for a specific cross section property, and σ describes that cross section (these are referred to as micro cross-sections, and relate directly to their macroscopic counterparts). Here, n is the number of neutrons in the volume being considered (which in our case, is a sphere, so $v = \frac{4}{3}\pi r^3$, and N is the number of neutrons present in our simulation). If we let σ_{sc}, σ_{cp} and σ_f describe the cross sections for our elastic scattering collisions, capture collisions, and fission collisions respectively, then we can describe the total cross section as $\Sigma_t = \sigma_{sc} + \sigma_{cp} + \sigma_f$. Then we can determine $\lambda_t = (n \cdot \Sigma_t)^{-1}$. Putting all this together, we can determine the length of the path our neutron will travel to be:

$$L = -\lambda_t \ln(\xi)$$

So to summarise, our randomly sampled (Monte Carlo method!) next (unit vector) direction and distance is given by:

$$\begin{aligned}
L &= -\lambda_t \ln(\xi_1) \\
\theta &= \operatorname{asin}(-1 + 2 \cdot \xi_2) \\
\phi &= 2\pi\xi_3
\end{aligned}$$

where ξ_1, ξ_2, ξ_3 are all uniformly distributed random variables on $[0, 1]$. The last thing to do is to determine the actual differential for our neutron. This is a straightforward 3D vector calculation, and is given:

$$\begin{aligned}
\mathrm{d}x &= L \cdot \cos(\theta) \cdot \cos\left(\phi\right) \\
\mathrm{d}y &= L \cdot \cos(\theta) \cdot \sin\left(\phi\right) \\
\mathrm{d}z &= L \cdot \sin(\theta)
\end{aligned}$$

Our decision process for which collision event occurs is relatively simple. We distribute probabilities of each event occurring according to the proportion of the total cross section they represent, and use a random variable ξ to decide which one occurs.

When we talk about these corss section values, we use Barns units. $1\text{barn} = 10^{-24}\text{cm}^2$. The relevant cross sections for Uranium-235 and Plutonium-239 are given in table 3.1. The important values for us are that of the thermal neutrons (as we are assuming monenergetic neutrons with energy at that level). To highlight the effect that the energy of a neutron has on its ability to engage in a fission reaction however, we include the same values for neutrons travelling at considerably faster (relativistic) energies for contrast. A quick observation would note that fission reactions are generally, maybe unintuitively, less likely to occur when the bombarding neutrons are too fast – though the physical explanation for this delves into quantum theory, and is out of scope for this project.

	Thermal (Barns)		
Material	Scatter	Capture	Fission
Uranium-235	10	99	583
Plutonium-239	8	269	748
	Fast (Barns)		
Uranium-235	5	0.07	0.3
Plutonium-239	5	0.05	2

Table 3.1: Averaged cross section data for Uranium-235 and Plutonium-239. Here, a "thermal" neutron is taken to be travelling at 2200m/s, and the values provides are in Barns (10^{-24}cm^2). This data retrieved from the JEFF nuclear data repository [7].

3.3.1 Alternative Approaches

Fluid Dynamics
There are simplified models, such as the one described in [8], which are more akin to a fluid dynamics approach. In a fluid dynamics approach, instead of tracking the behaviour of individual particles, you model the population of neutrons as a fluid which moves about within the medium. The behaviour of the neutrons can then be described by balance equations which act as flow in and out of the system. This method has the benefit of being considerably more computationally feasible than a particle simulation, but sacrifices accuracy in its representation of a system – particularly given the nature of a chain reaction somewhat necessitating the tracking of individual particles due to it being dependent on energy of individual particles and their orientation.

Monte Carlo Integration
Another method which is keeping in the spirit of working with Monte Carlo related methods, would be to evaluate the given integral directly. Doing so would require functions which approximate the required behaviours for a given material (for example, $f(\vec{r}, \vec{v}' \to \vec{v})$), though these approximations are likely not impossible given the abundance of experimental data available (one could also simply use data as a sort of reference table instead of having an analytic function to represent it). If you have a way to functionally describe all components of the equation, then to save ones sanity, instead of attempting to find an antiderivative for that function you could use Monte Carlo integration to evaluate it. Given the inherent dimensionality of the problem and the potential for sensitivity to parameters, it is possible this approach will be quite computationally expensive however, and so perhaps should be done with aid of hardware that surpasses the ability of a ThinkPad T440p.

3.3.2 Limitations of our Model

We might note that, in building our model, we've made a great deal many assumptions about the properties of our system. This would be an astute observation, and in fact we should make no claim to precision in our model whatsoever. Instead of determining a precise value for critical density, or reliably measuring properties surrounding the situations we've constructed, we instead set the goal of merely observing the trends we would expect to find in such a system.

What we have is not so much a spherical cow model of a bomb, as it is a cow-shaped model of a bomb.

Why do we place such a restriction on ourselves? This is because the assumptions we make limit our model considerably. For example, our assumption that all neutrons in the medium have the same kinetic energy takes away from the accuracy of our model, in that the system breaks the laws of thermodynamics – our collisions result in no energy lost (in way of a neutron being slowed), but themselves create energy (a new neutron with the same energy can be produced).

Similarly our assumption that there is not an external source of neutrons could be considered an inaccuracy. It is possible to construct your aparatus so as to limit the presence of external neutrons past what we inject into our experiment, however it is foolish to assume one could entirely rid a system of external influence – this is especially significant for our simulation when you consider the scale we've limited ourselves to (a note on which is below).

We would be remiss to not note the computational restriction we face as well. Assume that we could rid ourselves of the above assumptions and have a perfectly physical model of the physics of our system. Then even then, we could not trust our results, as to do so would require the simulation of a number of neutrons on order far greater than what my laptop is capable of handling – at the point you wish to run a simulation like that, you should be asking for super computer time. As such, we have a significantly reduced quantity of neutrons present in our system. We somewhat account for this by scaling our system to accommodate for this, in that instead of dealing with a bomb at a regular diameter such as the 17.32cm radius Los Alamos Trinity test, we reduce the scale of our system to be physically infeasible itself as well.

In short, our model should be considered extremely unphysical, and is more of an academic interest than an actual experiment we would seek results from. Nonetheless, it is fun to see a miniature nuclear reaction!

4 Results

It is difficult to compare our results directly to literature, due to hardware limitations resulting in a maximum number of simulated neutrons that is far below what would be required for more natural geometries. Instead, we can make observations about the behaviour of the simulation output, and comment on whether it is aligned with what we would expect to occur.

4.1 U-235 Simulations

4.1.1 Density Variation

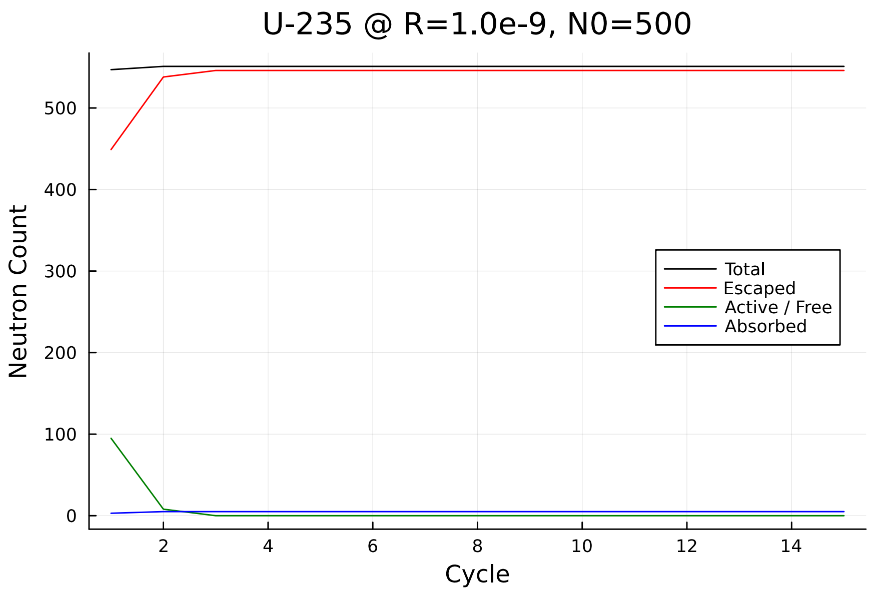

Figure 4.1: A "large" sphere with radius 10^{-9}cm, and a starting population of 500 neutrons, run for 15 simulation cycles.

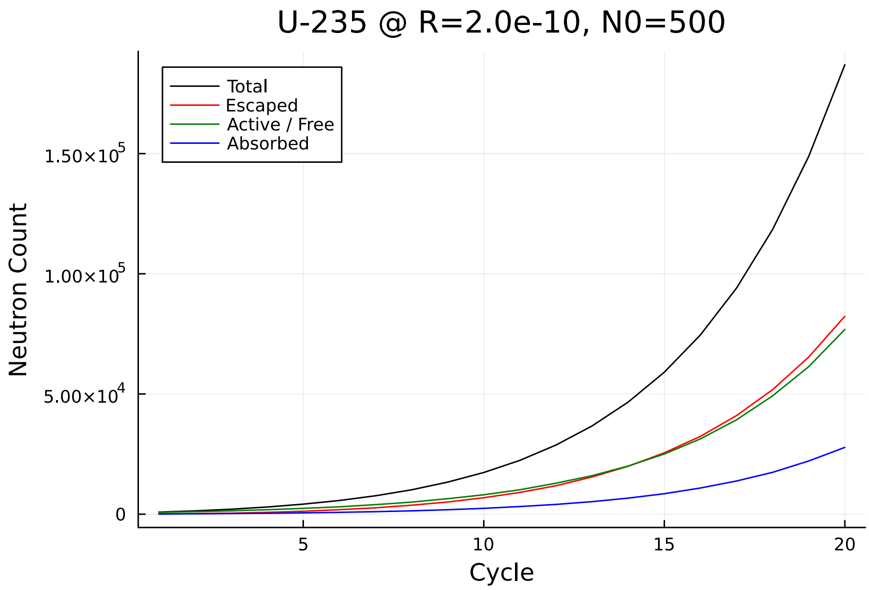

Figure 4.2: A "medium" sphere with radius $2 \cdot 10^{-10}$cm, and a starting population of 500 neutrons, run for 20 simulation cycles.

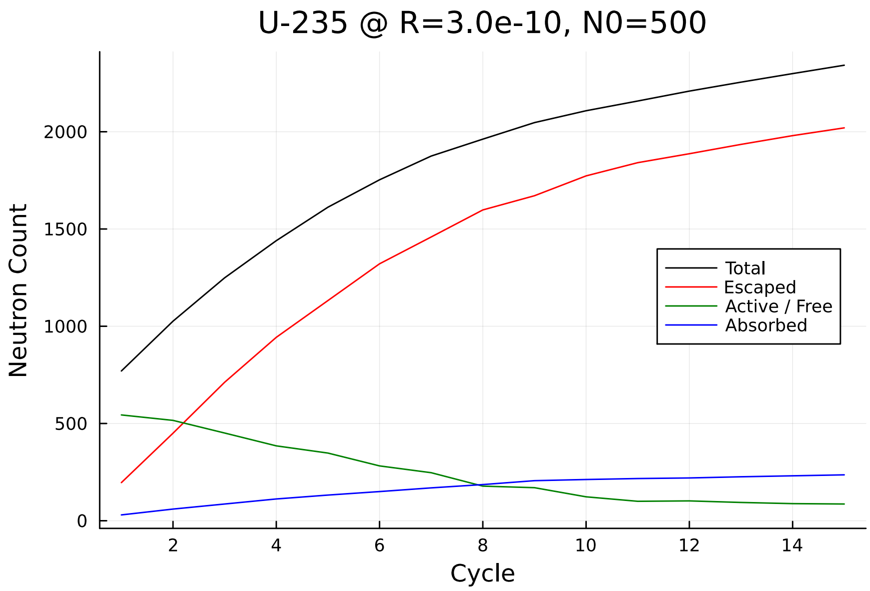

Figure 4.3: Another "medium" sphere with radius $3 \cdot 10^{-10}$cm, and a starting population of 500 neutrons, run for 15 simulation cycles.

4.1.2 Critical Density Analysis

Figures 4.1 - 4.3 show how different populations of neutrons in the medium grow under the dynamics of the system they're in. The only property that varies between these graphs is the radius of the sphere of Uranium in which the 500 neutrons interact. Figure 4.1 shows that almost all our neutrons escape almost immediately, while some are absorbed. No sustained fission reaction occurs in this case - we might posit that the sphere is too large (and thus the neutrons too sparse in our Uranium mass) to interact to a degree which encourages the production of other neutrons. This would be supported by the fact that the total population of neutrons remains largely unchanged from the initial count of 500.

This is in stark contrast to what we observe in, say, figure 4.2. Here we see sphere of smaller radius (increasing density), and observe that our neutron population grows in what appears to be an exonential manner. Here, we are observing a self-sustaining fission reaction which has become super-critical. While some neutrons are still escaping, we see that the number of active neutrons is still growing exponentially, and so the reaction will self sustain.

Figure 3.3 shows a more middle ground between the two. Theoretically it is possible to have a fission reaction system which is self sustaining, without being super-critical or sub-critical. In practice, however, this is impossible as it requires a perfect balance of conditions which is not feasible in the real world. This figure depicts behaviour approaching that boundary, where the population of neutrons eventually decays to a sub-critical state, however does so at a slower rate than figure 4.1 which had a sphere of larger radius and so reached that state of non-reaction much faster.

We can see the relationship between radius of the sphere and the neutron population growth rate more clearly in figure 4.4.

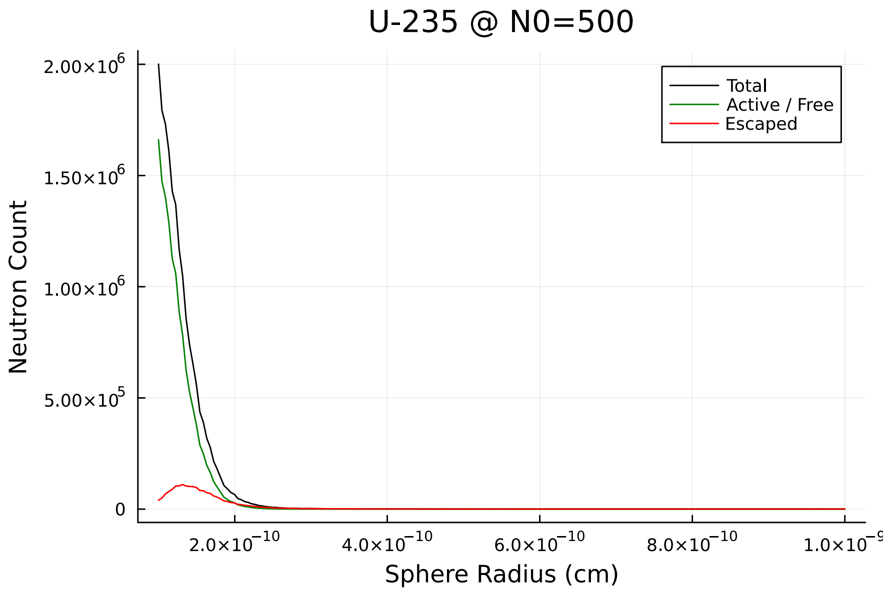

Figure 4.4: Neutrons present in a mass of Uranium condensed into sphere of given radius (i.e. density is leftwards increasing in the graph).

There is a point (around $3 \cdot 10^{-10}$cm) for which a sphere of greater radius will not result in a burn up situation - i.e., the number of neutrons either remains the same or decreases such that the reaction fizzles out. For spheres with a radius smaller than this, however, we see an exponential rise in the amount of neutrons as radius decreases. This is consistent with behaviour expected from super-critical systems, that is to say, it identifies the critical density for Uranium (when there are that many neutrons present). As we stated in our limitations, the number of neutrons present is incredibly unrealistic, and so we are unable to determine from this what the actual critical density of Uranium might be, unfortunately. However we are still able to identify behaviour, as the system scales nonetheless.

Note that there seems to be a dip in escaped neutrons as the sphere continues to decrease in radius. This is a misnomer, and is actually due to floating point errors - this comes about in the calculation of the euclidean distance of a neutron from the origin, and as distances decrease in size these values become smaller, until the code can no longer support their precision.

4.2 Pu-239 Simulations

4.2.1 Density Variation

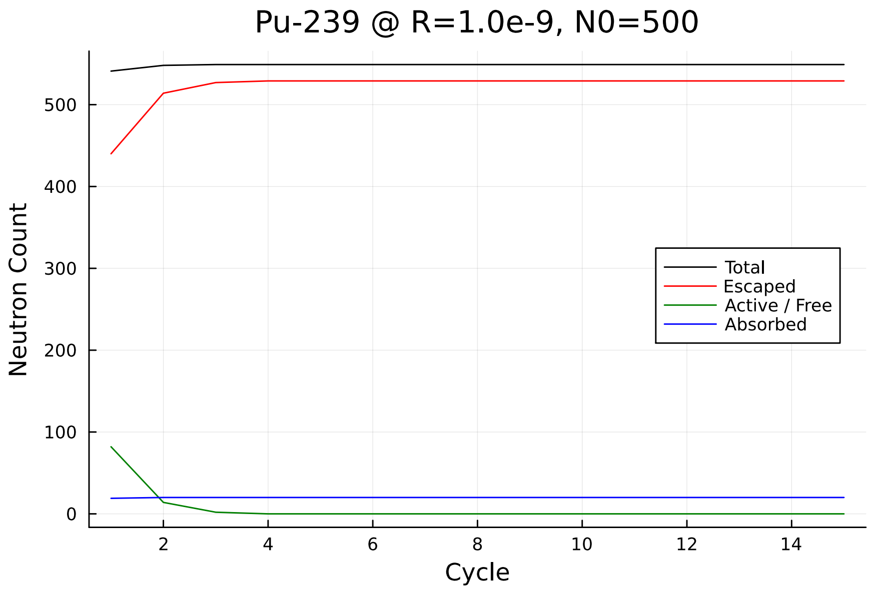

Figure 4.5: A “large” sphere with radius 10^{-9}cm, and a starting population of 500 neutrons, run for 15 simulation cycles.

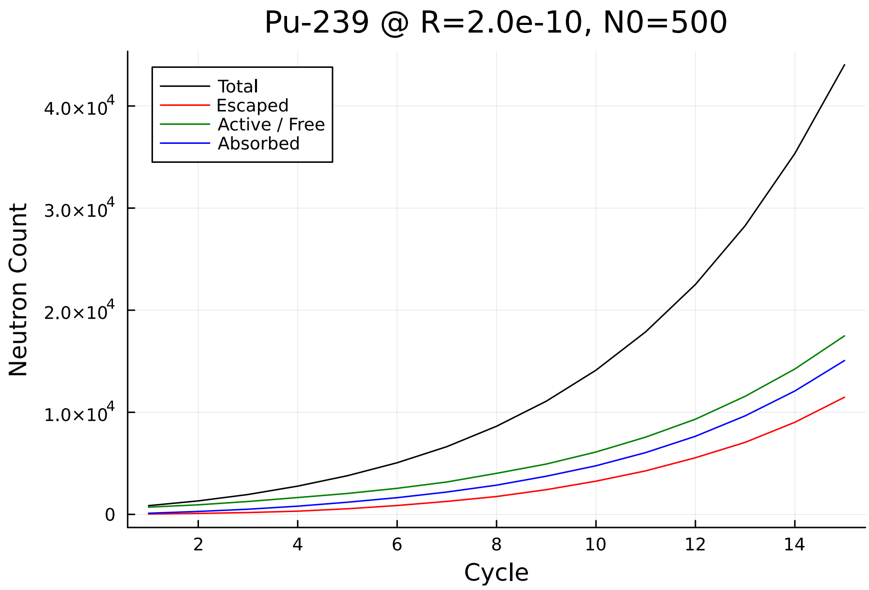

Figure 4.6: A "medium" sphere with radius $2 \cdot 10^{-10}$cm, and a starting population of 500 neutrons, run for 20 simulation cycles.

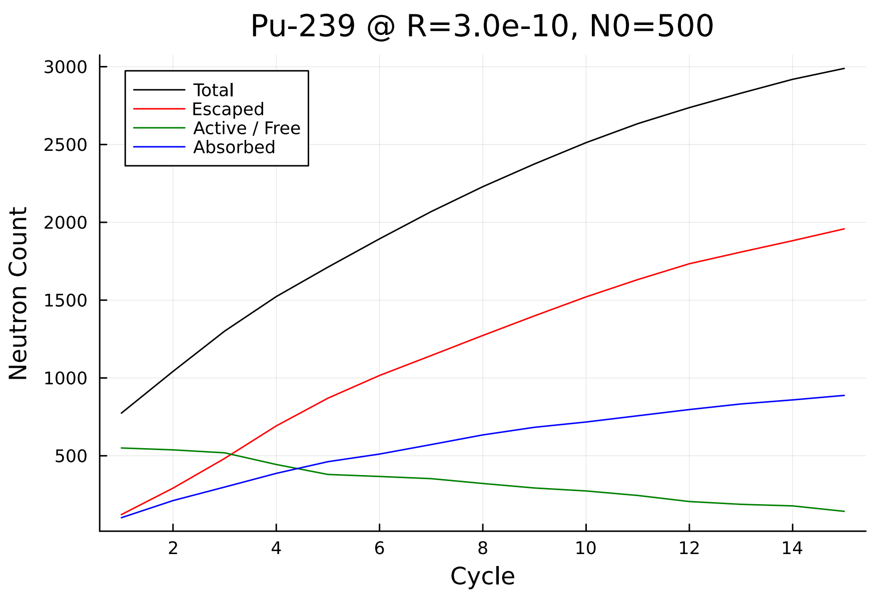

Figure 4.7: Another "medium" sphere with radius $3 \cdot 10^{-10}$cm, and a starting population of 500 neutrons, run for 15 simulation cycles.

4.2.2 Critical Density Analysis

We largely include Plutonium in our simulations for two reasons: 1. because the bomb developed at Los Alamos had a Plutonium core, and it seemed only fitting to include a Plutonium simulation given the origins of the work in this; and 2. so we have something to compare the Uranium simulations to.

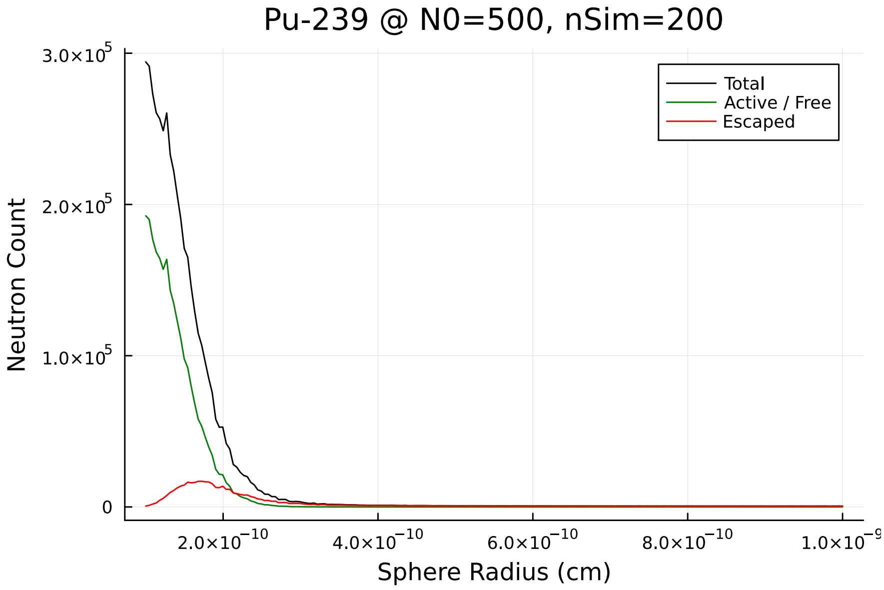

Figure 4.8: Neutrons present in a mass of Uranium condensed into sphere of given radius (i.e. density is leftwards increasing in the graph).

When it comes to the Plutonium results, we see much the same behaviour as we did for Uranium, and for the same reasons. We only have to note that the orders to which the neutrons grow is somewhat greater for Uranium than for Plutonium. For example, for a sphere of radius $2 \cdot 10^{-10}$cm Plutonium grew to a population of approximately 40000 neutrons, whereas Uranium sat comfortably at approximately 200000. If we recall back to our table which described the average cross section data for Uranium and Plutonium, we note that the average cross section values for capture and fission events are both greater for Plutonium than for Uranium. That is to say, a thermal neutron, on average, will have to travel farther through a Plutonium medium in order to experience a fission event, than it would if it were in a Uranium medium. Additionally, from these values, the probability of a fission reaction occurring sits at approximately 78% for Plutonium, whereas it sits at approximately 85% for Uranium. Thus, we would expect there to be more fission reactions for a Uranium medium, and thus more opportunity for neutron development. The trend therefore is similarly consistent for comparisons between materials.

5 Conclusions

5.1 What did we achieve?

In this project we sought to simulate a nuclear fission chain reaction, for an albeit contrived example, but academically interesting one nonetheless. We first built the theory surrounding nuclear fission and neutron transport codes, with notes on the historical significance of their development, and then constructed an experiment around that that was achievable given the limitations in time and available hardware. From this we were able to identify trends in our results that are consistent with physically observed behaviour – essentially we simulated a nuclear bomb going off, but if that bomb was about a picometer in radius!

5.2 Future work?

Neutron Reflector
When it comes to nuclear reactors, one goal of your system is to keep the neutron count in equilibrium so as to ensure a sustained reaction that doesn't grow too quickly and lead to super-critical conditions (i.e., an explosion). However, there is a case where you would want this rapid growth in reactions - in the case that you want an explosion! Whereas nuclear reactors have devices designed to regulate neutron energy and count, a nuclear bomb has the opposite goal. However, one of the larger causes for loss of neutrons is that they simply leave the medium you are trying to contain them within. As such, one method often used (which was invented at Los Alomos for the Trinity test) is to have a "neutron reflector". This is an outer casing around your bomb which biases the reflection angle when it comes to elastic scattering collision events for neutrons operating within the bounds of the bomb medium. This decreases the loss of neutrons to the environment, and thus maintains density of neutrons for longer, making it easier for a sustained and super-critical fission reaction to develop. One such extension could be then to include support for such a structure into the simulation, and to observe how it affects the critical density of both isotopes.

Other Fission Reactions
Currently in the simulation, if a neutron's collision is deemed to produce a fission event, we only support the case that one neutron is ejected from the atom our neutron has collided with. This is referred to as an (n,2n) reaction. However, it is possible for more outputs – an (n,3n) reaction is possible for example, where two excess neutrons are ejected from the target atom. This would increase the number of neutrons present in the medium, and is more physically accurate.

More Precise Scattering Variants
Currently only in-elastic scattering is supported, however this is insufficient for a particle simulation that wishes to be more accurate. When a neutron collides with an atom, it should be affected by the momentum of that atom, instead of randomly picking a direction to head in next. Similarly, for cases of fission events, the resulting neutron should be affected by the direction the colliding neutron approached. These will affect where subsequent fission reactions occur in the mass

Neutron Energy Distributions

In simplifying our model to assume a uniform, averaged neutron energy, we ignore many effects. For example, there is a significant difference between mean free-paths for thermal and fast neutrons, and each have their own purpose. For example, in a nuclear reactor you wish to have more thermal neutrons as they caise fission reactions over longer time scales, whereas fast neutrons will result in more fission events in shorter periods. Some analytic approximations to energy distributions for neutrons within medium are available, and these could be incorporated into our model to more accurately represent the behaviour of neutrons. This would well be accompanied by a more precise implementation of scattering methods as described above, as they are also somewhat dependent on energies of participating neutrons.

Reaction Medium Geometries

We could also support different geometries. Currently we assume a sphere, which is quite simplistic. Some more academic structures such as a cube would not be difficult to implement and provide some interesting analytics, however some other geometries such as a cylinder could be useful for simulations on reactor cores for example.

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