Dylan J. Frank
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Introduction

The United States has refrained from nuclear weapon detonations for over 30 years, in accordance with the Comprehensive Nuclear-Test-Ban Treaty of 1996. Given recent geopolitical developments, it is crucial to maintain and verify an effective stockpile. However, due to significant costs and constraints imposed by treaties on scientific experiments, laboratories heavily rely on computational physics codes. codes deal with the physics and mathematics governing how radiation interacts with matter, known as radiation transport. They come in both stochastic and deterministic forms, each specialized based on computational and statistical requirements. For instance, evaluating the effects of weapons on large urban areas for either emergency response or defense strategy may necessitate a rapidly efficient deterministic code that utilizes numerical methods to solve complex equations. On the other hand, more complex tasks, such as designing a radiotherapy plan for cancer patients, demand highly detailed geometric and nuclear data. These can only be accurately obtained through stochastic methods like Monte Carlo sampling [1].

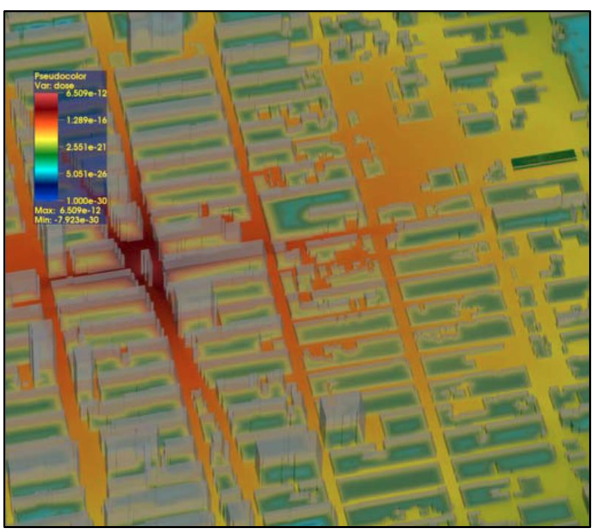

Figure 1: Deterministic Simulation of Nuclear Detonation over Manhattan.

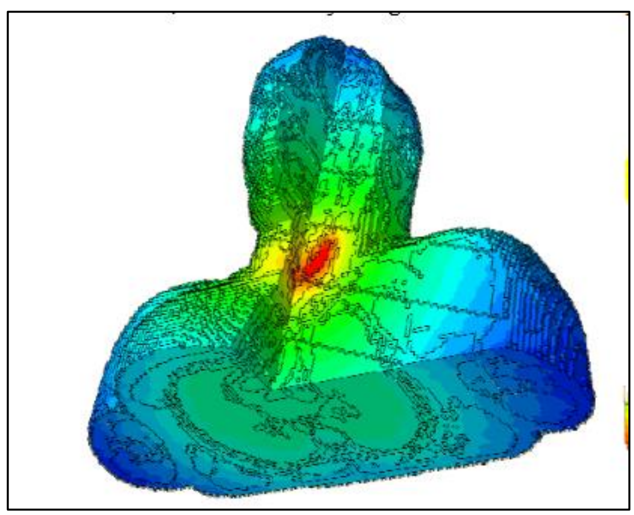

Figure 2: Monte Carlo simulation of Radioiodine Treatment for Thyroid Cancer. [2]

Primer to Nuclear Physics

Before diving into the equations and computation relevant to radiation transport, we must be familiar with some basic concepts in nuclear physics. [3]

Neutrons

Neutrons are fundamental particles nestled within the nucleus of an atom. Unlike protons, which bear a positive electric charge, neutrons are electrically neutral, rendering them impervious to electromagnetic forces. In terms of mass, they closely resemble protons. While protons play a pivotal role in determining an atom's chemical properties, the concentration of neutrons exerts a strong influence on nuclear stability and behavior, a topic we'll delve into in the following sections.

Radiative Capture

When a neutron collides with a nucleus, there is a possibility that the nucleus will absorb the neutron, this is sometimes referred to as *parasite absorption*. The nucleus returns from an excited state to a ground state by emitting gamma rays. This process can be represented in conventional notation as:

$$ {}^{\mathrm{A}}_{\mathrm{Z}}\mathrm{X} + {}^{1}_{0}n \rightarrow {}^{\mathrm{A+1}}_{\mathrm{Z}}\mathrm{X} + \gamma \qquad (1) $$

Here, A represents the sum of protons and neutrons (n), Z is the number of protons, and X serves as a placeholder for the chemical symbol, determined by Z.

Fission

Nuclear fission is initiated by the absorption of a neutron, leading to increased nuclear instability. This prompts the overcoming of nuclear binding forces by repulsive forces between protons, resulting in the fragmentation of the nucleus. The energy released, described by $E=mc^2$, is substantial due to the disparity in mass between the fragments and the original nucleus. In engineering terms, the emission of high-energy prompt neutrons is crucial. These neutrons play a pivotal role in sustaining a chain reaction of fission, a fundamental mechanism for both nuclear power plants and weapons.

In terms of applications, nuclear fission serves as the primary energy source for commercial nuclear power plants and plays a significant role in the energy released during a nuclear explosion. For instance, consider the induced fission reaction of Uranium-235, which releases 200 MeV of energy. This capacity to harness and control nuclear fission is what makes it feasible to generate electricity on a large scale and develop powerful weaponry.

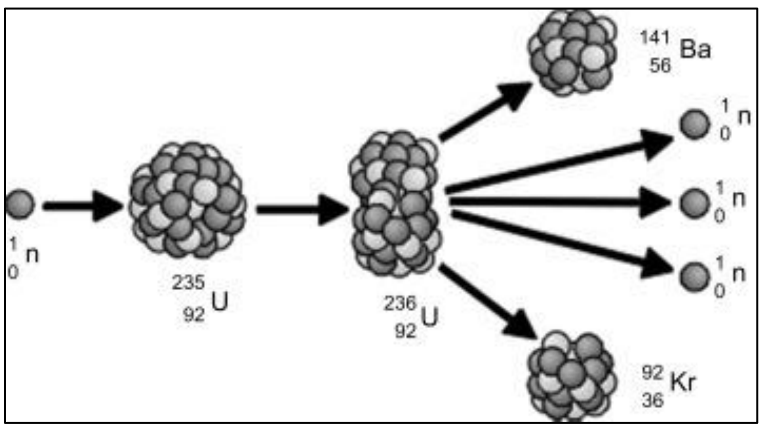

Figure 3: Diagram of the Fission of Uranium-235 [4]

Scattering

Scattering simply describes the collision between a neutron and an atomic nucleus. A collision can be elastic, where 100% of the neutron's kinetic energy is retained, or partially inelastic, where some of the neutron's kinetic energy is transferred to the target nucleus. If the probability of scattering in any particular direction is the same in all directions, the scattering is said to be *isotropic*, otherwise it is considered to be *anisotropic*. Elastic scattering is more favorable for interactions with heavy-nuclei like uranium, while inelastic scattering is more profound with light target nuclei such as hydrogen.

Cross Section

Microscopic cross sections, represented by the Greek letter σ , quantify the effective target area of a nucleus and are measured in units of barns (where 1 barn equals 10^{-24} square centimeters). The microscopic cross section is contingent on the energy of the incident neutron. In general, the cross section is inversely proportional to energy, meaning that fast energy neutrons are less likely to interact with matter. There exists extensive libraries such as ENDF/B (American), JENDL (Japanese), and KEDAK (German), that host experimentally-measured cross sections data for nearly all nuclide and at a myriad of energies. Take for example the fission cross section of Plutonium-239 [5]:

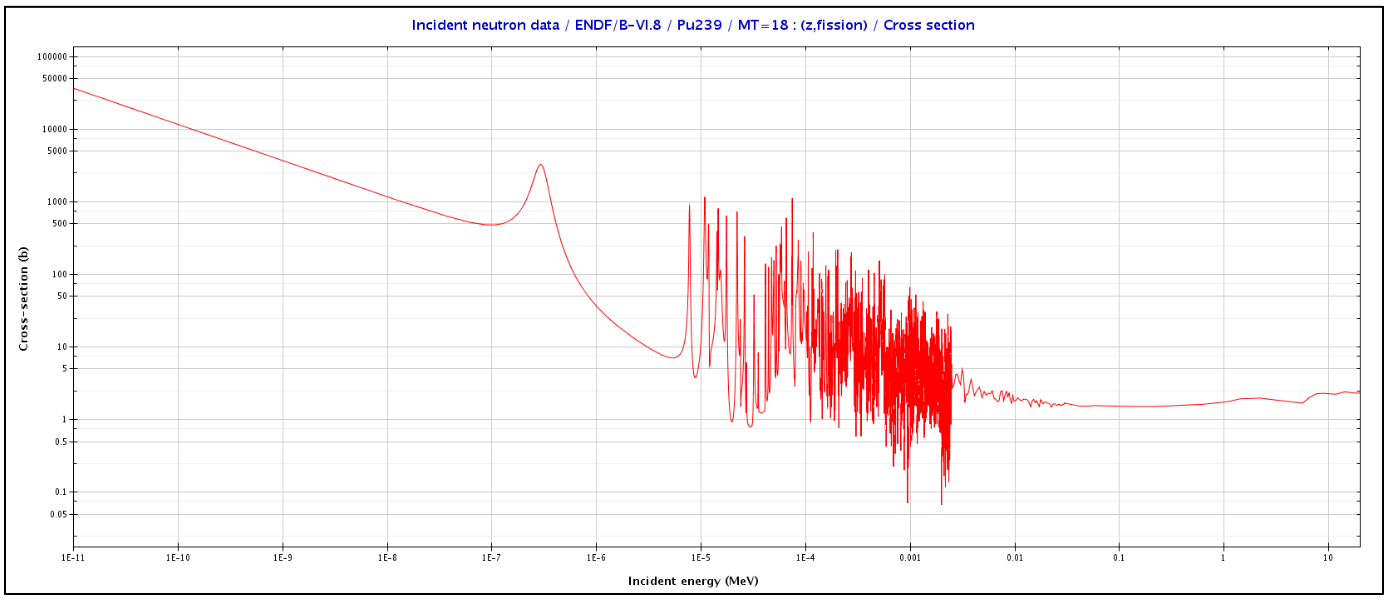

Figure 4: Microscopic Fission Cross Section for Plutonium-239

In computation, it is often more advantageous to utilzize the macroscopic cross section, which is defined as $\Sigma = \sigma N$. Where N is the atom density of the material (atoms / cm2), thus resulting in Σ having a unit of cm^{-1} which represents the probability of a nuclear reaction per centimeter traveled by the neutron in a medium. The inverse of the macroscopic cross section is referred to as the *mean free path* (λ), or how far can the neutron travel in the medium before confronting a specific type of nuclear reaction.

Monte Carlo Method

Monte Carlo methods represent a sophisticated class of computational techniques employed across diverse disciplines, including radiation transport simulations, where the prominent MCNP (Monte Carlo N-Particle) code holds particular prominence [6]. These methodologies hinge on the generation of random samples from experimental data and find validation through statistical principles such as the Law of Large Numbers (LLN). In the realm of radiation transport, MCNP leverages stochastic processes to model the intricate interactions of particles with matter, offering invaluable insights into the intricate dynamics of radiation propagation in various environments.

The Law of Large Numbers, denoted as $\lim_{n \to \infty}$ P(sample mean) = μ, asserts that as the sample size (n) approaches infinity, the sample mean converges in probability to the population mean (μ) [7].

Rejection Sampling

We can demonstrate the effectiveness of the integrative Monte Carlo method by randomly sampling points on the XY plane to approximate π. The Python code for this as well as the code for all simulations in the succeeding sections is available on the GitHub repository, *dyl-frank/Intro-to-MC-Transport* [8].

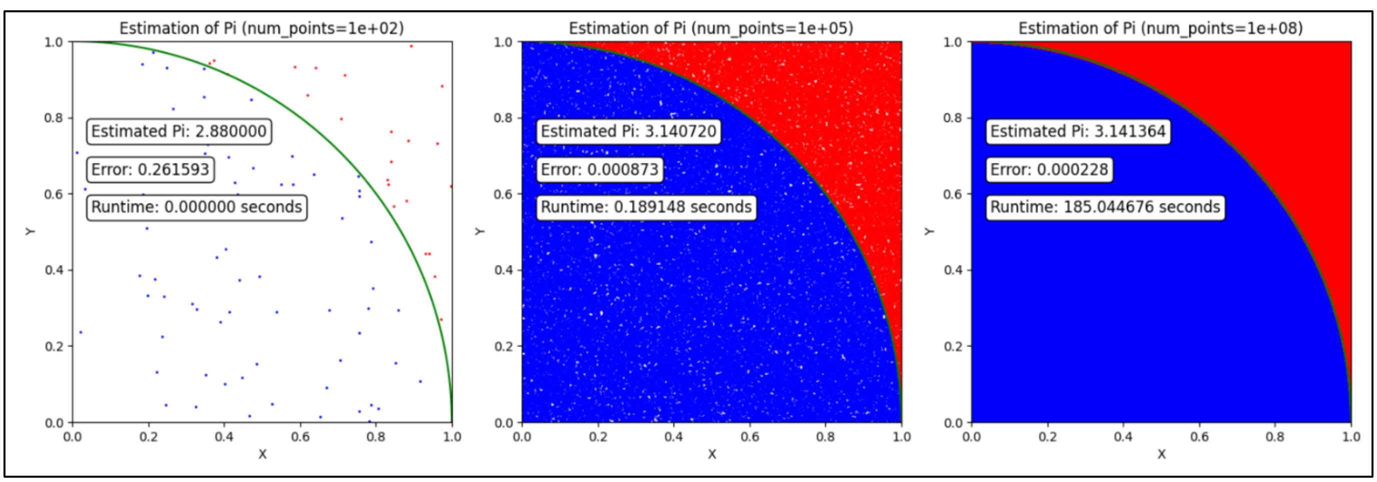

Figure 5: Results from Monte Carlo Approximation of pi

As evident from the results, the estimations of π demonstrate a remarkable level of accuracy. It is worth noting that the accuracy of these estimations is directly influenced by the number of sampled points, as elucidated by Eq.3

Problem statement:

For our Monte Carlo radiation transport code, we will define the following scenario:

- A plutonium sphere with a radius of R1
- Surrounding the sphere is a layer of water extending from R1 to R2.
- Then, there is a plutonium shell extending from R2 to R3 followed by another layer of water beyond R3.

Additional Assumptions:

- All scattering is assumed to be elastic and isotropic.
- All neutrons, including prompt neutrons from fission, possess an energy of 14 MeV.
- Each fission reaction emits exactly 3 prompt neutrons in an isotropic distribution.

The task is to calculate the positions of all captured neutrons within this defined geometry as well as the neutron flux through each cell.

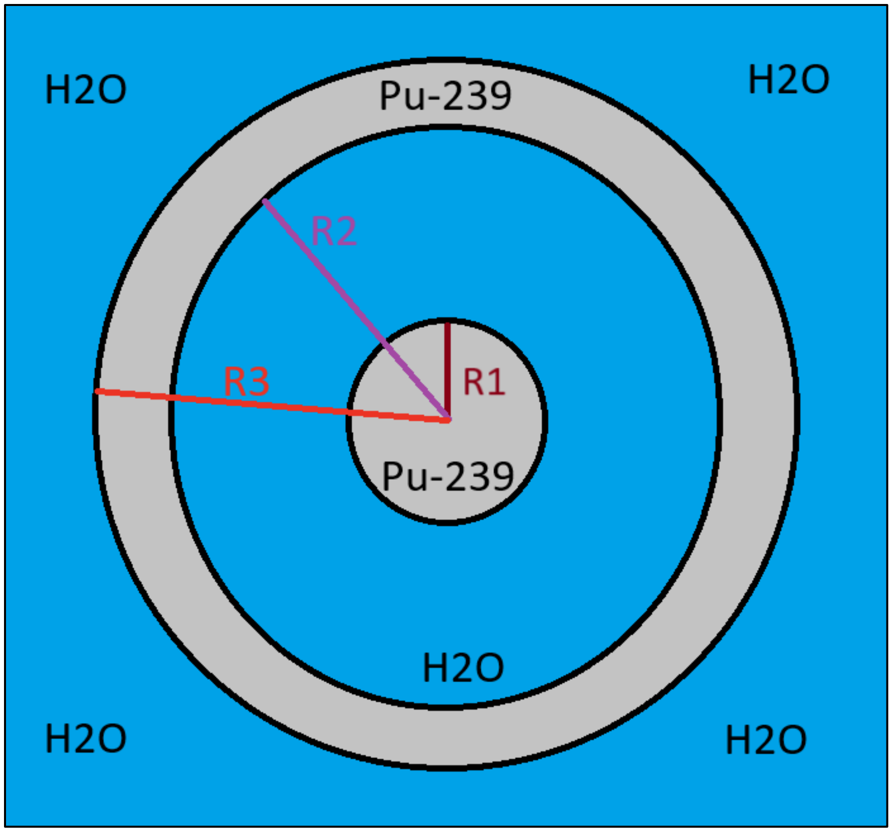

Figure 6: Diagram of the Model Simulated

Solution

The complete solution to this problem is available on the GitHub repository [8], however here is a high level overview of the code courtesy of ChatGPT 3.5.

This Python script performs a Monte Carlo simulation for neutron transport. It starts by initializing various parameters and nuclear data for Pu-239 and H2O. The simulation takes place in three defined cells with specified boundaries. The program then defines a `Particle` class, representing a neutron, with attributes for position, scattering events, origin, and status (dead or alive).

There are two functions, `Plutonium` and `Water`, which simulate the movement of neutrons within the defined cells based on their initial positions and scattering events. The particles move and interact according to specified probabilities of scattering, absorption, and fission.

A `process_particle` function determines which cell a particle is in and calls the corresponding function for further processing.

The program initializes a specified number of particles, assigns them to threads for parallel processing, and runs the simulation. It tracks the number of fissions and captures in each cell. The final results are printed, including the compute time, total number of particles simulated, total fissions, and fissions per initialized particle.

Additionally, a summary table is generated, displaying statistics for each cell, including the number of captures, density, and neutron flux. The simulation's progress is monitored, with a timeout feature implemented to ensure the simulation does not run indefinitely. The script provides valuable insights into neutron transport within defined cell boundaries.

Results

The python code was rans with the following parameters, R1 = 5, R2 = 10, R3 = 12, Initial_paticles = 100, random_seed = 1699490753.8066308. The following results were achieved:

```
Time out!
Simulation Complete!
Compute Time:     637.2268497943878 s
Total Number of Particles Simulated: 103
Total Number of Fissions: 72486
Fissions per Initialized Particle: 724.86
```

Cell	Number of Captures	Density (neutrons per cm^3)	Flux (Neutrons per cm^2 per second)
Cell 1	1485	13.1303	6.82775e+10
Cell 1 (Normalized)	14.4175	0.127478	6.62888e+08
Cell 2	8742	77.2963	1.11535e+10
Cell 2 (Normailized)	84.8738	0.750449	1.08287e+08
Cell 3	71030	628.043	1.21123e+11
Cell 3 (Normalized)	689.612	6.09751	1.17595e+09

Figure 7: Results from an MC Simulation

Additionally, the following plots have been created as a visual aid to understanding the propagation of neutron radiation. Note that there are disparities in uniformly sampling spherical angles as seen in figures, however this issue is being resolved as of the time writing this.

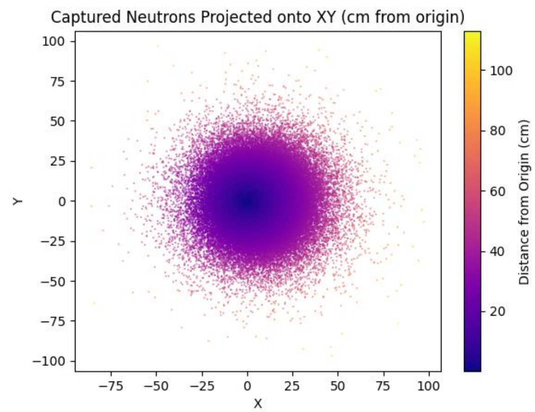

Figure 8: 2D Captured Neutron Plot

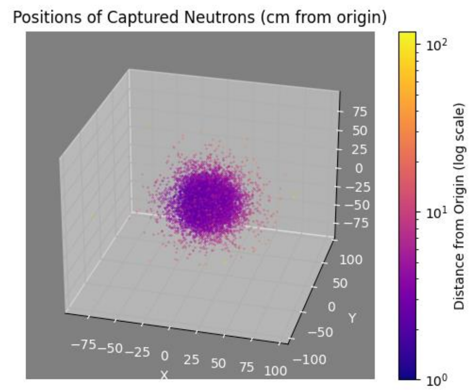

Figure 9: 3D Captured Neutron Plot

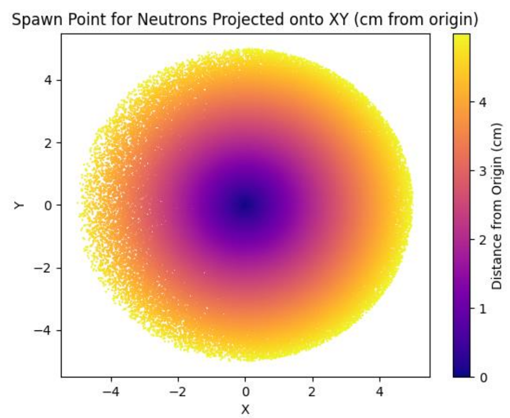

Figure 10: 2D Spawned Neutron Plot

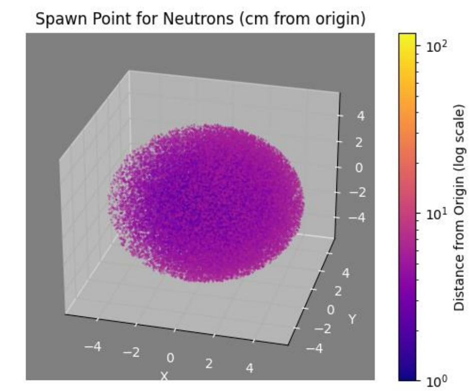

Figure 11: 3D Spawned Neutron Plot

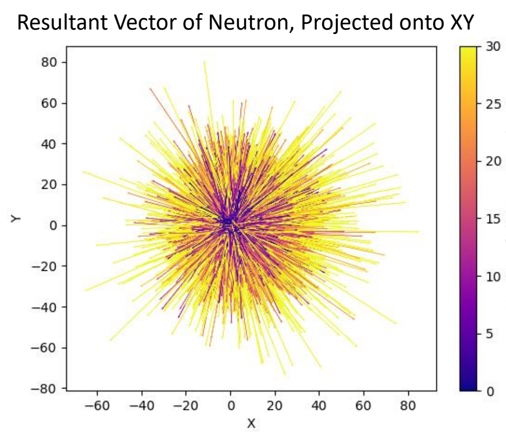

Figure 12: 2D Neutron Tracks

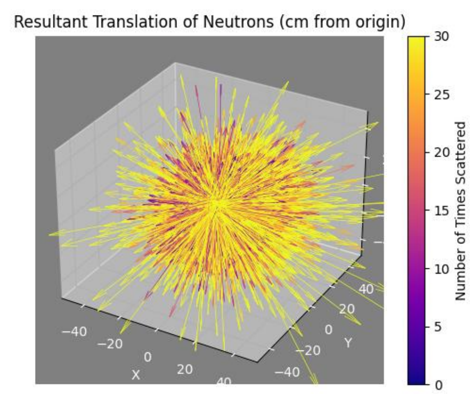

Figure 13: 3D Neutron Tracks

Takeaways

Radiation transport codes play a pivotal role in safeguarding global security and fostering peace. They hold immense potential in tackling pressing issues such as healthcare, climate change, and nuclear arsenal management. Through optimization, Monte Carlo codes can efficiently sample extensive repositories of nuclear data, providing a precise portrayal of the physical environment. Moreover, the progress in supercomputing empowers scientists and policymakers to gain deeper insights into the repercussions of a nuclear detonation, aiding in strategic preparedness and response. Furthermore, coupling radiation transport codes with computational fluid dynamics (CFD) presents an innovative approach to simulate dynamic explosions, offering a comprehensive understanding of complex phenomena. This integration facilitates the exploration of various scenarios, contributing to more effective risk mitigation strategies.

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