Critical Mass Determination Project

supercritical uranium monte carlo coding project for nuclear physics 1 at UVA.

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1 Background

When learning modern and nuclear physics as part of my undergraduate degree, we discussed the exponential decay of unstable nuclei. Although it's impossible to predict when an individual radioactive atom will decay, it is well understood that a large number of atoms of the same unstable isotope will reliably decrease in number at the same exponential decay rate. The number of radioactive atoms at time t follows the following equation:

$$N(t) = N_0 * e^{-\lambda t} \tag{1}$$

where N_0 is the initial population of atoms and λ is the decay constant. Interestingly, the statistics of the *population* are quite predictable; whereas the statistics of *individual* nuclei are not. We cannot predict when an individual nucleus will decay. Instead, we can only predict what will happen for large numbers of nuclei. I proceeded with the supercriticality project under this premise: **if I could describe how the populations of free neutrons and fission centers change over time, I might be able to accurately model a supercritical nuclear chain reaction.**

But what computational models enable us to simulate the evolution of populations over time? In my undergraduate computational physics course, an example we studied was the Susceptible, Infected, Recovered (SIR) model of epidemiology. The SIR model attempts to describe the time evolution of a contagious disease as it spreads throughout a population [2]. However, the SIR model is easily adapted to many other problems where different populations interact and their numbers change over time. The simplest SIR model comprises just three ordinary differential equations and tracks how a population of susceptible people (S) become infected patients (I) and eventually recover (R) from their illnesses.

$$\frac{dS}{dt}(t) = -\beta S(t)I(t) \tag{2}$$

$$\frac{dI}{dt}(t) = \beta S(t)I(t) - \gamma I(t) \tag{3}$$

$$\frac{dR}{dt}(t) = \gamma I(t) \tag{4}$$

Here, the rate of change of each population depends on interactions with the other populations. These interactions are moderated by the coefficients β and γ that indicate the strength rate of the interactions. The initial conditions usually consider $S_0 = N - \delta$, $I_0 = \delta$, and $R_0 = 0$ with N as the total population and δ a small number of initially sick "patient zero" cases. As time progresses, the S and I populations intermingle, which pulls people from the S camp into the I camp. Simultaneously, time allows the infected patients I to recover and transition into the recovered population R. Given sufficient time, the end-behavior of the evolution is steady state with the entire population having gone through the infection-recovery process and is just $R_f = N$, $S_f = 0$, and $I_f = 0$. See Figure 1 on page 3.

As we can see in the simple example SIR model, it only takes a small number of sick patients to quickly infect a large population in a matter of months. Notably, after infecting a small number of people, the (I) population grows rapidly during days 25-35. Is it possible that the population of infected patients is supercritical during that time? I wanted to test and see if I could apply this method to the physics of nuclear explosions.

2 How it works

I wrote a simple Python program that aims to model the physics inside a nuclear bomb. The program is designed to simulate at what mass of uranium the bomb goes supercritical, which is when the number of neutrons created per generation reaches 2. Since there are many ways to modify the SIR

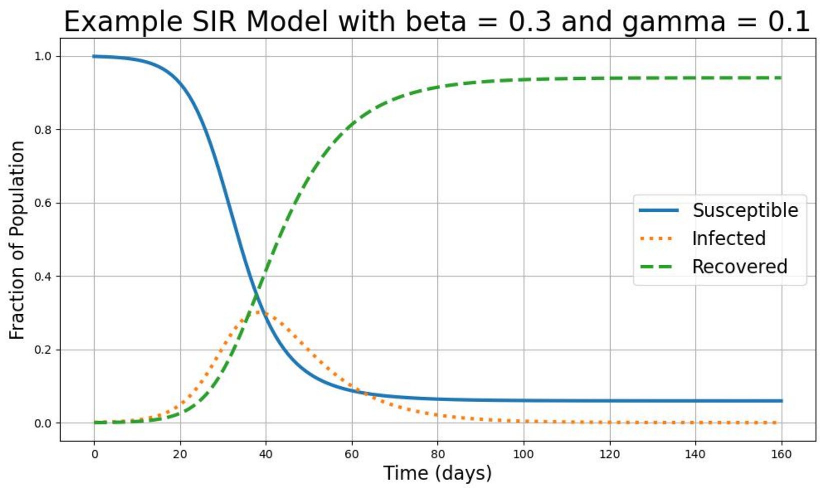


Figure 1: A visualization of the simple SIR model [1] The initial population is $S = 1000$, $I = 1$, and $R = 0$. $\beta = 0.3$ and $\gamma = 0.1$. As time progresses, the infected and susceptible populations mix, which grows the infected population. Then, the infected patients recover with time.

model, I built the simulation to run in a couple of different models; however, I only kept one model in the final draft that I felt worked the best. This model emulates the basic SIR model described above with small changes related to neutron-nucleus interactions. The other previous attempts used a more complicated model that seeks to also keep track of the number of neutron generations, and a very old attempt used random walk dynamics inside the uranium core.

3 Simple SIR Approach

For the first model, I adapted the SIR model to reflect the different populations of interest, the free neutrons and the uranium atoms. To do so, I made the following assumptions:

- The fission centers ^{235}U are the "susceptible" population S because they get used up as they interact with free neutrons.
- Initial free neutrons from the neutron source are in the I population, since they can "infect" a fission center, converting it to energy and even

more neutrons.

- Each fission adds more neutrons to I and subtracts fission centers from S.

- As neutrons scatter too far and exit the sphere, they leave the I population and enter the R population of "removed neutrons".

- Finally, there's a fourth population called P, which is just tallying the number of fissions produced.

In implementing this version, there are only 2 rates to consider: the fission and ejection rates. First, we need the fission rate that describes the interaction between free neutrons and uranium fission centers, leading to the production of energy and new generations of neutrons. Second, we need the ejection rate to see how quickly neutrons leave the bomb structure. If the construction of the bomb is just right, then the neutrons should reproduce so quickly that the bomb goes supercritical, despite many neutrons also leaving the bomb.

I've constructed the following ordinary differential equations for the simple model:

$$\frac{dS}{dt}(t) = -\beta S(t)I(t) \tag{5}$$

$$\frac{dI}{dt}(t) = \beta k S(t)I(t) - \gamma I(t) \tag{6}$$

$$\frac{dR}{dt}(t) = \gamma I(t) \tag{7}$$

$$\frac{dP}{dt}(t) = \beta S(t)I(t) \tag{8}$$

The only fundamental differences between these equations and the simple SIR model equations above is the inclusion of the k parameter for $\frac{dI}{dt}(t)$ and the new $\frac{dP}{dt}(t)$. The k value is a multiplicative factor denoting the average number of new neutrons produced after any one fission event, which we can easily find online is approximately 2.6 [5]. The final equation for $\frac{dP}{dt}$ is just tallying the number of fissions produced so that we can later count the average amount of total energy released.

However, even though we have the equations, we are still missing the coupling constants β and γ, the rates at which fission and ejection occur. How can we go about finding these values? In the practice of epidemiology, these constants are usually calculated empirically [4]. γ is the inverse of the average length of an infection, and β is the estimated transmission rate. Taking for example COVID-19, in Algeria in 2020, these parameters were estimated to have the following values: $\beta = 0.0561215$ and $\gamma = 0.0455331$. Their ratio $R_o = 1.23$, called the basic reproduction number, describes the number of additional cases each sick person will create [4]. However, since we're tasked with simulating the supercriticality condition without the supplement of experimental data on nuclear bombs, we'll have to estimate the fission and ejection rates another way.

The fission rate is related to the fission probability, the likelihood that a single neutron will force a ^{235}U nucleus to fission. To calculate the fission rate, we should start by finding this probability for a single neutron to cause a uranium nucleus to fission. We can find this using the method discussed in class given the number density of uranium n and the cross section for fission $\sigma_{fission}$. The mean free path $x_{fission}$ to fission is:

$$x = -\frac{1}{n\sigma_{fission}} ln(C)$$

where C is a random number between 0 and 1. However, since we're working with large numbers of neutrons, we can apply the central limit theorem to our random number C, taking the mean value of the random distribution from 0 to 1. As such, we choose $C = 0.5$.

$$x_{fission} = -\frac{1}{n\sigma_{fission}} ln(0.5) \tag{9}$$

The probability of fission occurring within the mean free path is given by:

$$P = e^{-xn\sigma_{fission}} \tag{10}$$

Now that we have the probability of a single fission event occurring for one neutron, we can begin to translate this into the rate for a population of neutrons to fission a group of ^{235}U nuclei in a time interval. The probability P of a reaction occurring with rate r in a time interval t is:

$$P = 1 - e^{-rt}$$

and solving for r,

$$r = -\frac{ln(1-P)}{t} \tag{11}$$

In order to find the fission rate, all we need is the probability for a fission to occur and the time interval over which it takes place. We discussed in class that the time for one neutron generation is approximately 10 ns; we'll use this as the time interval for our fission rate. Moreover, we said that the total time for the nuclear explosion is around 80 generations, which takes us to a little less than 1 µs.

Finding the neutron ejection rate is a bit more involved than the fission rate. We need to find the probability that a random neutron will exit our bomb given the size of the bomb and the neutron mean free path for scattering. We can find the mean free path for scattering the same as before:

$$x_{scatter} = -\frac{1}{n\sigma_{scatter}} ln(0.5)$$

by just swapping $\sigma_{fission}$ for $\sigma_{scatter}$. However, we've only found the average distance neutrons travel between scattering events; yet, we're interested in the probability a neutron scatters outside our bomb. How do we relate the scattering length to the geometry of the bomb?

4 Monte Carlo Integration for Ejection Probability

In consultation with classmate Brannon Semp, I've devised the following method to calculate the average ejection probability from the mean free path. Given that the bomb has a spherical geometry, the free neutrons can roam anywhere within the sphere. At any given time t, any individual neutron will be located at a random position within the sphere. After a small time step Δt, the neutron will have moved one mean free path from its original position in a random direction. If the neutron moves outside the sphere, its probability of ejection is 1. If it stays inside, the probability is 0. To transition from the individual neutron to the average neutron, we simply need to integrate this probability over the entire sphere. It is most efficient to carry out this task using monte carlo integration.

The probability a random neutron will scatter out of the sphere is given by the following piecewise function:

$$P(\vec{x}) = \begin{cases} 1: & \|\vec{x} + \Delta\vec{x}\| \geq R \\ 0: & \|\vec{x} + \Delta\vec{x}\| < R \end{cases} \tag{12}$$

Given an initial position $\vec{x}$ and small displacement $\Delta\vec{x}$ within a sphere of radius R, we only need to integrate over all positions and directions within the sphere to calculate the total probability. We are integrating over five dimensions: three are for the initial position, whereas only two are needed for the displacement, since we assume in spherical coordinates that the magnitude of $\Delta\vec{x}$ is constant (mean free path) and only the angles ϕ and θ vary. In order to cancel the dimensions of length and angle contributed by the integration, we will need to divide by the volume of the sphere and its solid angle at the end.

After monte carlo integration of the probability function over all space and angles within the sphere, we arrive at the following formula:

$$P_{ejection} = \frac{N_{inside}}{N_{total}} \frac{1}{\Omega V} \tag{13}$$

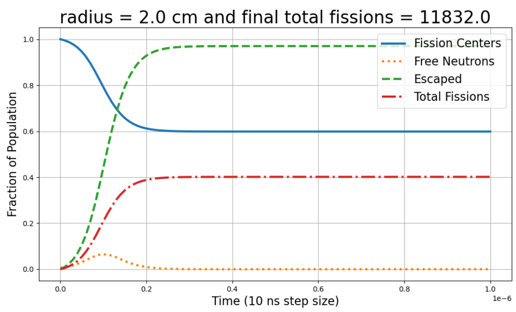
with N_{inside} representing the number of points $\|\vec{x} + \Delta\vec{x}\|$ inside the sphere and N_{total} representing the total number of points tested during integration. Ω is the solid angle of the sphere 4π and V is the volume of the sphere $\frac{4}{3}\pi R^3$. Since monte carlo integration relies on random numbers, the more points we choose, the more reliable our result becomes. For each radius R, I average the fission probability of five different runs of integration with 10^6 test points.

Now that we have the ejection probability for the average neutron, we can simply convert it to a rate just as we did before for the fission probability. Finally, with all of these calculations, we're ready to implement our SIR model for the physics of a nuclear bomb.

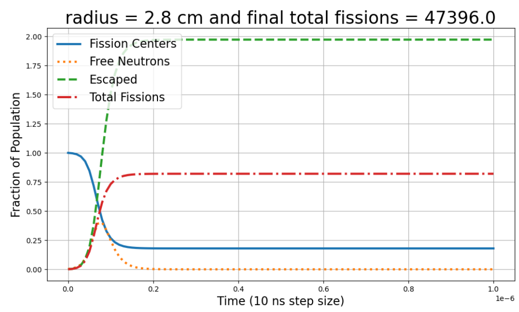
5 Results

Below in Figure 2 on page 8, I've included plots demonstrating the results of my simulation model [1]. I've sampled across various bomb radii from 2 cm to 12 cm and tallied up the total number of fissions produced after 1 µs of simulation. At small radii, there is not much fission because the free neutron ejection rate is large and there are not many scattering centers available. However, as the bomb size increases, the ejection rate shrinks, the number of scattering centers grows, and so too does the total number of fissions.

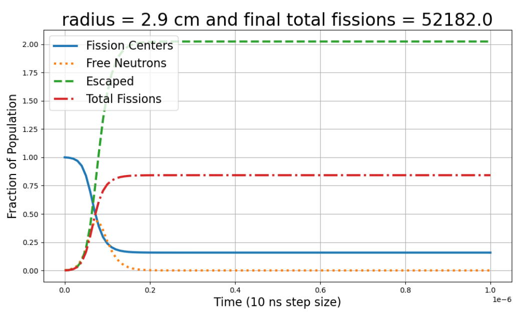
Figure 2: Plots of the neutron and scattering center populations over time for various bomb radii.



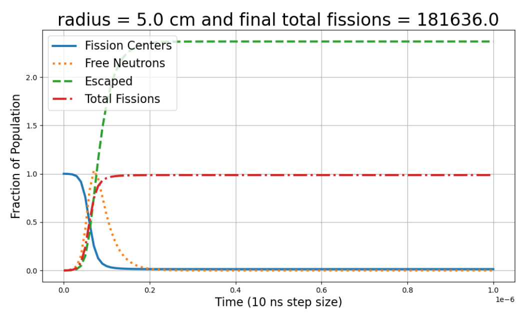
(a) radius = 2 cm, fissions = 11,832



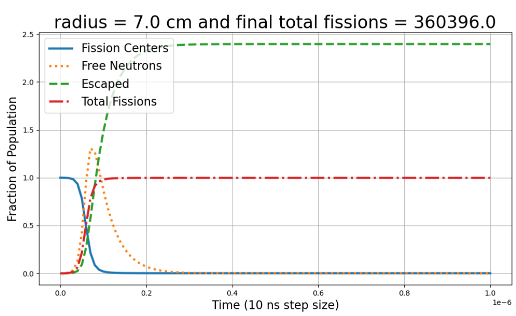
(b) radius = 2.8 cm, fissions = 47,396



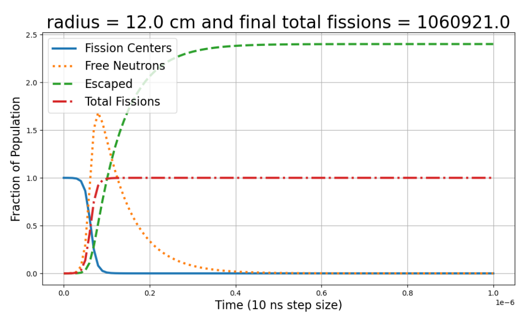
(c) radius = 2.9 cm, fissions = 52,182



(d) radius = 5 cm, fissions = 181,636



(e) radius = 7 cm, fissions = 360,396



(f) radius = 12 cm, fissions = 1,060,921

We see from the figure that of the plots shown, the ones with final *Escaped* population (total neutrons that were ejected) higher than 2.0 correspond to bomb configurations where supercriticality occurred. In the plots shown, this transition takes place between a radius of 2.8 cm and 2.9 cm.

6 Assorted Questions and Answers

What follows are several paragraphs answering various questions presented at the end of the project description. I found most of my results from a useful book called *The Physics of the Manhattan Project, Third Edition* by Bruce Cameron Reed.

What is the cross-section for fission (of ^{235}U) as a function of the energy of the incident neutron? I found the easiest way to answer this question was to look at the *Evaluated Nuclear Data File* (ENDF) provided by the National Nuclear Data Center hosted through Brookhaven National Laboratory [3]. Using the database, we can generate a simple plot of the total cross-section of ^{235}U and neutron interactions as a function of incident neutron energy as illustrated in figure 3 on page 10.

What other scattering processes occur and their cross-sections? What's really neat about the ENDF website is that we can isolate the different types of interactions between ^{235}U and free neutrons. For example, we can isolate elastic, non-elastic, and inelastic collisions. We can also separate out different fission modes, as well as number of neutron products. We can even look at the gamma ray produced by an excited ^{235}U nucleus after bombardment by a neutron!

In short, other scattering processes that occur are different variations of classical scattering, different versions of fission, neutron emission, and gamma emission. We can find all their cross-sections online [3].

How many neutrons are released from each fission and what are their energies? ^{235}U releases on average about 2.6 neutrons per fission [5]. In my simulation, I chose a slightly more conservative value of 2.4, since I haven't chosen to consider various fission modes in my code.

The secondary neutrons produced by fission have a range of energies; however, the average energy of the released neutrons is about 2 MeV. The

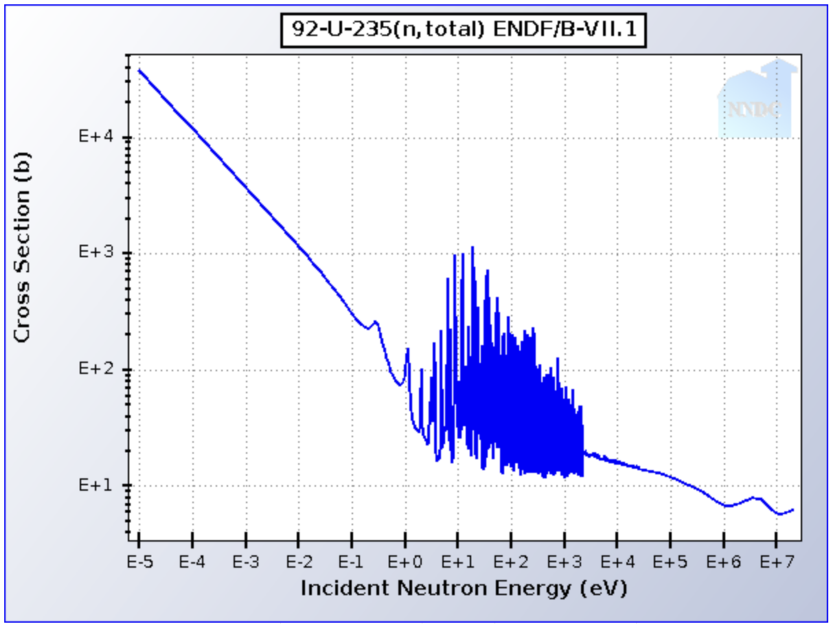


Figure 3: A log-log plot of the cross section in barns as a function of incident neutron energy in electron volts for interactions between free neutrons and ^{235}U. The cross section is highest for slow neutrons and decreases as energy grows.

energy distribution of produced neutrons after fission of ^{235}U is shown in figure 4 on page 11 [5].

How much energy is released by each fission? How much variation is there? The energy release during one fission event varies depending on the type of fission reaction and the fission products present. However, taking as an example the fission of ^{235}U into barium and krypton with three neutrons, we find that the energy release is 173.3 MeV [5].

If you include a neutron reflector, what are the relevant cross sections? Historically, the neutron reflector was called the *tamper* and it consisted of a shell of dense material surrounding the fissile core [5]. Tungsten-carbide (WC) was the tamper material used in *Little Boy*. The dominant reaction happening in the tamper is that of free neutrons colliding elastically with the tungsten-carbide lattice. The important cross sections would be for

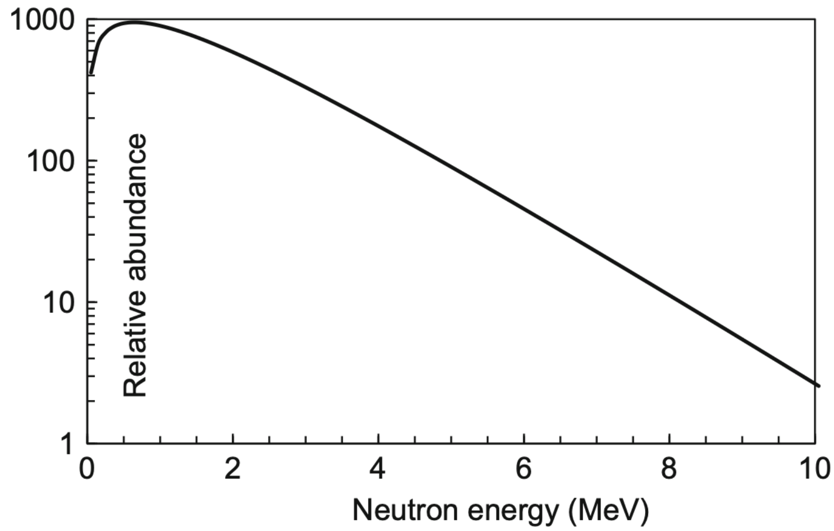


Figure 4: Energy distribution of neutrons emitted following fission of ^{235}U. The most probable energy is slightly less than 1 MeV, but the average value is around 2 MeV.

elastic scattering between these particles at various neutron energies. This would involve the cross-sections of the different naturally-occurring isotopes of tungsten (^{180}W, ^{182}W, ^{183}W, ^{184}W, ^{186}W) as well as ^{12}C.

Assuming you use k = 2 to define supercriticality, can you find a value for k by looking at the results of a single "seed" neutron? For a ^{235}U mass of a given size, what type of variation do you see in the value of k resulting from multiple trials of single seed neutrons? My simulation is easily modifiable to look at the results of a single seed neutron. However, since my solution uses non-stochastic ordinary differential equations, my results do not change appreciably with repeated runs of single seed neutrons. The main point of variation in my results in how I calculate the average neutron ejection probability. Since that method relies on monte carlo integration, I average the results of five integration attempts to hopefully converge closer to the true result.

Can you estimate the fraction of ^{235}U that has fissioned when your device has produced energy equivalent to 15 kTons of TNT? How can you compute such a number? Exploding one ton of TNT yields approximately 4.2×10^9 J, which means that 15 tons would be about 63×10^9 J [5]. This energy release is roughly equivalent to what would be released by the fission of 0.9 kg of ^{235}U given that a single fission is approximately 173.3 MeV.

References

[1] Taylor Colaizzi. *nuclear-bomb*. `https://github.com/taylorjcolaizzi/nuclear-bomb`. Accessed: 2025-11-17. 2025.

[2] Majid Bani-Yaghoub Hadeel AlQadi. "Incorporating global dynamics to improve the accurary of disease models: Example of a COVID-19 SIR model". In: *PLoS One* 17.4 (2022). DOI: `https://doi.org/10.1371/journal.pone.0265815`.

[3] Brookhaven National Laboratory. "Plotted cross section". In: *National Nuclear Data Center: Evaluated Nuclear Data File* (2025).

[4] Dilip Kumar Bagal Mohamed Lounis. "Estimation of SIR model's parameters of COVID-19 in Algeria." In: *Bulletin of the National Research Centre* 44.180 (2020). DOI: `https://doi.org/10.1186/s42269-020-00434-5`.

[5] Bruce Cameron Reed. *The Physics of the Manhattan Project Third Edition*. Springer, 2015.