Monte-Carlo Project — Study of Uranium Criticality

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Introduction

This project uses Python (Google Colab) to simulate uranium criticality by evolving the minimal model from the practical work (TP) towards a more realistic approach. The method involves criticizing the limits of the initial model (infinite medium, fixed parameters) before introducing a probabilistic model integrating losses and random multiplicity. Finally, we link these probabilities to real physics by integrating neutron energy and cross-sections derived from the bibliography cited at the end of the report.

I — Minimal TP Model: Description, Interpretation, and Limits

I.1 Description of the model and physical interpretation

Theoretical Reference Model – At the basis of neutron kinetics lies the deterministic continuous-time model. The evolution of the number of neutrons $N(t)$ is described by the fundamental differential equation:

$$\frac{dN}{dt} = (k-1)\,\lambda\,N(t) \quad \Longrightarrow \quad N(t) = N_0\,e^{(k-1)\lambda t}$$

This model predicts a strict exponential evolution. It is this reference dynamic that we seek to simulate, although the numerical approach of the TP is different.

Discrete Approach of the TP – To simulate this phenomenon, the TP uses a simplified model in *successive generations* (discrete). The model relies on the following hypotheses:

- infinite medium (no leakage);
- homogeneous and constant isotopic composition;
- any interaction with ^{235}U causes fission;
- each fission produces exactly two neutrons.

The fission probability is equated to the atomic proportion p of ^{235}U: a neutron produces 2 neutrons with probability p, and 0 otherwise. The key parameter is then the mean multiplication factor: $m = 2p$.

We interpret m as the average number of neutrons produced in the next generation per active neutron:

- $m < 1$: extinction on average;
- $m = 1$: critical regime (average stability);
- $m > 1$: growth on average.

For natural uranium ($p \simeq 0.007$), we obtain $m \simeq 0.014 \ll 1$: the model thus predicts very rapid extinction.

This model allows visualizing the sub-critical / critical / super-critical transition. However, it conflates distinct mechanisms into p and does not aim for a realistic threshold.

I.2 Criticality threshold and structural limits

The critical threshold of the model is defined by $m = 1$, i.e., $p_c = 0.5$. The unrealistic nature of this value highlights the absent mechanisms:

- absence of leakage (infinite medium);
- absence of capture without fission;
- multiplicity fixed at 2;
- absence of energy dependence (constant probabilities).

The rest of the project introduces these effects progressively: (i) explicit losses, (ii) random multiplicity, (iii) probabilities motivated by $\sigma_f(E)$, $\sigma_c(E)$, and $\sigma_s(E)$.

II — First Improved Model

II.1 Motivation

The minimal model is intentionally extreme: any interaction boils down to *fission* (probability p) or *extinction* (probability $1-p$), with a multiplicity fixed at 2 neutrons. This leads to dynamics that are too "clean" and does not distinguish between physical mechanisms that have very different effects on the duration of the chain. We therefore introduce an **effective** probabilistic model that separates these contributions, while remaining simple to simulate via Monte-Carlo.

II.2 Improved Model

To each neutron, we associate three exclusive outcomes:

- **fission**: production of new neutrons;
- **loss**: disappearance;
- **scattering**: the neutron *survives* and remains active in the next generation.

We denote p as the proportion of ^{235}U, and we introduce *effective* probabilities p_{f} (fission), p_{L} (loss), and p_0 (scattering), with the constraint: $p_{\mathrm{f}} \geq 0,\ p_{\mathrm{L}} \geq 0,\ p_0 = 1 - p_{\mathrm{f}} - p_{\mathrm{L}} \geq 0$.

Consistent with the code, we link these probabilities to p by:

$$p_{\mathrm{f}} = \alpha\, p, \qquad p_{\mathrm{L}} = \beta(1-p), \qquad p_0 = 1 - \alpha p - \beta(1-p),$$

where α represents global fission efficiency, and β regulates the intensity of losses.

In the implementation, we fixed $\alpha = 0.6$ and $\beta = 0.4$, which guarantees $p_{\mathrm{f}} + p_{\mathrm{L}} \leq 1$ over the tested range of p. Conditionally on a fission, the multiplicity ν is random:

$$\nu = \begin{cases} 1 & \text{with probability } 0.25, \\ 2 & \text{with probability } 0.50, \\ 3 & \text{with probability } 0.25. \end{cases}$$

Even with the same mean, this variability increases the dispersion of trajectories, especially near the critical regime.

II.3 Monte-Carlo Simulation

In a real reactor, the number of neutrons is of the order of 10^{18}. It is impossible to simulate every neutron individually. We therefore simulate a **reduced sample** (here a few thousand) which provides a *statistical estimate* of global behavior, at the cost of statistical uncertainty (noise) which we reduce by averaging multiple realizations.

We simulate a trajectory generation by generation. Denoting Z_g as the number of active neutrons at generation g:

- initialization: $Z_0 = 1$;
- for each active neutron, draw a real number $r \sim \mathcal{U}(0,1)$:
  - if $r < p_{\mathrm{f}}$: fission, add $\nu \in \{1,2,3\}$ neutrons;
  - else if $r < p_{\mathrm{f}} + p_{\mathrm{L}}$: loss, add 0 neutrons;
  - else: scattering/neutrality, add 1 neutron (the neutron is kept).
- stop at extinction ($Z_g = 0$) or at the ceiling $T_{\max}$.

We repeat N independent trajectories to estimate mean quantities and their variability.

III — Results and Interpretation

III.1 Measurement and Estimator

For each value of p, we simulate N independent trajectories and measure $T = \min(\text{extinction generation}, T_{\max})$. The estimator is: $\widehat{\mathbb{E}}[T](p) = \frac{1}{N}\sum_{j=1}^{N} T^{(j)}(p)$.

III.2 Computational Cost (Complexity)

A trajectory is simulated by processing all neutrons present at each generation. $C_{\text{traj}} \propto \sum_{g=0}^{T-1} Z_g$. Thus, for a grid of M values of p and N trajectories per point: $C_{\text{total}} \propto M\,N\,\mathbb{E}\left[\sum_{g=0}^{T-1} Z_g\right]$. This cost can increase very quickly when p approaches the critical zone, as trajectories become longer and the population Z_g can grow significantly.

III.3 Results

(i) $\widehat{\mathbb{E}}[T](p)$ increases with p. In both models, increasing p increases the probability of fission, thus lengthening the average time before extinction.

(ii) Interpretation of the gap: In our implementation, the "scattering/neutrality" outcome preserves the neutron: it remains active and can attempt an interaction again, which mechanically lengthens the chains, even in the presence of losses. Furthermore, the variability of ν increases the dispersion of trajectories compared to the binary TP model.

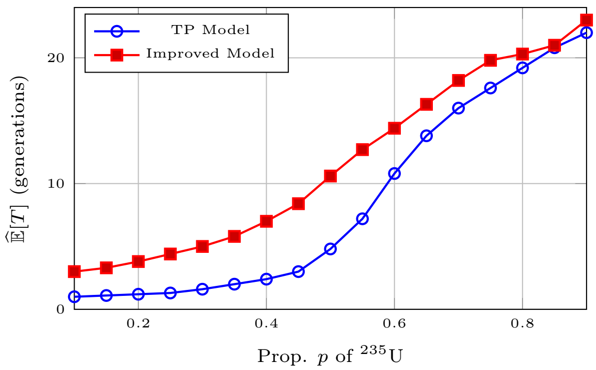

Figure 1: Comparison of models.

VI — Physical Model: Energy, Capture, and Inelastic Scattering

VI.1 Why introduce energy and cross-sections

In the previous models, the probabilities p_f, p_L, p_0 were fixed effective parameters. Here, we link these probabilities to the **microscopic physics**. Each neutron carries an energy E, and reaction probabilities depend on cross-sections $\sigma(E)$ (interpolated from ENDF data). We simulate an infinite medium of natural uranium:

$$N_{235} = 0.007, \qquad N_{238} = 0.993.$$

VI.2 Complete Interaction Probabilities

Unlike the simplified model, a neutron now has four possible destinies at each interaction, the sum of whose probabilities is 1:

- **Fission** (n, f): Production of new neutrons (mainly on ^{235}U at low energy).
- **Radiative Capture** (n, γ): The neutron is absorbed and disappears without producing descendants. This is the main "death" mechanism.
- **Inelastic Scattering** (n, n'): The neutron loses a large amount of energy (excitation of the target nucleus).
- **Elastic Scattering** (n, n): Simple bounce, low energy loss.

Microscopic probabilities are calculated at each step according to the neutron's energy E and the nucleus encountered (drawn according to macroscopic sections Σ_{tot}).

VI.3 Fission: Multiplicity and Watt Spectrum

When a fission occurs, the multiplicity ν follows a probabilistic law based on physical averages (e.g., $\bar{\nu} \approx 2.43$). Crucial point: neutrons are born **fast** (average energy ≈ 2 MeV) following a Watt distribution. To cause new fissions on ^{235}U, they must be slowed down (thermalized).

VI.4 Slowing Down and Resonant Captures

The neutron's destiny depends on how it loses its energy:

- **High energies (> 0.1 MeV):** The collision with ^{238}U is often *inelastic*. The neutron abruptly loses its energy, falling into the keV range.
- **Resonance domain (10 eV - 1 keV):** This is the "danger zone". While slowing down via successive elastic collisions, the neutron traverses this zone where the capture cross-section σ_c of ^{238}U is immense.

VI.5 Results and Physical Interpretation

The simulation carried out with 1000 initial neutrons shows an evolution radically different from the simplified model, characterized by an average effective multiplication factor of:

$$k_{eff} \approx 0.9833 < 1$$

The temporal evolution (Fig. 2) is explained in two phases:

1. The Initial Peak (Transient) The sudden rise at the beginning is artificial. We injected the initial neutrons at thermal energy (0.025 eV). At this energy, the fission cross-section of ^{235}U is maximal (≈ 584 barns), causing an immediate burst of fissions.

2. Extinction (Asymptotic Regime) Once the first generation passes, new neutrons are born fast (MeV). To cause a fission, they must slow down. However, in pure natural uranium (without a moderator like water), the majority of neutrons are **captured by the resonances of** ^{238}U before reaching thermal energy. The system is physically **sub-critical**. The population decreases exponentially until extinction, which validates the physical consistency of the model (unlike the infinite growth of the previous model).

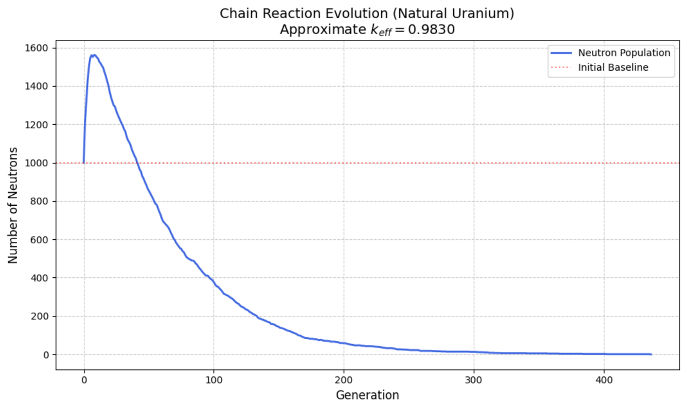

Figure 2: Population Evolution (Physical Simulation).

Conclusion

This project allowed us to progressively build a Monte-Carlo neutron transport simulator. Starting from a simplified mathematical model (infinite medium, fixed probabilities) which predicted an unrealistic criticality at $p = 0.5$, we arrived at a complete physical model integrating energy spectra and nuclear cross-sections (ENDF).

The final results demonstrate that natural uranium enriched to 0.7% is intrinsically **sub-critical** ($k_{eff} \approx 0.98$) in the absence of a moderator. The introduction of *inelastic scattering* and *radiative capture* allowed us to reproduce the stifling effect of the reaction by ^{238}U (resonant captures). This work illustrates the necessity of moderators in thermal reactors and the power of Monte-Carlo methods for solving complex integral problems where analytic intuition is no longer sufficient.

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