The Analytical and Numerical Approximation of a Three-Component Decay Chain

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NPRE 247

Computer Project 1

October 21, 2018

Introduction and Analytical Solution

Three component decay chain is very important in nuclear physics. One of the reasons for its importance is the ^{135}Xe decay chain that tracks the decay and production of ^{135}Xe, often called a reactor poison due to its high cross-section [1]. The decay of ^{135}Xe looks like this three-component decay chain

$$^{135}_{54}Xe \rightarrow {}^{135}_{55}Cs \rightarrow {}^{135}_{56}Ba \tag{1}$$

The ability to understand three component decay chains also allows a nuclear engineer to understand all forms of decay and the rates at which they happen. An analytical solution to the three-component decay chain starts with the differential equations of each isotope

$$\frac{dN_1(t)}{dt} = -\lambda_1 N_1(t) \tag{2}$$

$$\frac{dN_2(t)}{dt} = -\lambda_2 N_2(t) + \lambda_1 N_1(t) \tag{3}$$

$$\frac{dN_3(t)}{dt} = \lambda_2 N_2(t) \tag{4}$$

Where λ is the decay constant of the reaction. The solution to (2), the decay of the parent, is simple with the knowledge that decay is exponential and the solution becomes

$$N_1(t) = N_1(0)e^{-\lambda_1 t} \tag{5}$$

Which is called the radioactive decay law. The solutions for (3) and (4), the production and decay of the first daughter and the growth of the (assumed stable) second daughter, follow a different solution called decay with production. The general form of decay with production looks like

$$N(t) = N_O e^{-\lambda t} + \int_0^t dt' Q(t') e^{(t-t')} \tag{6}$$

Where Q(t) is the rate of production of the isotope. If Q(t) has no time dependence and is instead a constant Q_o, the integral can be evaluated to give

$$N(t) = N_O e^{-\lambda t} + \frac{Q_O}{\lambda}[1 - e^{-\lambda t}] \tag{7}$$

If one applies this integration to (3) and (4), one obtains the decay and production of the first daughter and the production of the assumed stable second daughter, which take the form

$$N_2(t) = N_2(0)e^{-\lambda_2 t} + \frac{\lambda_1 N_1(0)}{\lambda_2 - \lambda_1}[e^{-\lambda_1 t} - e^{\lambda_2 t}] \tag{8}$$

$$N_3(t) = N_3(0) + N_2(0)[1 - e^{-\lambda_2 t}] + \frac{N_1(0)}{\lambda_2 - \lambda_1}[\lambda_2(1 - e^{-\lambda_1 t}) - \lambda_1(1 - e^{\lambda_2 t})] \tag{9}$$

Equations (5), (8), and (9) are the analytical solutions for the parent, first daughter, and second daughter respectively [2]. If one assumes that the daughters have no initial value, such as in the problem parameters, then any terms multiplied by $N_2(0)$ or $N_3(0)$ disappear. Their sums make up the analytical solution for the total, which should be constant.

Numerical Solution

There is another way to approximate the number of isotopes of each type in a decay chain that is less intensive and easier on processors. The numerical solution calculates the number of isotopes over specific jumps forward in time, instead of a calculation for each point in time. The numerical solution does this through forward differencing. Forward differencing comes from the concept of the slope of the function, specifically defining the slope as

$$\frac{N(t + \Delta t) - N(t)}{\Delta t} = \frac{dN(t)}{dt} \tag{10}$$

From this point, one can solve for $N(t+\Delta t)$ quite simply, giving

$$N(t + \Delta t) = \frac{dN(t)}{dt}\Delta t + N(t) \tag{11}$$

This is a forward difference. However, since the form of the derivative is known, the forward difference can be extremely generally written as

$$N(t + \Delta t) = \lambda N(t)\Delta t + N(t) \tag{12}$$

From here one would only need to plug in the correct N(t) and λ values to find the value of N(t) that is Δt away from one already known.

Problem 1

Description

The first problem is to plot the numerical solution of the first daughter for three different values of Δt: coarse, medium and fine. To start, the parameters say that both daughters are not present in the sample initially while the parent is initially at 100 atoms. The parameters also give half-lives of 1.1 hour and 9.2 hours to the parent and first daughter, which, in conjunction with the equation

$$\lambda = \frac{\ln(2)}{t_{1/2}} \tag{13}$$

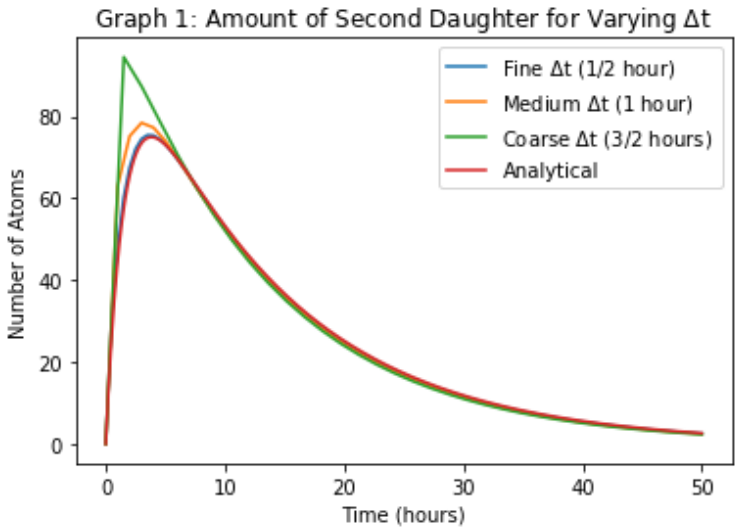
Gives λ values of .6301338005 1/h for the parent and .0753420848 1/h for the first daughter. These two lambda values and the initial amounts of the isotopes, when put into the numerical solution for the first daughter, gives the equation

$$N_2(t + \Delta t) = \Delta t \frac{\lambda_1 N_1(0)}{\lambda_2 - \lambda_1}\left[e^{-\lambda_1 t} - e^{\lambda_2 t}\right](\lambda_1 - \lambda_2) + \frac{\lambda_1 N_1(0)}{\lambda_2 - \lambda_1}[e^{-\lambda_1 t} - e^{\lambda_2 t}] \tag{14}$$

Which can then be graphed from the start time of 0 hours to the end time of 50 hours using varying values of Δt.

Results

For the three different values of Δt the values chosen were: ½ hours, 1 hour, and 3/2 hours. These values were chosen through testing and put into a python plot with the analytical solution to make Graph 1.



Discussion

As can be seen, the smaller the Δt value, the more accurate and precise the numerical solution is compared to the analytical. This can be seen most plainly in the graphs of the solutions with a coarse and fine Δt value, especially at the maximums. The coarse solution has the most incorrect maximum of about 93.52 atoms, which is about 26% off the analytical solution's maximum of about 74.94 atoms.[1] The fine solution, on the other hand, fits its description, and its maximum of about 75.46 is only 0.69% off the analytical solution's. All of the solutions are approximately similar near 0 hours and infinity, with the coarse solution showing the most variance from the analytical at 50 hours. In exact terms, the coarse solution is

[1]Note: due to the way the analytical solution was calculated in python, with np.arange(), it is technically also an approximation with a Δt of 1/60 hours, or 1 minute. However, this is precise enough to allow the analytical solution to be used as representative of the actual decay.

11.07% off the analytical solution at 50 hours. The medium solution is about 4% to 7% off the analytical across the whole graph. Interestingly, while the maximums of the numeric solutions were all higher than the analytical, the values at 50 hours were all lower. All of this leads a conclusion that the more time steps taken with less time in between leads to a more accurate solution.

Problem 2

Description

Problem 2 is to plot the numerical solutions of all the isotopes involved and their total from time 0 hours to an end time of 50 hours. The numerical solution for the first daughter is shown in equation 14, and the numerical solutions for the parent and second daughter come from combining equations 5 and 9 with equation 12, respectively. This gives

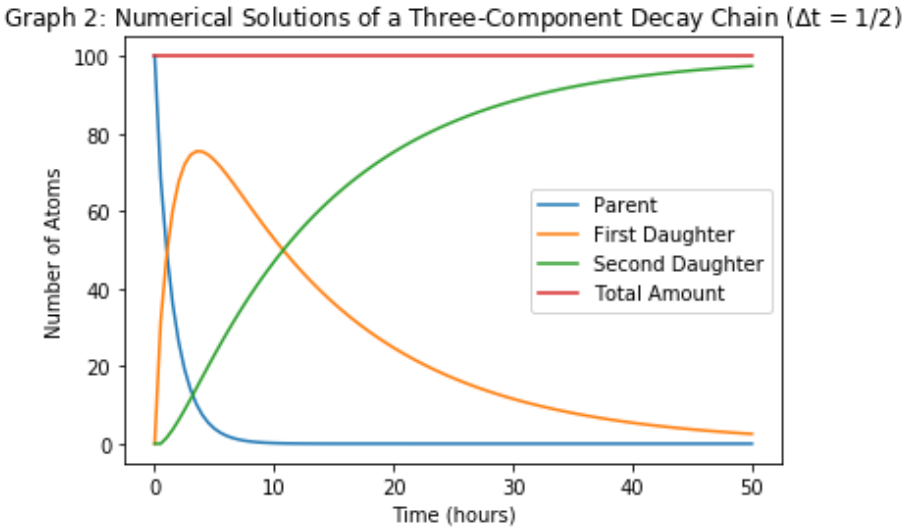
$$N_1(t+\Delta t) = \Delta t\left(-\lambda_1 N_1(0)e^{-\lambda_1 t}\right) + N_1(0)e^{-\lambda_1 t} \tag{15}$$

$$N_3(t+\Delta t) = \Delta t\left(\frac{\lambda_2\lambda_1 N_1(0)}{\lambda_2-\lambda_1}\left[e^{-\lambda_1 t} - e^{\lambda_2 t}\right]\right) + \frac{N_1(0)}{\lambda_2-\lambda_1}\left[\lambda_2(1-e^{-\lambda_1 t}) - \lambda_1(1-e^{\lambda_2 t})\right] \tag{16}$$

As the numerical solutions of the parent's decay and the second daughter's growth, which can be graphed from 0 to 50 hours with varying time steps like the first daughter. The total is the sum of all three solutions

Results

The Δt that was chosen for this problem was the fine Δt of 0.5 hours from problem 1 because the fine Δt value led to very little variance from the analytical solution as shown in problem 1. Plotting these four numerical solutions with fine time steps against their start and end times in python gives the graph of Graph 2 on the next page.



Discussion

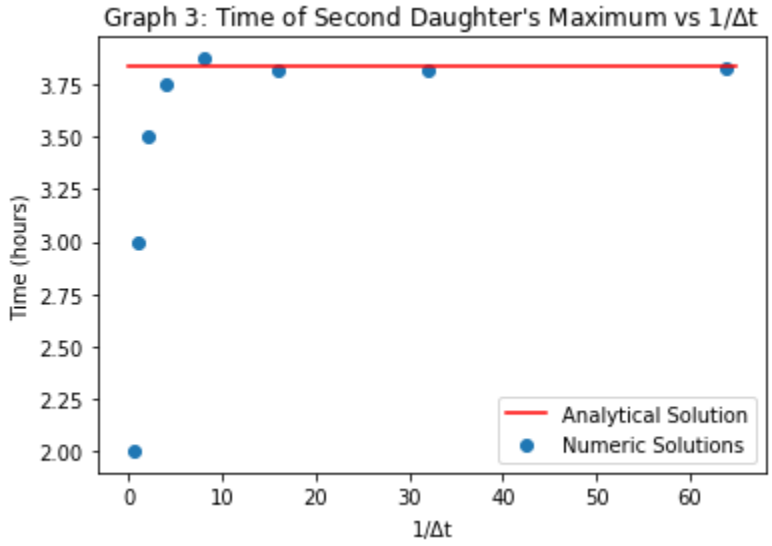
The parent goes through a simple exponential decay from 100 atoms to an asymptote of 0 atoms. This is in line with the exponential decay law and the initial conditions, the function reaches its halfway point around 1.1 hours. The second daughter increases to a maximum and then also decays exponentially to a lower bound of 0 atoms. As problem 1 showed, this is rather accurate to the actual growth and decay of first daughter. One can also see that the number of atoms is about half its maximum around 9.2 hours after it reaches its maximum, which fits the initial half-life. The second daughter, because it is stable, grows in a curve that starts exponential but becomes logarithmic to an upper bound of 100 atoms. The second daughter cannot grow beyond its bound for the same reason that the total amount is stable: the conservation of atoms. Since the number of atoms are conserved during a decay (not counting an α particle as an atom) the collective number of atoms of any isotope cannot exceed the initial amount, in this case, 100 atoms.

Problem 3

Description

The third problem was the times of the maximum solution of varying Δt values against the inverse of those Δt values and compare the times of the maximums to the analytical solution. This is similar to problem 1, but with a specific eye towards the maximum of the second daughter. The math, therefore, is practically identical but the coding is different, involving fetching the indices of maximums and multiplying them by their Δt values.

Results



The calculation started with a Δt of 1/64 hours, increasing multiplicatively by 2 until it reached a Δt of 2 hours. Any value of Δt higher than 2 was too similar to be feasibly distinguished from each other. Because the x-axis is 1/Δt, as one moves further along the x-axis, the Δt values decrease instead of increase.

Discussion

Much like the actual values of the maximums, the time at which they occur also becomes more accurate and precise as Δt is decreased. The vertical distance between maximum times decreases as Δt decreases, to the point of being barely noticeable. This speaks to the increasing accuracy of the solutions while the decreasing distance from the analytical solution's line speaks to increasing precision.[2] These results corroborate the conclusion from problem 1: the more time steps taken with less time in between leads to a more accurate solution.

[2] Again, the way the analytical solution was calculated in python is also an approximation, but it is an approximation with high accuracy and precision of its own.

References

[1] IAEA. 2004. “Physics and Kinetics of TRIGA Reactors”: 15-18. https://ansn.iaea.org/Common/documents/Training/TRIGA%20Reactors%20(Safety%20and%20Technology)/pdf/chapter2.pdf

[2] Shultis, J. Kenneth, Richard E. Faw. 2017. “Chapter 5: Radioactivity” *Fundamentals of Nuclear Science and Engineering Third Edition* : 97-131.