A Nuclear Decay Chain Two Ways: ^{213}Bi

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Abstract

Atom counts are modeled as the result of radioactive decay for ^{213}Bi, an alpha particle-emitting medical isotope used in the treatment of leukemia and other cancers. Two models are implemented: a slower naive counting Monte Carlo method, as well as a faster Markov chain approach. We compare these models to theoretical expectations and find both to be largely consistent with theory and each other, though some interesting differences are noted, particularly in parameter sensitivity and the ability to keep track of alpha decays. Half-lives of radioisotopes are treated as parameters, and naive Monte Carlo, due to its random nature, is found to be more sensitive to hypothetical adjustments.

1 Introduction

Common helium nuclei, composed of two protons and two neutrons, are often referred to as *alpha particles* in medical contexts. These particles are prized in radioisotope applications like Targeted Radionuclide Therapy (TRNT) due to their short penetration depth (40-80 μm), minimizing damage to healthy tissue [1]. Due to helium's relative scarcity in the atmosphere, alpha particles are typically produced in reactors through the radioactive decay of heavier elements like bismuth-213 (^{213}Bi), whose decay chain is shown in Figure 1. Of the five isotopes pictured, only the top four are radioactive, and each has an associated timing value, or half-life τ, the time required for 50% of a sample of that radioisotope to decay.

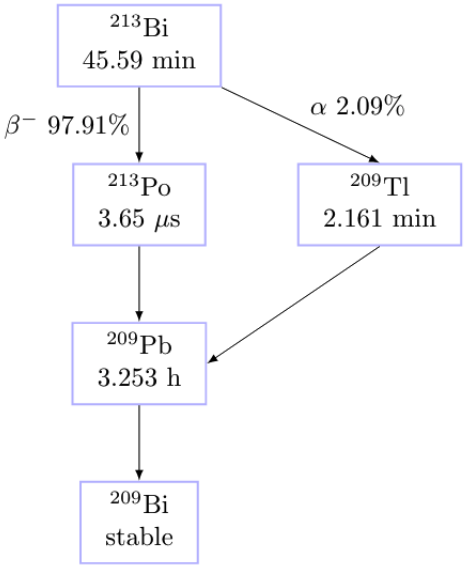

Figure 1: ^{213}Bi nuclear decay chain. Adapted from [1], [5], [6], [7], and [8].

^{213}Bi alpha-decays are relatively rare, as shown in Figure 1. So given the randomly spontaneous nature of radioactive decay, what would a starting sample of ^{213}Bi atoms look like after some time has passed? What would the final distribution of atoms look like? Could we count how many potentially life-saving alpha particles were produced?

2 Mathematical Background

Facts and results detailed in this section are paraphrased from Shultis and Faw [4].

In general, it's not possible to determine when any single nucleus will spontaneously decay. However, it is possible to observe and describe aggregate decay behavior in a sample of atoms. We can use continuous maths to model this discrete scenario. For a large sample of size N, in a small time interval Δt, some proportion of atoms ΔN will spontaneously decay. This suggests $\frac{\Delta N}{N}$ is the probability any one nucleus in the sample decays. It should be clear that as Δt gets smaller, so does the probability. This tiny decay probability approaches a constant λ defined

$$\lambda = \lim_{\Delta t \to 0} \frac{(\Delta N/N)}{\Delta t}.$$

This λ is called the *decay constant* and is unique to each radioactive isotope. Shultis and Faw interpret λ as the decay probability per infinitesimal time interval.

If we consider a sample of N radionuclides (atoms) with decay constant λ, $N(t)$ represents the expected or average number of atoms that ***have not*** decayed at time t. The probability any atom decays within an interval dt is λdt, and the expected number of decays occuring in dt at time t is $\lambda dt N(t)$. This number must equal the decrease $-dN$ in the number of atoms, so we write the differential equation

$$\begin{aligned} -dN &= \lambda N(t) dt \\ \frac{dN(t)}{dt} &= -\lambda N(t). \end{aligned} \tag{1}$$

So given a sample of radioactive atoms and a decay constant λ, we can compute how many undecayed atoms $N(t)$ should remain after time step t. The familiar solution to this differential equation can be written

$$N(t) = N_0 e^{-\lambda t}. \tag{2}$$

We will use this calculation to sanity-check our models later. Since the half-life τ of each radioisotope tells us when half the sample will have decayed, we can use this fact and (2) to solve for λ in terms of τ :

$$\begin{aligned} N(\tau) &= \frac{1}{2} N_0 = N_0 e^{-\lambda \tau} \\ \frac{1}{2} &= e^{-\lambda \tau} \implies \tau = \frac{ln2}{\lambda} \\ \lambda &= \frac{ln2}{\tau}. \end{aligned} \tag{3}$$

This relationship between τ and λ is especially useful. Since our differential equation solution specifies the number of undecayed atoms remaining at time t, the probability $\overline{P}(t)$ that any one nucleus ***doesn't*** decay within an interval of length t is

$$\overline{P}(t) = \frac{N(t)}{N_0} = e^{\lambda t}. \tag{4}$$

This means the complement $P(t)$, the probability any one nucleus *does* decay within the interval is 1 minus (4):

$$P(t) = 1 - \overline{P}(t) = 1 - e^{\lambda t}. \tag{5}$$

The decay chain diagram in Figure 1 gives us the half-life of each radioisotope, and since we know the relationship between τ and λ, we can compute λ and find a decay probability within a time-step of arbitrary length for each isotope. Now we have everything we need to describe our models.

3 Models

For both the naive Monte Carlo and Markov chain models, we start with 100,000 ^{213}Bi atoms and zero each of the other isotopes. Given the decay behavior implied by Figure 1, we count all five isotopes for 10,000 time steps of width $1s$ and return a final vector representing the distribution of atoms among the isotopes. These five atom counts are this paper's dependent variables. The radioisotope half-lives, τ_1, τ_2, τ_3 and τ_4, serve as model parameters.

3.1 Naive Counting Monte Carlo

A basic form of the naive counting Monte Carlo algorithm is described in Newman [3]; corresponding Julia [2] code can be found in file *decay_naive.jl*. The idea is to maintain a set of bins or vectors with which to count the isotopes, with one vector for each. For this paper 10,000 time steps are used, and so each isotope vector is of that size. The algorithm is "naive" in the sense that it is not efficient. A nested for loop is used, so the relatively slow running time is $O(n^2)$. We note it's a counting algorithm, so for this discrete scenario it counts total alpha decays, giving us an idea about how many α-particles might be available for treatment.

For each $1s$ time step, we append the current count of undecayed nuclei to each isotope vector. In the first time step, the vectors each have one entry: ^{213}Bi has 100,000 and the others have zero. For each isotope we determine randomly, based on probability formula (5) above, how many nuclei in the sample are expected to decay in that time step. We tally up decays within each step, decrementing and incrementing the current count for each isotope. The algorithm works from the bottom of the decay chain upward, first counting lead-209 (^{209}Pb) decays, then polonium-213 (^{213}Po), thallium-209 (^{209}Tl), and finally ^{213}Bi to avoid double-counting. A final vector of isotope counts is returned, and alpha particles (decays to ^{209}Tl) are also tallied and displayed.

Due to this algorithm's random nature, we anticipated the need to batch execute this procedure multiple times to produce more accurate final atom count vectors. These batch runs were collected in a dataframe and column means were returned.

3.2 Markov Chain

Markov chains are a natural choice for studying nuclear decay chains, as they're useful for keeping track of state transitions. For this paper we maintain five states, one for each isotope, modeled in the 5x5 transition matrix A shown below. The columns left-to-right and rows top-to-bottom represent the decay chain isotopes in this order: ^{213}Bi, ^{213}Po, ^{209}Tl, ^{209}Pb, and ^{209}Bi:

$$A = \begin{pmatrix} 1-dp4 & 0 & 0 & 0 & 0 \\ dp5 & 1-dp2 & 0 & 0 & 0 \\ dp6 & 0 & 1-dp3 & 0 & 0 \\ 0 & dp2 & dp3 & 1-dp1 & 0 \\ 0 & 0 & 0 & dp1 & 1 \end{pmatrix}.$$

Each entry of A is filled in terms of decay probabilities from column isotope to row isotope, computed with (5) according to Figure 1. For instance, note the lower-right entry 1. This represents the transition from ^{209}Bi to itself. Since we know ^{209}Bi is stable, there is no next state to move into, and thus this probability is 1. The same logic applies to the rest of the matrix. For four radioisotopes, we might expect only four decay probabilities are needed, but due to ^{213}Bi's decay paths two additional probabilities $dp5$ and $dp6$ are found in the first column. We compute these as joint with $dp4$, assuming independence of events. Each column in A adds to 1.

In a Markov chain model, advancing the clock 10,000 steps means exponentiation of matrix A. The initial counts of 100,000 ^{213}Bi atoms and zero for the others are represented as an initial state vector $\mathbf{x}_0 = [100000, 0, 0, 0, 0]$. Exponentiating matrix A 10,000 times and multiplying by the initial state vector yields a final isotope atom count vector $A^{10000}\mathbf{x}_0^T$. On current computer equipment, this calculation is fast, but we should note this isn't a counting algorithm, and so counting alpha particles is problematic and not attempted. This model's code is found in file *decay_markov.jl*.

4 Accuracy & Results

The solution (2) to our decay chain's differential equation (1) can be used to check model accuracy. Given ^{213}Bi's half-life of $\tau = 45.59 \cdot 60$ seconds, and its decay constant $\lambda \approx 0.00025339883766905944$, we find that $N(10000) = 7934.2$ undecayed ^{213}Bi atoms should remain in the sample at time $t = 10,000$.

First we look at the Markov chain, which returns final vector $\mathbf{u} = [7934, 2, 8, 61848, 30208]$. Note that for this particular setup this final vector never changes, since the Markov chain is deterministic. For ^{213}Bi in the first position, this result is spot on when compared to $N(10000)$, and the execution completes in less than 1 second. The Monte Carlo method is slower and not as accurate. One typical batch of 5 executions returns final vector $\mathbf{v} = [7976, 2, 8, 61812, 30226]$ in about 9 seconds. Let $\mathbf{x} = \mathbf{u} - \mathbf{v}$. The Euclidean norm, or magnitude of $\mathbf{x}$, defined

$$\|\mathbf{x}\| = \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2} \tag{6}$$

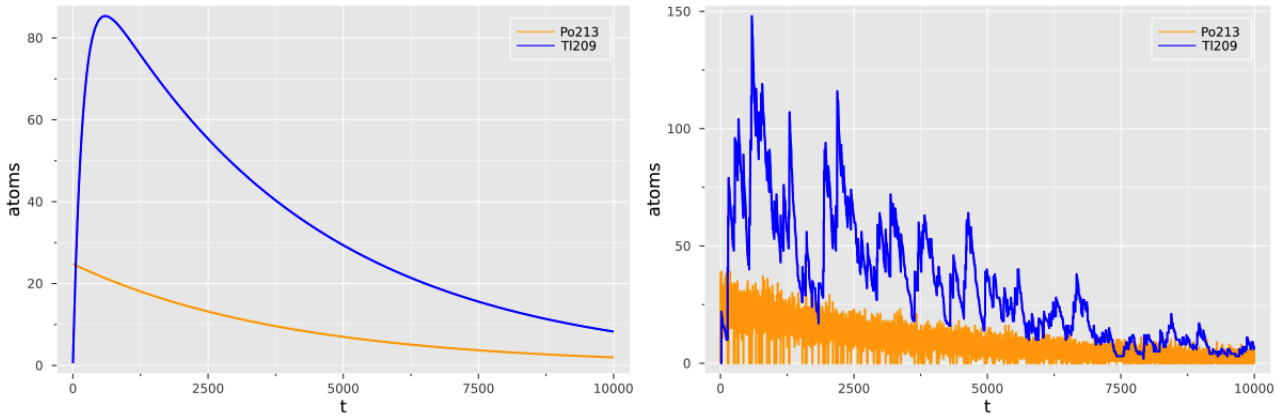

Figure 2: Atom counts for ^{213}Po and ^{209}Tl. Markov chain (left) and naive Monte Carlo (right).

can be used as a similarity score for **u** and **v**. A smaller score indicates more similar vectors, and by this measure, these 5 executions score 273.6. After 500 executions, the Monte Carlo method returns final vector $\mathbf{w} = [7938, 2, 8, 61853, 30199]$ for a similarity score of $\|\mathbf{u}\text{-}\mathbf{w}\| = 10.7$. Additional executions close the gap between vectors **u** and **v**! How many executions would it take for the Monte Carlo vector to converge on the Markov chain vector? Interestingly, after 5000 executions, the gap only closed a bit further, yielding a final vector $\mathbf{z} = [7938, 2, 8, 61852, 30201]$, for a similarity score of $\|\mathbf{u}\text{-}\mathbf{z}\| = 9$. A run of 10,000 executions gave us vector $[7936.0, 2.0, 8.0, 61848.0, 30205.0]$ and a similarity score of 3.6. This suggests the Monte Carlo vector will eventually converge on the Markov chain vector!

In terms of atom counts, the two models were largely consistent with each other. They also both closely matched the expected number of undecayed ^{213}Bi atoms given by solution equation (2), provided that the Monte Carlo method completes sufficient iterations to close the gap between final vectors. The final atom counts for ^{213}Bi, ^{209}Pb, and ^{209}Bi were so alike that the corresponding plots were visually identical, and for the sake of brevity we won't show them here.

Figure 2 highlights one aspect of the models' differing behavior. For isotopes ^{213}Po and ^{209}Tl, the Monte Carlo method on the right presents a much more erratic picture, due to the algorithm's randomness strategy. The scale of the graphs is also quite different, with the Monte Carlo method showing generally higher atom counts for both isotopes over 10,000 seconds. The Markov chain's smoothness is a result of the model's pre-set probabilities.

We kept track of alpha particles with the Monte Carlo method. Sets of 5, 10, and 100 executions yielded mean total alpha decays (particles) per run of 1911, 1955, and 1925 respectively. The Markov chain can't count alpha decays, but since the ^{209}Tl decay path has a probability of 2.09%, we might expect this to be a good estimate for the number of alphas available for medicine. However, the Monte Carlo method suggests there are fewer alpha decays than expected, closer to 1.9%. This discrepancy is likely an opportunity to dig deeper.

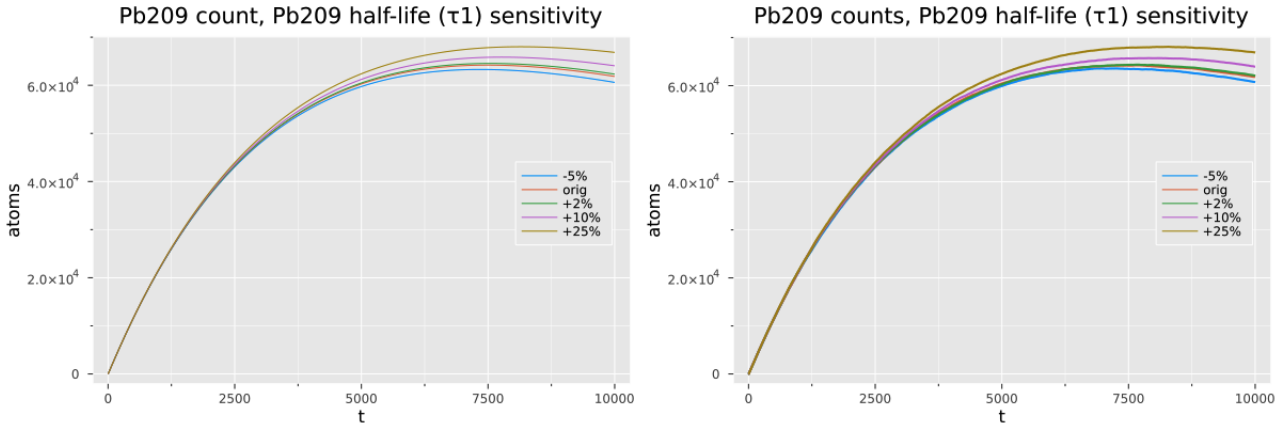

Figure 3: Sensitivity plots for ^{209}Pb atom counts. Markov chain (left) and naive Monte Carlo (right).

5 Sensitivity Analysis

5.1 Plots

All four τ half-life parameters were adjusted to visualize the effects of tuning on the models. In general, τ_2 and τ_3 (^{213}Po and ^{209}Tl half-lives) had no discernible effect on either model, for any of the atom counts. As such we only present plots for τ_1 (^{209}Pb) and τ_4 (^{213}Bi). For the atom counts of ^{213}Bi, ^{209}Pb, and ^{209}Bi, the models' sensitivity to changes in both τ_1 and τ_4 were indiscernible. Figure 3 illustrates this lack of sensitivity for ^{209}Pb and τ_1, and thus similar plots for ^{213}Bi and ^{209}Bi are omitted.

However, ^{213}Po and ^{209}Tl tell a different story. See Figures 4 and 5. For isotopes ^{213}Po and ^{209}Tl, the two models' sensitivity plots are wildly different. The Markov chain shows no sensitivity at all, yet the Monte Carlo model has it in heaps! Again we see scale differences in the plots, with those of Figure 5 about twice that of Figure 4. The shorter half-lives of these isotopes seem to amplify the effect of the Monte Carlo method's randomness! The Monte Carlo method is clearly more sensitive to changes in τ_1 than the Markov chain. For brevity, we omit plots that tell an identical story for τ_4.

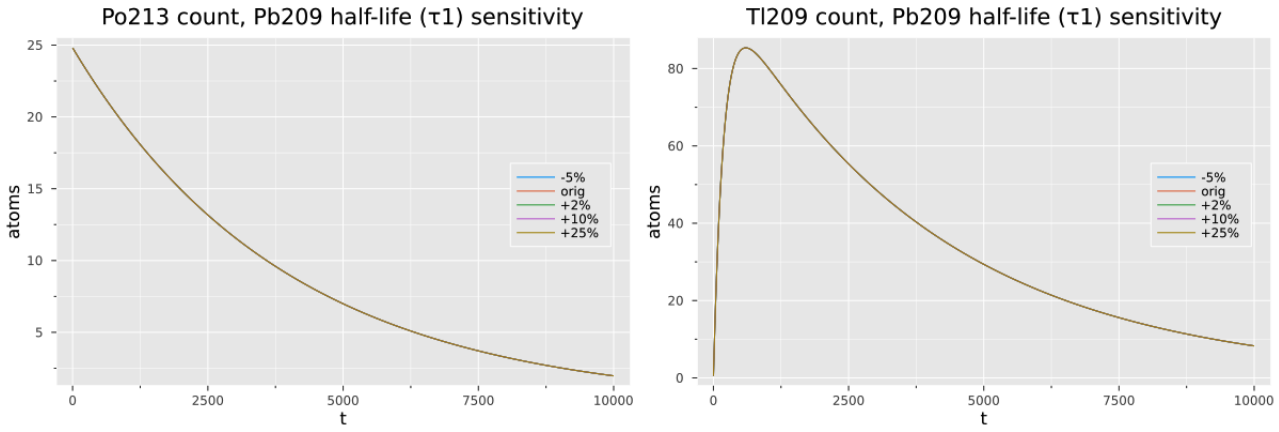

Figure 4: Markov chain sensitivity plots for ^{213}Po and ^{209}Tl, tuning parameter τ_1.

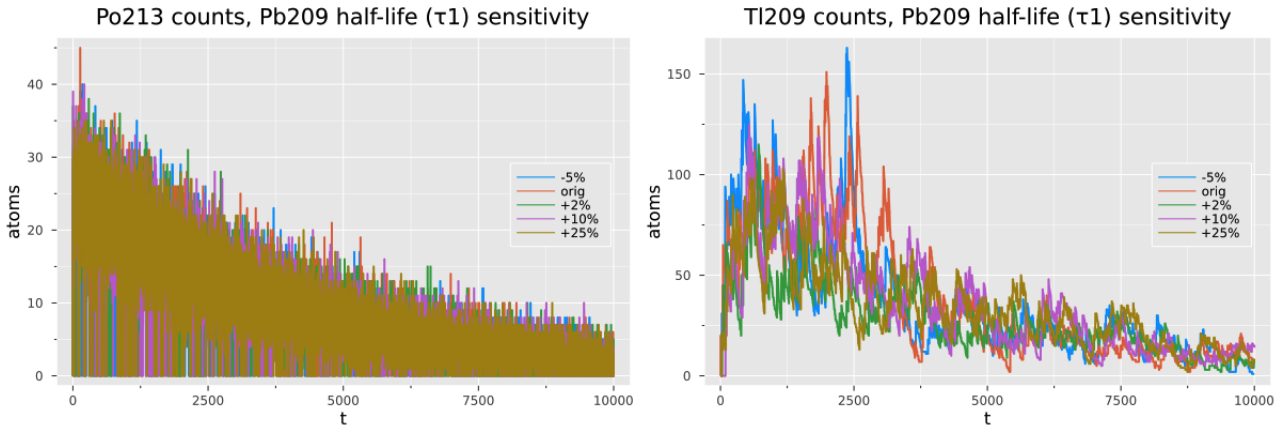

Figure 5: Naive Monte Carlo sensitivity plots for ^{213}Po and ^{209}Tl, tuning parameter τ_1.

5.2 Vector Similarity

As an additional measure of model sensitivity, we revisit the Euclidean norm as mentioned above (6). Table 1 shows test vector similarity scores for vectors returned by the models before and after parameter tuning. Lowest scores for each comparison are highlighted. Out of eight comparisons, the Markov chain model yields a lower score for five, and the Monte Carlo model yields lower scores for three. This suggests again that the Markov chain is less sensitive to parameter changes, since the test vectors produced are more similar to the original vectors in 5/8

cases. However, we note that for this comparison only single runs of the Monte Carlo method were used. A better comparison would be with test vectors produced by a large batch Monte Carlo run, but due to time constraints and increasing code complexity, this question will have to wait.

model	Δ	parameter	norm(orig-test)
Markov	-5%	τ_1	**1755.7**
Monte Carlo	-5%	τ_1	1851.4
Markov	-5%	τ_4	**1231.2**
Monte Carlo	-5%	τ_4	1243.4
Markov	+2%	τ_1	**664.7**
Monte Carlo	+2%	τ_1	1017.7
Markov	+2%	τ_4	500.3
Monte Carlo	+2%	τ_4	**437.8**
Markov	+10%	τ_1	**3132.5**
Monte Carlo	+10%	τ_1	3163.4
Markov	+10%	τ_4	2535.0
Monte Carlo	+10%	τ_4	**2292.4**
Markov	+25%	τ_1	7064.7
Monte Carlo	+25%	τ_1	**6816.6**
Markov	+25%	τ_4	**6431.2**
Monte Carlo	+25%	τ_4	6596.2

Table 1: Final vector similarity scores as a result of parameter tuning.

6 Conclusion

We've shown that both Monte Carlo and Markov chain methods are viable options for modeling radioisotope nuclear decay chains. The two models are broadly similar and consistent, though for the two most radioactive isotopes we studied, ^{213}Po and ^{209}Tl, the Monte Carlo method is much more sensitive to changes in half-life parameters τ_1 (^{209}Pb) and τ_4 (^{213}Bi). This is a discrete problem, so the Markov chain's continuous configuration prevents it from counting total alpha decays without some code modifications, but for this purpose the Monte Carlo method shines.

Further research should apply these same techniques to larger decay chains, such as those of Thorium and Uranium. Experimentation with the timestep width should also be pursued. Perhaps by combining other more complex decay chains with $1min$ or $1ms$ timesteps new interesting behavior will become apparent. Model-checking could also be expanded. We computed $N(t)$ for the isotope in the first position, ^{213}Bi, since that's the only non-zero atom count we have when we start. A strategy for checking the accuracy of the other isotope counts needs development, perhaps simply by starting with more non-zero atom counts or possibly re-sampling all isotopes during execution.

One odd thing about this project is the nature of the half-life parameters. By definition these don't change! But given how radioactivity works, it's difficult to imagine any other parameters that would affect this decay system. Perhaps half-lives and decay constants are different in some parallel universe.

References

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