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A Simple Monte Carlo Simulation To Illustrate The Uranium-238 Decay Series And Nuclear Stability Principles

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Abstract:
The uranium-238 radioactive series is a well-known multi-step decay chain involving multiple alpha and beta-negative decays, ultimately resulting in the stable lead-206 isotope. In this work, we use computational simulations with Monte Carlo method to analyze the stochastic timing of decay events and to evaluate hypothetical decay pathways. Initially, by considering only mass and charge conservation, we identify 3,003 theoretical decay chains. However, many of these chains are unphysical due to energy constraints and nuclear stability. By incorporating additional nuclear physics principles, such as decay energy and nuclear shell stability, we confirm that only the well-established uranium-238 decay series is physically possible. This approach demonstrates a practical application of computational techniques to analyze nuclear decay chains.
***Key Word**: Uranium-238; Radioactive series; Nuclear decay; Simulation; Monte Carlo method.*

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I. Introduction

The uranium-238 (U-238) radioactive series refers to the decay chain of U-238, a naturally occurring radioactive isotope. Through a series of alpha and beta-negative decays, the unstable U-238 nucleus decays into various other nuclei such as thorium, radium, and lead. The uranium-238 decay series has significant applications in various fields due to its long-lived nature as a radioactive element. The decay products of U-238 are used in scientific research, energy production, medicine, and industrial processes.

The U-238 series plays a crucial role in geochronology, particularly in the method known as uranium-lead dating. By analyzing the ratio of U-238 to its final decay product, lead-206, it is possible to date rocks, minerals, and even the Earth itself. This method is widely used to determine the age of geological formations, providing a timeline for Earth's history over billions of years [1-4]. U-238 decays to thorium-234 in its early stages. U-Th dating is used to date calcium carbonate materials, such as coral and cave deposits, providing insights into past climates and environmental changes [5-7].

Radium-226, a decay product of U-238 series, was historically used in radiation therapy for treating cancer[8]. While modern treatments have moved to more advanced radioactive isotopes, radium was once widely used in brachytherapy treatment. Radioisotopes in the U-238 decay series that emit alpha particles are being researched for their potential in targeted cancer therapy. Alpha particles are highly ionizing and can destroy cancer cells with minimal damage to surrounding healthy tissues [9].

Radon-222, a naturally occurring gas in the U-238 decay chain, is used in industrial processes like gas flow tracing and radiographic inspection. It is also used in environmental monitoring to assess radon levels in buildings and the environment, as high radon levels pose health risks [10-12]. Thorium-234 and other isotopes in the series are used in industrial radiography for non-destructive testing. These isotopes emit radiation that can penetrate materials and are used to inspect the internal structure of objects without causing damage. This technique is widely used in industries such as aerospace, automotive, and construction to detect cracks, flaws, or weaknesses in materials and components.

The U-238 series, particularly radium-226 and radon-222, is used in environmental studies to trace the movement of groundwater [13]. Radium and radon are naturally dissolved in groundwater and can help in studying the hydrological properties of aquifers and the flow rates of water systems. This is vital for understanding water resource management and contamination risks. Isotopes in the U-238 series, including thorium-230, are used in oceanography to study sedimentation rates and ocean currents [14]. By analyzing the accumulation of thorium isotopes in marine sediments, is possible to infer the historical patterns of oceanic processes over time.

Detailed study of this series provides valuable information about the nuclear processes involved and the properties of the different isotopes [15,16].

It is straightforward to see that a total of 8 alpha particles and 6 beta-negative particles are necessary to U-238 transforms into the stable Pb-206. The mass number of each element of the series is given by *A = 4n + 2*, where *n* is an integer number. According to literature the following decay chain is assumed to be correct [17-19],

$$ {}^{238}_{92}U \xrightarrow{\alpha} {}^{234}_{90}Th \xrightarrow{\beta} {}^{234}_{91}Pa \xrightarrow{\beta} {}^{234}_{92}U \xrightarrow{\alpha} {}^{230}_{90}Th \xrightarrow{\alpha} {}^{226}_{88}Ra \xrightarrow{\alpha} {}^{222}_{86}Rn \xrightarrow{\alpha} {}^{218}_{84}Po \xrightarrow{\alpha} {}^{214}_{82}Pb \xrightarrow{\beta} {}^{214}_{83}Bi \xrightarrow{\beta} {}^{214}_{84}Po \xrightarrow{\alpha} {}^{210}_{82}Pb \xrightarrow{\beta} {}^{210}_{83}Bi \xrightarrow{\beta} {}^{210}_{84}Po \xrightarrow{\alpha} {}^{206}_{82}Pb. \quad (1) $$

Alternatively, in a more concise form,

$$ {}^{238}_{92}U \rightarrow 8\,{}^{4}_{2}\alpha + 6\,{}^{0}_{-1}\beta + {}^{206}_{82}Pb. \quad (2) $$

An important computational technique that uses random sampling to solve mathematical problems involving complex systems or uncertainty is the Monte Carlo method [20,21]. It is used to approximate solutions to problems that may be difficult or impossible to solve analytically. Monte Carlo simulations are a powerful method used to model and study radioactive decay, which is inherently a random process [22-24]. These simulations rely on random sampling techniques to solve problems that are deterministic in principle but too complex for traditional analytical approaches. In the context of radioactive decay, Monte Carlo methods are used to simulate the behavior of large numbers of radioactive atoms, predict decay patterns, and estimate associated radiation exposure or detection scenarios. Studies focus mainly on the exponential decay law and the probability of an individual nucleus decaying within a given time frame, related to the half-life of the nucleus [23].

In this study, we investigate the decay chain of uranium-238, culminating in the stable lead-206 isotope, due to its importance in various applications. At first, taking into account only the principle of conservation of mass and charge, the order in which the alpha and beta particles are emitted does not matter (see Equation 2). The question is similar to put eight identical balls of a given color (alpha particles) and six identical balls of another color (beta particles) into a box with fourteen empty spaces. In other words, it is the number of ways of picking 8 unordered outcomes from 14 possibilities; or the number of ways of picking 6 unordered outcomes from 14 possibilities,

$$ C_{14,8} = C_{14,6} = \frac{14!}{6!\,(14-6)!} = 3{,}003. \quad (3) $$

A central question that plays an important role is: Among the 3,003 possible pathways how to reach in the true pathway described in scheme given in Equation (1)? In what follows, using a simple code written in Fortran language and some basic principles of nuclear physics, we answer this question. Monte Carlo method is used only to simulate the sequence of decay events (alpha or beta decays). No further details on the decay constants or half-lives of individual nuclei are necessary. We use a simple Fortran code and Monte Carlo methods to generate and evaluate all possible decay pathways. While this approach neglects decay constants and half-lives of individual nuclei, it provides a useful framework for understanding the variety of potential decay sequences. Table 1 summarizes the isotopes, decay modes, and half-lives involved in the U-238 decay chain.

II. The Generation Of The 3,003 Different Possible U-238 Decay Chains

First we have to generate all the 3,003 different pathways to transform U-238 into Pb-206 after the emission of 8 alpha particles and 6 beta-negative particles, regardless of the order of emission. However, to generate manually all the 3,003 sequences would be virtually impossible. In this sense, a Fortran code was developed to list all the possible ways in the U-238 radioactive decay chain. Since beta-negative emission only changes the atomic number *Z* by +1, and the alpha emission changes the mass number *A* by -4 and the atomic number *Z* by -2, the maximum *Z* is 98 after 6 initial and consecutive beta emissions. On the other hand, in the case of 8 initial and consecutive alpha emissions, the lower *Z* is 76,

Table 1. List of isotopes in the U-238 radioactive decay chain, decay modes and half-lives.

Parent nucleus	Main decay mode	Daughter nucleus	Parent half-life [25]
^{238}U	alpha	^{234}Th	4.468 x 10^9 y
^{234}Th	beta	^{234}Pa	24.10 d
^{234}Pa	beta	^{234}U	1.159 min
^{234}U	alpha	^{230}Th	2.455 x 10^5 y
^{234}Th	alpha	^{226}Ra	7.538 x 10^4 y
^{226}Ra	alpha	^{222}Rn	1,600 y
^{222}Rn	alpha	^{218}Po	3.822 d
^{218}Po	alpha	^{214}Pb	3.097 min

^{214}Pb	beta	^{214}Bi	27.06 min
^{214}Bi	beta	^{214}Po	19.71 min
^{214}Po	alpha	^{210}Pb	163.6 μs
^{210}Pb	beta	^{210}Bi	22.20 y
^{210}Bi	beta	^{210}Po	5.012 d
^{210}Po	alpha	^{206}Pb	138.376 d

$76 \leq Z \leq 98, 206 \leq A \leq 238.$ (4)

Then, in the 3,003 possible pathways there are the possibility to form 207 different nuclei. The main features of the Fortran code used to generate the pathways are:

1. Starting with the initial uranium-238 nucleus, a random number between 0 and 1 is generated. By convention, we adopted that if the random number is greater than or equal to 0.5 an alpha particle is emitted, otherwise a beta-negative particle is emitted.
2. The process is repeated for each nucleus formed after a beta or alpha emission.
3. After a total of 14 emissions (beta-negative and/or alpha particles), if the final nucleus is the stable lead-206 the pathway is said to be a right pathway, otherwise a wrong pathway.
4. Some instructions within the code are used to discard wrong pathways.
5. Some instructions within the code are used to discard repeated pathways.
6. Only right and unique pathways are stored.
7. About 190,000 sequences are generated to obtain the 3,003 right pathways (most were wrong or right but repeated pathways).

This method ensures that all 3,003 possible decay chains are generated efficiently, reducing computational complexity while maintaining accuracy. A schematic view of the algorithm used to generate the decay sequences is shown in Figure 1.

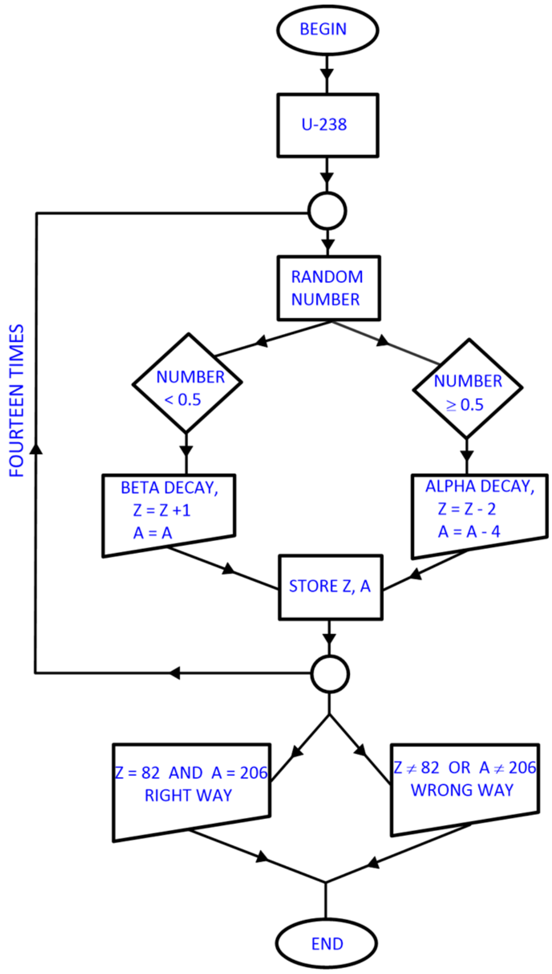

Figure 1. The flowchart algorithm used to determine the decay sequences after 14 alpha and/or beta-negative emissions.

III. Filtering The 3,003 Pathways

Once again, it should be noticed that in all generated sequences the principle of conservation of mass and charge is always obeyed,

$^{A}_{Z}X \rightarrow {}_{Z+1}^{A}Y + {}_{-1}^{0}\beta + \bar{\nu}_e$, (5)

for beta-negative decay, where X and Y are respectively the parent and daughter nuclei and $\bar{\nu}_e$ is the antineutrino, and

$$^{A}_{Z}X \rightarrow {}^{A-4}_{Z-2}Y + {}^{4}_{2}\alpha, (6)$$

for alpha decay. While all decay sequences obey conservation laws, additional nuclear physics principles help to narrow down the possibilities:

Nuclei not listed in the atomic mass table

After considering all the 207 nuclei described in (4), nuclei not listed in the atomic mass table [26] (for example $^{230}_{76}Os$, $^{222}_{82}Pb$ and $^{206}_{93}Np$) are discarded resulting in only 101 nuclei. Sequences containing one or more parent-nucleus that generate daughter-nuclei not listed in the atomic mass table are also removed. As a result of this step, the valid pathways are reduced to 2,989.

Energy considerations

An important quantity related to nuclear reactions or decays is the reaction energy or Q-value.

Let us consider the hypothetical nuclear reaction,

$$A + B \rightarrow C + D. \quad (7)$$

From the law of energy conservation we can write

$$(m_A + m_B)c^2 + T_A + T_B = (m_C + m_D)c^2 + T_C + T_D, \quad (8)$$

where m_A, m_B, m_C and m_D are the masses of nuclei *A*, *B*, *C* and *D;* T_A, T_B, T_C and T_D are their respective kinetic energies, and *c* is the speed of light in vacuum. The difference between final and initial kinetic energies is defined as the reaction energy or *Q*-value,

$Q = T_C + T_D - T_A - T_B = (m_A + m_B - m_C - m_D)c^2.$ (9)

If $Q > 0$, the reaction if accompanied by a liberation of kinetic energy at the expense of the rest energy (exoergic reaction). On the other hand, if $Q < 0$ the reaction involves an increase in the rest energy at the expense of the kinetic energy (endoergic reaction). In this last case the process cannot happen spontaneously because it requires energy input. For example, polonium-210 does not spontaneously decay by beta emission:

$^{210}_{84}Po \rightarrow {}^{210}_{85}At + {}_{-1}^{0}\beta + \bar{\nu}_e, \qquad Q = -3.98$ MeV. (10)

In Figure 2 is shown the *Q*-values for the U-238 decay chain where the highest value is represented by the alpha emission of Po-214 (7.834 MeV), and the lowest value by the beta emission of Pb-210 (0.064 MeV). Elimination of nuclei that present a negative *Q*-value for beta and alpha emissions within the Fortran code resulted in a much lower quantity of right sequences, that is only 432 right pathways.

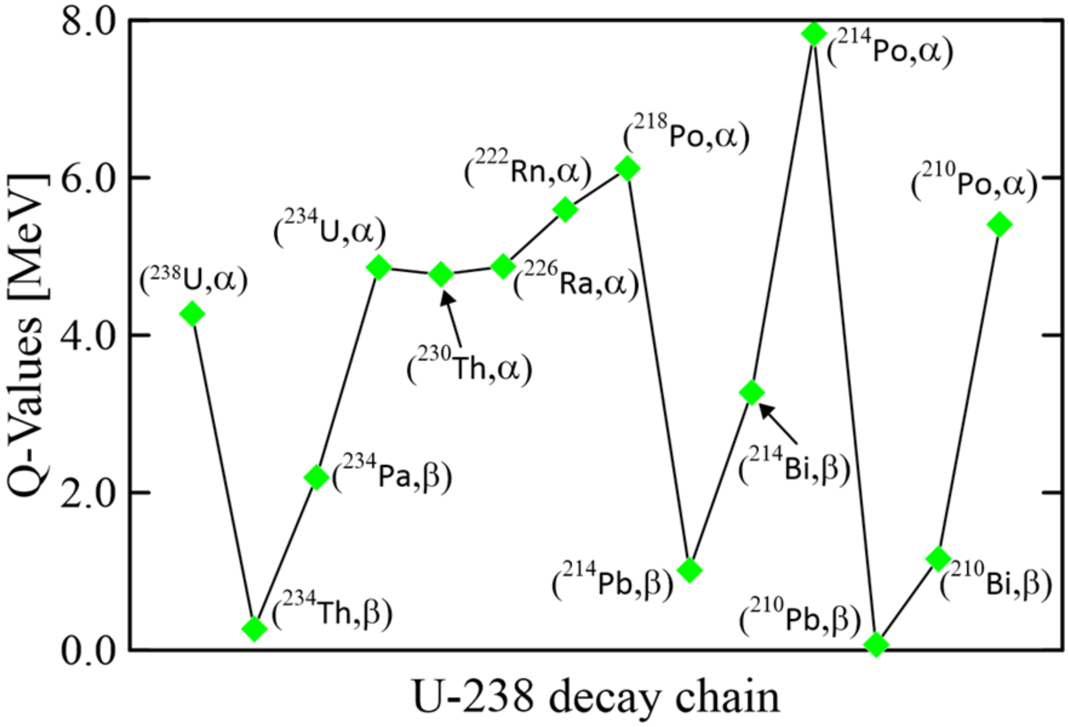

Figure 2. The Q-values for the nuclei of the uranium-238 decay series.

Nuclei with excess of neutrons

In a stable nucleus, the balance between neutrons and protons is crucial to maintaining nuclear stability. The strong nuclear force is the force that binds protons and neutrons together within the nucleus. This force is strong enough to overcome the electrostatic repulsion between the positively charged protons. However, the nuclear force is only effective over short distances, and it acts equally between proton-proton, neutron-neutron, and neutron-proton pairs. While neutrons help to reduce the electrostatic repulsion between protons, too many neutrons can lead to an imbalance. The increased neutron count can stretch the nucleus, reducing the effective range of the strong nuclear force, which weakens the overall binding of the nucleons.

When the number of neutrons significantly exceeds the number of protons, the nucleus becomes neutron-rich and energetically unstable. This neutron excess causes instability because the additional neutrons do not contribute to stabilizing the nucleus through the strong nuclear force but instead increase the overall energy of the system.

Neutrons do not experience the electrostatic repulsion that protons do, but when there are too many of them, the configuration of the nucleus becomes energetically unfavorable. The nucleus then has a higher total energy, making it unstable. In an attempt to achieve a lower energy state and restore balance, the nucleus will undergo beta-negative decay.

In neutron-rich nuclei, there is an increasing neutron-neutron interaction. While neutrons help provide extra binding to offset the proton-proton repulsion in stable nuclei, too many neutrons lead to a situation where their interactions do not sufficiently bind the nucleus. The Pauli exclusion principle also plays a role here, as adding more neutrons means placing them in higher energy states, making the nucleus less stable. Thus, the nucleus tries to reduce this excess energy and neutron-to-proton ratio by undergoing beta decay, converting a neutron into a proton to bring the nucleus closer to the valley of stability in the chart of nuclides.

In Figure 3 is displayed the number of neutrons as a function of the number of protons for the nuclei that may be formed in the U-238 series (lozenges) and the corresponding stable or longest-lived isotopes (circles). It can be seen that nuclei from Pt to Tl have an excess of neutrons and beta-negative emission predominates; on the other hand nuclei in the region U-Cf have a deficit of neutrons and do not undergo beta-negative emission, and all the other nuclei can decay via beta or alpha emission. Taking into consideration within the Fortran code that rich-neutron nuclei do not undergo alpha emission resulted in only 2 right sequences.

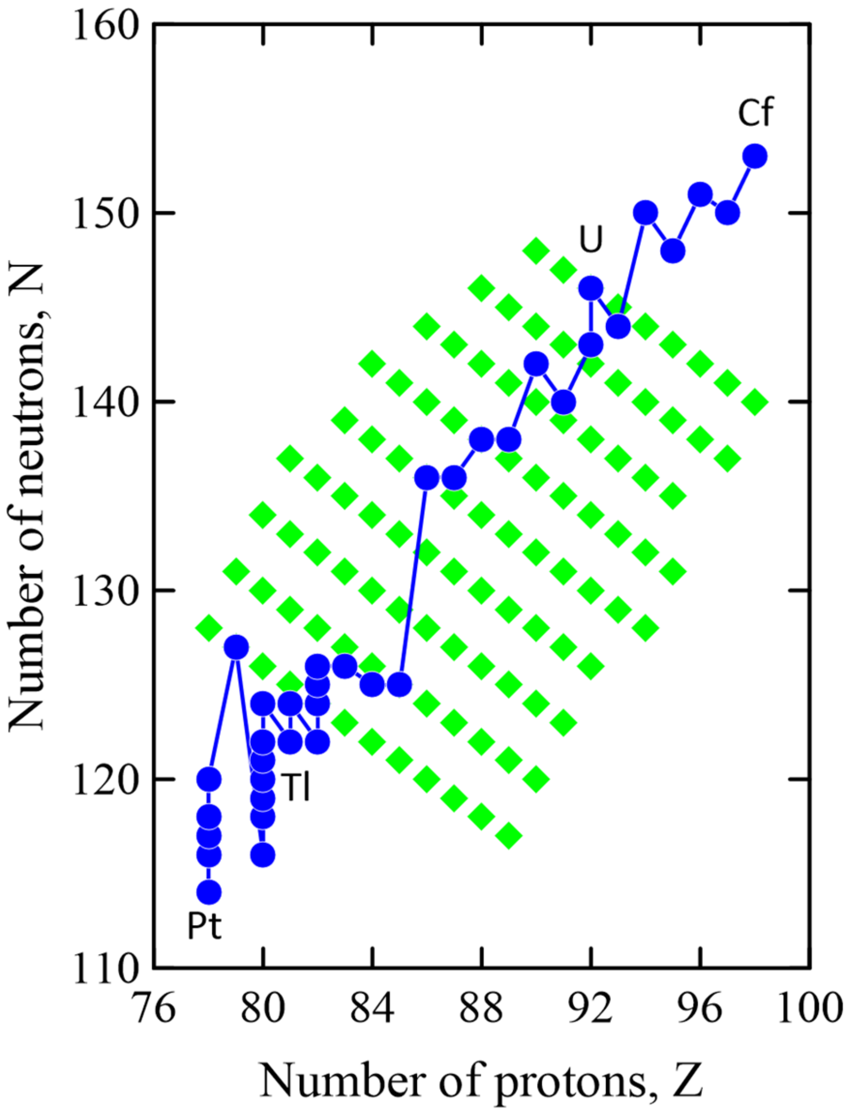

Figure 3. Number of neutrons versus number of protons for the nuclei that may be formed in the U-238 series (lozenges) and the corresponding stable or longest-lived isotopes (circles).

Lead isotopes

The magic number of protons (or neutrons) refers to specific numbers of nucleons that result in an exceptionally stable nuclear configuration. The magic number 82, for protons, is significant because nuclei with this number exhibit enhanced stability due to the complete filling of nuclear shells. Nucleons fill nuclear shells and when a shell is completely filled, the nucleus becomes more stable [15,16].

For nuclei with 82 protons, the proton energy levels in the nuclear potential are fully occupied. This complete filling results in a highly stable configuration that resists further decay. The element lead (Z = 82) has three stable isotopes: ^{206}Pb, ^{207}Pb, and ^{208}Pb. These are unusually stable compared to isotopes of elements with nearby proton numbers, and in particular the ^{208}Pb is doubly magic and is one of the most stable heavy nuclei. The thorium-232, uranium-235, and uranium-238 decay series all terminate at stable lead isotopes. This is because nuclei with 82 protons are particularly stable.

The magic number 82 for protons reflects the stability provided by a filled nuclear shell in the shell model. This configuration minimizes the nucleus's energy, making elements like lead highly stable. The presence of stable isotopes of lead and the termination of decay chains at Z = 82 highlight the importance of this magic number.

Taking into account the search for nuclear stability, the isotopes of thallium (Z = 81) decay by beta-negative emission, and the isotopes of polonium (Z = 84) decay by alpha emission, in both cases leading to isotopes of lead. Finally, when this information is inserted into the code resulted in the widely accepted U-238 decay scheme shown in Equation (1).

IV. Conclusion

The uranium-238 radioactive decay series is a crucial nuclear process with widespread applications across various fields. Through our Monte Carlo simulation of 3,003 potential decay sequences, we were able to identify the correct pathway. This study demonstrates the effectiveness of combining computational simulations with core nuclear physics principles.

In future work, incorporating decay constants and half-lives into the simulation will provide a more comprehensive understanding of the uranium-238 decay series. Additionally, exploring other radioactive decay series using similar methods may offer valuable insights into the behavior of different radioactive materials.

By utilizing Monte Carlo simulations and computational methods, this study models the complex decay pathways of U-238, revealing the multitude of potential decay sequences and enhancing our understanding of nuclear processes. Ultimately, these findings highlight the significance of the U-238 decay series in both theoretical research and practical applications, emphasizing its role in advancing diverse fields, from geochronology to cancer therapy.

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