MATH6103 - PROJECT

# Monte-Carlo Methods in Neutron Transport Codes

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# 1 INTRODUCTION

On July 16, 1945, the scientists working at Los Alomos on the Manhatten Project bared 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 two smaller atoms, and in the process release a relatively large 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 helps save lives, in fields such as medical imaging.

## 1.1 PROJECT GOALS

This project is about creating a toy box through which to demonstrate the physics the scientists at Los Alomons 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 Alomos 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.

# 2 Background

## 2.1 How did nuclear fission research start?

First time atom was split
Los Alomos
John von Neumann and Monte-Carlo method. Difficult integrals. Stochastic simulations.

## 2.2 Where is neutron transport used in modern life?

**Nuclear Weapons**
**Nuclear Fission Reactors**

## 2.3 Existing Work

Oppenheimer / Los Alomos - nuclear fission tests - critical density
Von Neumann - monte carlo methods - stochastic simulations
MCMP - closed source - commercial

# 3 Theory

## 3.1 Nuclear Fission

### 3.1.1 Fission Process

How does nuclear fission work. What is required, what is output.

Factors that affect the reaction

### 3.1.2 Neutron Transport

Transport equation

### 3.1.3 Collision Kernels

Neutron cross section

Scattering collision

- In-elastic (changes direction and speed. Assume this doesn't happen for simplicity) - Elastic (changes direction but not speed)

Capture collision

Fission collision

## 3.2 Transport Simulation

### 3.2.1 Algorithm for simulating

## 3.3 Alternative Approaches

Talk about fluid dynamics approaches

Monte-Carlo integration of integral

## 3.4 Assumptions and Limitations

Isotropic point source at the centre of the bomb that emits monoenergetic neutrons, with the bomb being a single isotope material with no imperfections. Not so much a spherical cow model as it is a spherical bomb model.

Instead, we make a couple concessions. As it isn't so much the volume of the medium that affects the criticality of our system, but the density of neutrons within that medium, we can hope to approximate the behaviour for regular systems by scaling down our medium to a point of similar density.

Low neutron count

# 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 Neutron Species Counts

### 4.1.2 Varying Density

### 4.1.3 Critical Density Analysis

## 4.2 Pu-239 Simulations

### 4.2.1 Neutron Species Counts

### 4.2.2 Varying Density

### 4.2.3 Critical Density Analysis

# 5 Conclusions

## 5.1 What did we achieve?

## 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 in real kinetic dynamics, this is infeasible. When a neutron collides with an atom, it should be affected by the momentum of the 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
**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.

# References