To: Dr. Palmtag

From: Grayson Gall

Subject: Forward Euler method applied to modeling a nuclear decay chain of length n

Date: September 17, 2021

Introduction

The purpose of this memo is present on overview of my application and implementation of the Forward Euler method in modeling an arbitrary nuclear decay chain. I was tasked with creating a user friendly program that will read input parameters from an input file to model the decay of an arbitrary number of nuclides in a decay chain with no additional source terms. However, my program does support additional constant source terms. The primary quantites we are interested in is the activity of the nuclides at some time t in our time domain. Additionally, my program utilizes the Richardson Extrapolation technique for estimating the error for a numerical solution where an analytic solution is unknown. I chose to implement my program in MATLAB because of its ease of use when handling matrices and plotting.

Theory

Analytic Solution

The nuclear decay of the first nuclide in a decay chain can be modeled by the differential equation

$$\frac{dN}{dt} = -\lambda N \tag{1}$$

And the decay of other nuclides in a decay chain can be modeled with similar decay equations

$$\frac{dN_i}{dt} = \lambda_{i-1} N_{i-1} - \lambda_i N_i \tag{2}$$

From equation two we can see that this is a highly coupled set of equations. For nuclides much lower in the decay chain the analytic solution depends on the solution of all the nuclides before it in the decay chain. Analytic solutions for the decay of these lower nuclides, while possible to derive is not trivial and for a decay chain of more than 3 or 4 nuclides becomes wholly impractical and inefficient.

Forward Euler Solution

Rather than solving for analytic solutions the Forward Eueler method discritizes the derivatives and then we solve for the decay of a nuclide one time step at a time. Each time step is a linear interpolation from the value at the previous time step. While it may not seem to make sense that we can approximate a smooth curve with a series of straight lines this approach is analogous to thinking about a circle as an infinitely sided polygon. After a certain number of sides or, in our case time steps, the series of straight lines begins to appear smooth and after a sufficiently large number of times there is little difference between the smooth curve and our model.

After we perform the discritization of our set of equations our governing equations in the forward Euler method with a uniform time step becomes

$$
\begin{bmatrix} N_1 \\ N_2 \\ N_3 \\ \vdots \\ N_i \end{bmatrix}^k = \begin{bmatrix} 1 - \lambda_1 \Delta t & 0 & 0 & \cdots & 0 \\ \lambda_1 \Delta t & 1 - \lambda_2 \Delta t & 0 & \cdots & 0 \\ 0 & \lambda_2 \Delta t & 1 - \lambda_3 \Delta t & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \lambda_{i-1} \Delta t & 1 - \lambda_i \Delta t \end{bmatrix} \begin{bmatrix} N_1 \\ N_2 \\ N_3 \\ \vdots \\ N_i \end{bmatrix}^{k-1} \tag{3}
$$

Where k denotes the kth time step

Note that the choice any given Δt does not guarantee that you will be able to find the number or number density for any given time of interest. To get around this issue I implemented a linear interpolation between the times surrounding the time of interest to get a more accurate answer for any arbitrary time within the time domain. This does, however, require at least one time step after the time of interest to execute. Though this should not matter very much as one or a few time steps after the time of interest will not significantly affect run times.

Error

This method while very simple to implement in MATLAB does carey some conditions for an accurate solution and is only a first order method which means that the magnitude of the error is directly proportional to our value of $\lambda \Delta t$ for each nuclide. And the largest error is thus proportional to the largest λ.

$$
\text{Absolute Error} \propto \lambda_{\max} \Delta t \tag{4}
$$

In the case of the first two or three nuclides in the decay chain the analytic solution is readily available so calculating the error for those is straight-forward we simply find the difference between the actual value and our calculated value at any given time.

$$
\text{Absolute Error} = |\text{Actual} - \text{Estimate}| \tag{5}
$$

However when there is not an analytic solution as readily available we need to use another method to estimate our error. I used the Richardson Extrapolation method.

Richardson Extrapolation

This method of error estimate requires at-least runs of the simulation using a time step of Δt and $\frac{\Delta t}{2}$. We then take the difference in the values of those two simulations and that difference will be an approximation of our error from the actual solution for the time step of $\frac{\Delta t}{2}$.

$$
\text{Error} \approx |N^{\Delta t} - N^{\Delta t/2}| \tag{6}
$$

And since we are primarily concerned with the numeric values of the activity of the nuclides in the decay chain the error we care about is for the activity so equation 6 becomes

$$
\text{Error} \approx \lambda |N^{\Delta t} - N^{\Delta t/2}| \tag{7}
$$

We can continue to do this calculation with different time steps until we have reached a time step with the required error. If we then take our error approximations and plot them with their respective time steps we should expect to see a linear relationship between time step and error.

Results

Nuclides A and B

Nuclide	Initial Number of Atoms	Half Life	Time Domain (hr)
A	3.6e10	10 hr	$0 \leq t \leq 50$
B	0	24 min	$0 \leq t \leq 50$

Table 1: Table of initial conditions for the nuclides

The first step after any piece of code is written is to test it to ensure that it is behaving in the expected manner. To do this I ran the forward Euler method for two nuclides, A and B, for 6 different time steps for a time domain from 0 to 50 hours. Plotting the results for each time step on a separate plot for both nuclide A and B. I then compared the activity at a time of 5 hours for each time step to the activity calculated analytically, created a power fit of the error to ensure a close to linear relationship. I then created a plot of the error and the fit. I also calculated fit and plotted the maximum absolute error for each time step. It is important to note that this is not the same as the error between the activities at 5 hours because the maximum error can occur at any point in the time domain.
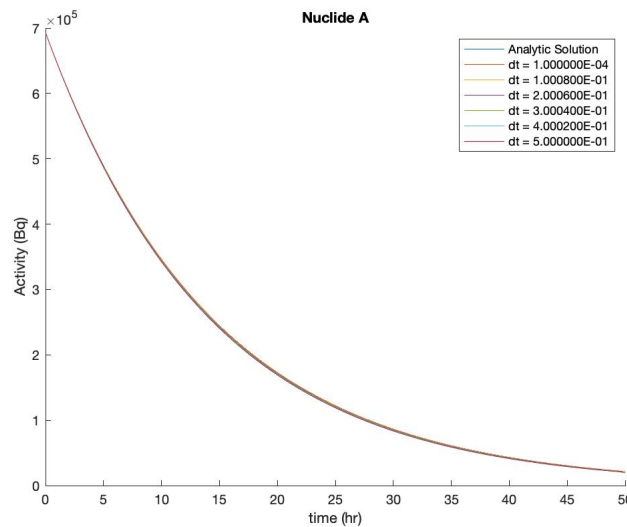

Figure 1: The activity of Nuclide A calculated over 6 different time steps
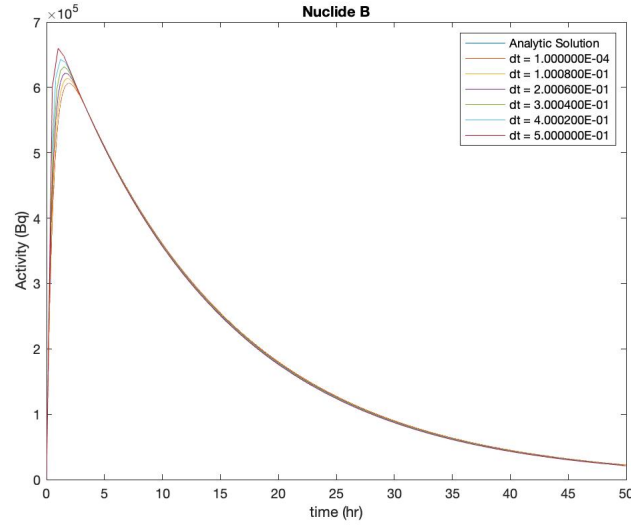
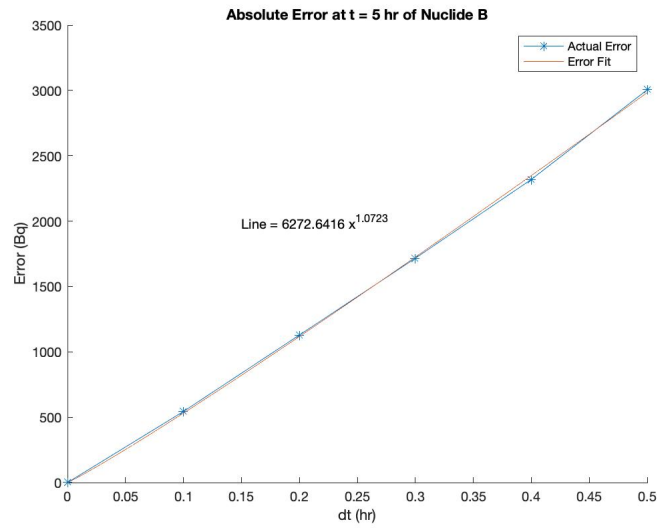Figure 2: The activity of Nuclide B calculated over 6 different time steps

Figure 3: The absolute error versus time step for Nuclide B at t = 5 hours

$$E(\Delta t) = 6272.6416\Delta t^{1.0723} \tag{8}$$
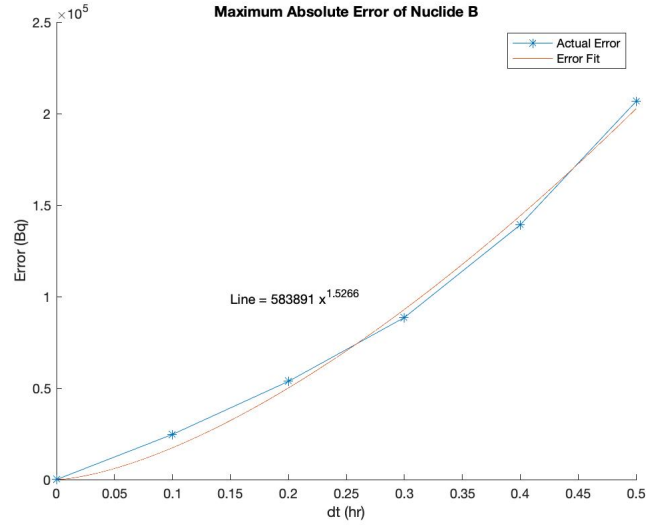
Equation for the absolute error at t = 5 hours

Figure 4: The maximum absolute error versus time step for Nuclide B

$$E_{\max}(\Delta t) = 583891\Delta t^{1.5266} \tag{9}$$

Equation for the maximum absolute error

Δt (hr)	Activity at t = 5 hr	Absolute Error at t = 5 hours	Maximum Absolute Error
0.5	5.074218e5 Bq	3.004662e3 Bq	2.067084e5 Bq
0.40002	5.081077e5 Bq	2.318751e3 Bq	1.391952e5 Bq
0.30004	5.087100e5 Bq	1.716484e3 Bq	8.853239e4 Bq
0.20006	5.092974e5 Bq	8.853239e4 Bq	5.365114e4 Bq
0.10008	5.098821e5 B1	5.365114e4 Bq	2.469157e4 Bq
1e-4	5.104260e5 Bq	5.196942e-1 Bq	2.291985e1 Bq
Analytic Solution	5.104265e5 Bq	0	0

Table 2: Activity of Nuclide B at t = 5 hours

Error Location (hr)	Δt needed (hr)
t = 5	1.289391e-3
$0 \le t \le 50$	2.441406e-4

Table 3: Time step needed for an error of 5 Bq

From figures 1 and 2 we can see that my implementation of the Forward Euler method is in very good agreement with the analytical solution. In figure 3 and equation 8 we can see that

the Forward Euler method follows a very near linear relationship, which is what we would expect to see.

However, when looking at the maximum absolute error we see a relationship closer to that of a quadratic equation. This most likely due to the shape of the decay of nuclide B. Since nuclide B has a sharp peak it will be harder for the Forward Euler method to resolve that portion of the curve and thus a smaller time step will be needed.

Case of 7 Nuclides

Nuclide	Initial Number of Atoms	Half Life (yr)	Time Domain (yr)
1	1.25e22	1e9	$0 \leq t \leq 10,000$
2	0	2	$0 \leq t \leq 10,000$
3	0	2	$0 \leq t \leq 10,000$
4	0	500	$0 \leq t \leq 10,000$
5	0	1000	$0 \leq t \leq 10,000$
6	0	1600	$0 \leq t \leq 10,000$
7	0	1	$0 \leq t \leq 10,000$

Table 4: Table of initial conditions for the nuclides

In order to ensure the accuracy of my solutions for the case of 7 nuclides I began by using the Richardson Extrapolation on the activity of nuclide 7 at the point t = 2000 yr. I started with an initial guess of a time step of 0.5 yr and continued to half it until i reached an error below 1 Bq. Using this I found that I needed a time step of 0.0625 yr to achieve this level of accuracy. See table 5 for the approximate error for every time step.

Δt (yr)	Activity at t = 2000 yr	Approximate Error (Bq)
0.5	4.746044e4 Bq	N/A
0.25	4.746320e4 Bq	2.761725 Bq
0.125	4.746458e4 Bq	1.380458 Bq
0.0625	4.746527e4 Bq	0.6901277 Bq

Table 5: Activities and Errors of Nuclide 7 at t = 2000 yr

I also used this data to create a line of best fit for the error of the simulation. From this fit we see that there is a nearly perfect linear relationship between time step and error.
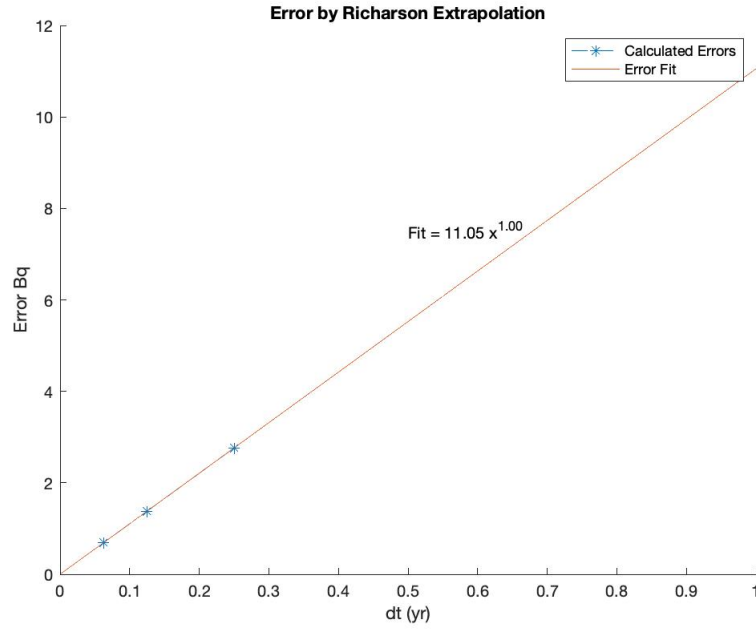
Figure 5: Plot of Error Approximation of Nuclide 7 at t = 2000 yr

$$E(\Delta t) = 11.05\Delta t^{1.00} \tag{10}$$

Equation for the approximate error of the activity of nuclide 7 at t = 2000 yr

After calculating the time step needed I ran the calculations for the entire 10,000 years, plotted the results and found the activity for each nuclide at t = 2000 yr. See apendix A for a plot of nuclide 3-7 on its own graph.
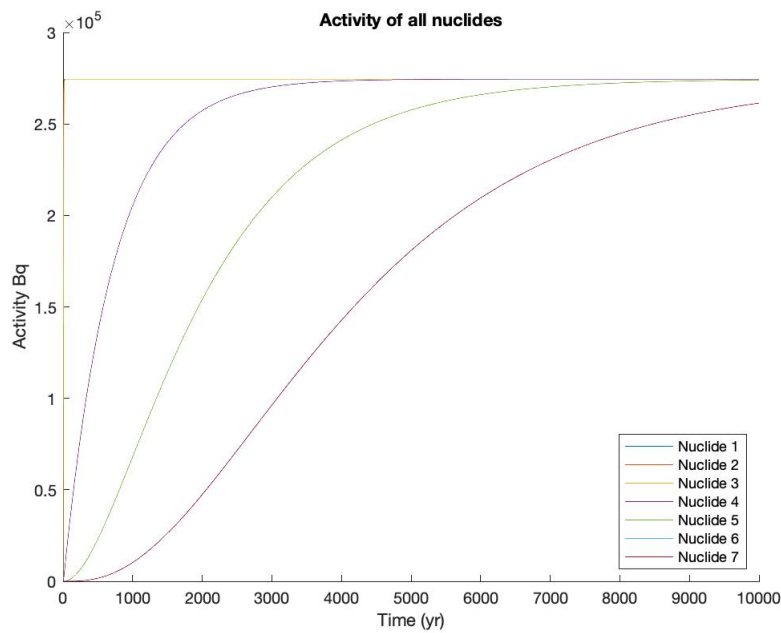

Figure 6: Plot of the activity of all 7 Nuclides

Additionally, on the individual plots of nuclide 1 and 2 I plotted the analytical solution and from there we can see excellent agreement
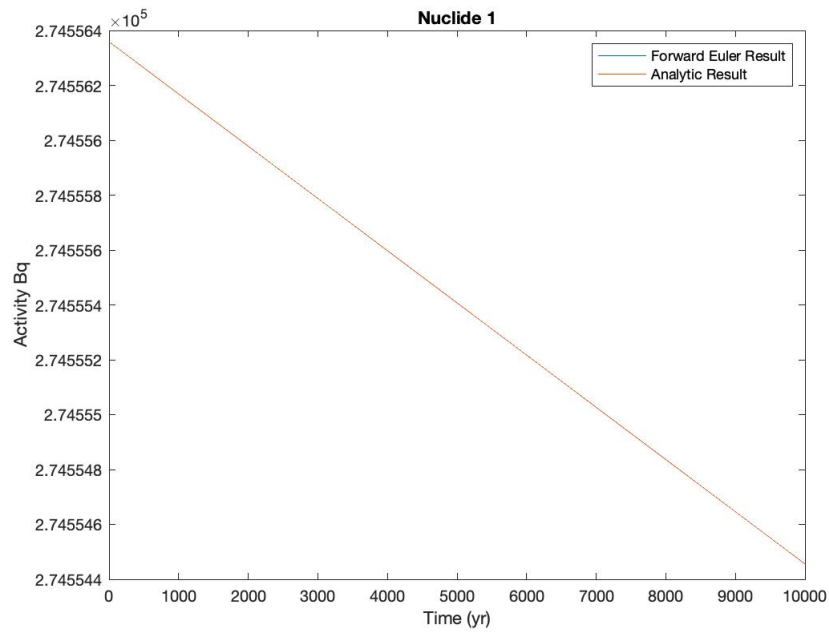
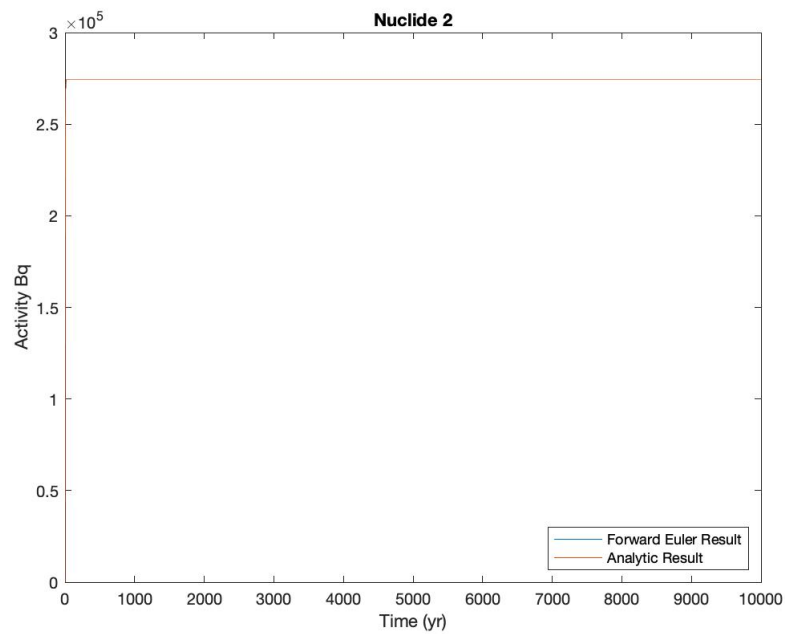Figure 7: Plot of the activity of N1 with analytic solution

Figure 8: Plot of the activity of N2 with analytic solution

Nuclide	Activity at t = 2000 yr (Bq)
1	2.745560e5
2	2.745560e5
3	2.745560e5
4	2.572603e5
5	1.540273e5
6	4.753181e4
7	4.746527e4

Table 6: Table of initial conditions for the nuclides

Finally, as another check for the error in my solutions I found the error between the activity of nuclide 1 and 2 and their respective analytic solutions at t = 2000 yr.

Nuclide	Error in Activity at t = 2000 yr (Bq)
1	3.945897e-7 Bq
2	3.950554e-7 Bq

Table 7: Table of Absolute Errors for Nuclide 1 and 2

This result also shows excellent accuracy with the time step selected by the Richardson Nicholson extrapolation.

The results also show the trends that we should expect for a decay chain that contains an extremely long lived head nuclide. The first 2 nuclides come into secular equilibrium very quickly. The third, forth and fifth will take slightly longer to reach secular equilibrium since they have slightly longer half-lives. Those longer half-lives prevent nuclide 7 from quickly coming into secular equilibrium with nuclide 1. We can also see that all of the nuclides are approaching the saturation activity. Since the first nuclide in the decay chain is so long lived the saturation activity is the initial activity of nuclide 1.

$$\text{Saturation Activity} = 2.745564e5 \text{ Bq}$$

Summary

While solving for an analytic solution is, at times a very good approach to solving a problem. There are cases when it will become impractical or even impossible to solve these kinds of problems analytically. This is where numerical methods come in and open so many doors for modeling and understanding the physical world. Additionally, when done well the application of a good a numerical method to a problem is not only accurate but also generalizable and re-usable. When writing code for a problem it is almost always best to write for an arbitrary case, one that can be applied over and over again to many different problems. This project has given me a great tool to use in future classes if I am faces with a similar problem. I also personally really enjoyed this project as it let me put the things I have learned in my CSC minor to good use to build reusable code and decrease user pre-formatting.

Future Work

While I did write my code to be generalized and it is if I were to expand upon this project in the future I would put all of the parts of the main script into an even cleaner and more digestible format for the average user. Some parts of the program in the post processing aspect are specific to this project but there are ways in which it could be improved and further generalized. My implementation of the Richardson error extrapolation technique for example is currently based on the error about a single point where as in the future I could base it off the root mean square error between the two time steps. This would take some effort to implement but I believe it would be a worth while addition to the code base. Other improvements could include an interactive UI for the user and further documentation.
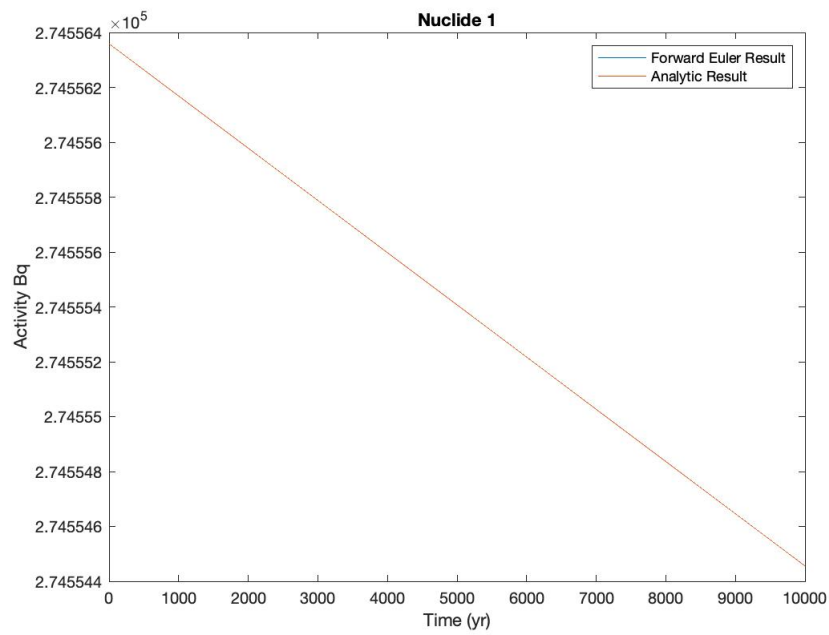
Appendix A

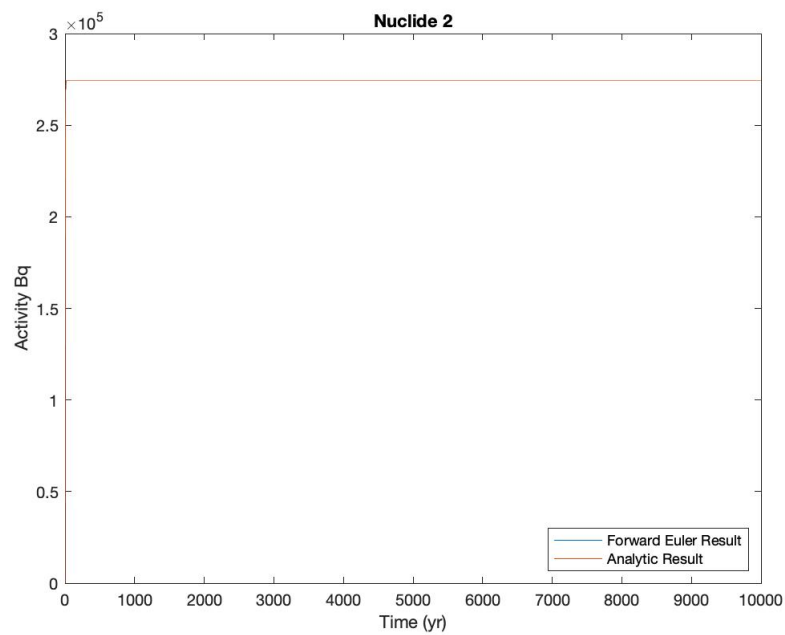Figure 9: Plot of the activity of N1 with analytic solution

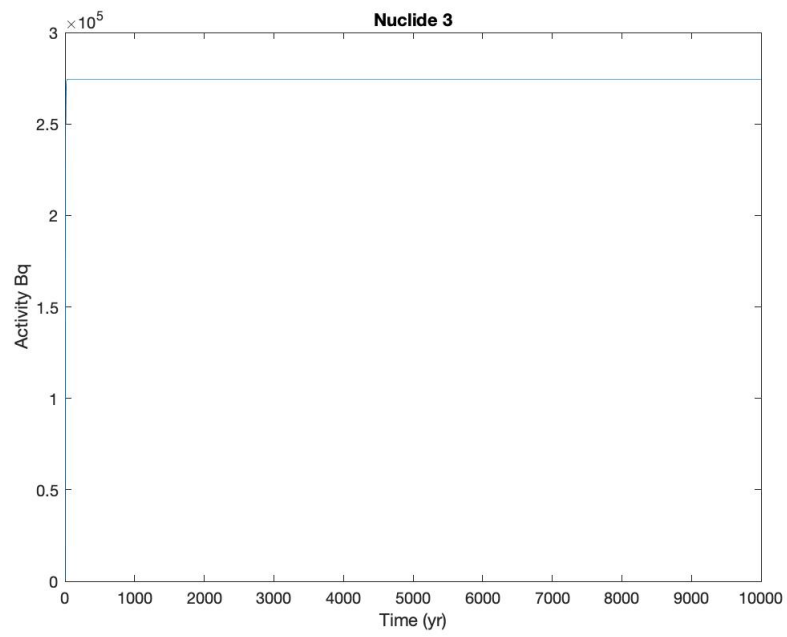Figure 10: Plot of the activity of N1 with analytic solution
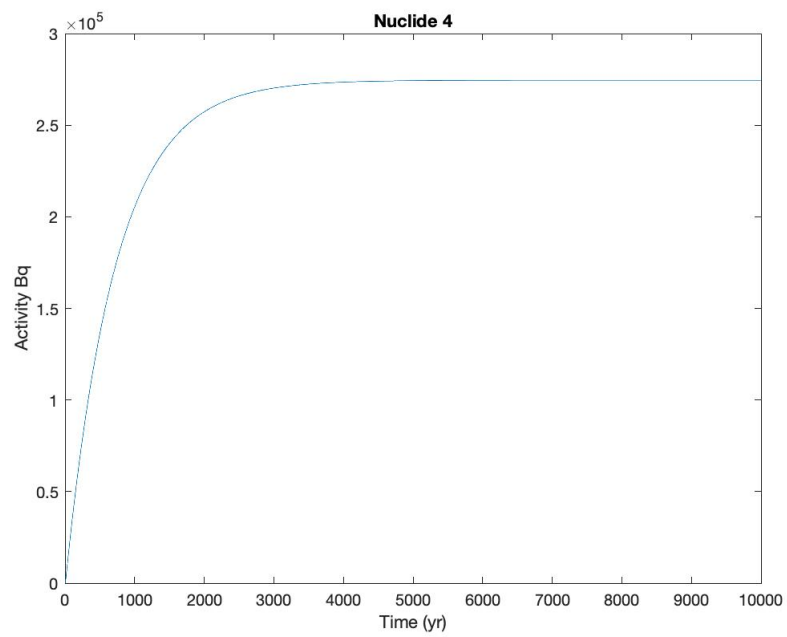
Figure 11: Plot of the activity of N3

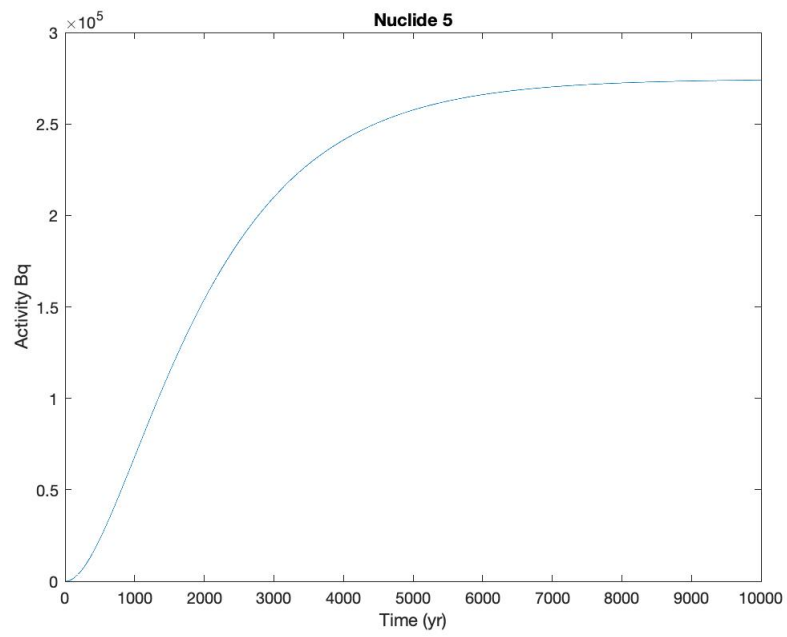Figure 12: Plot of the activity of N4

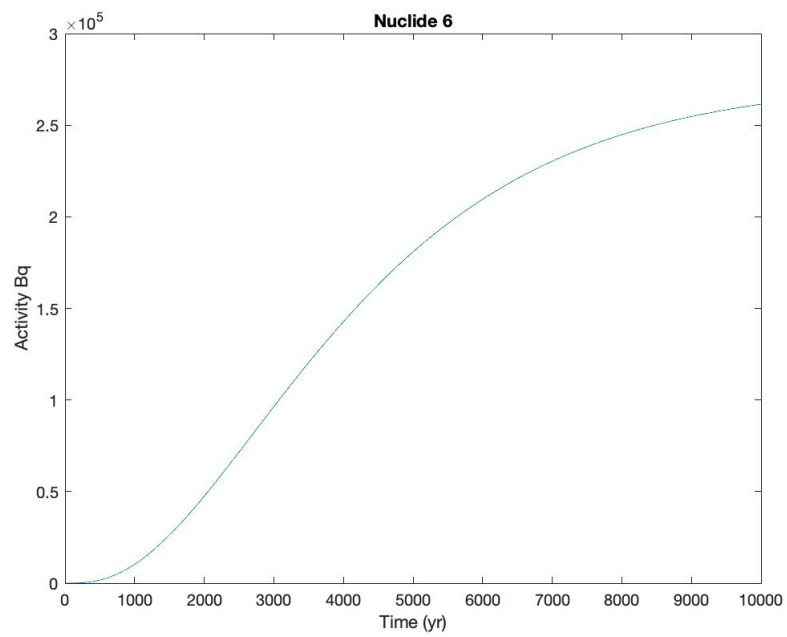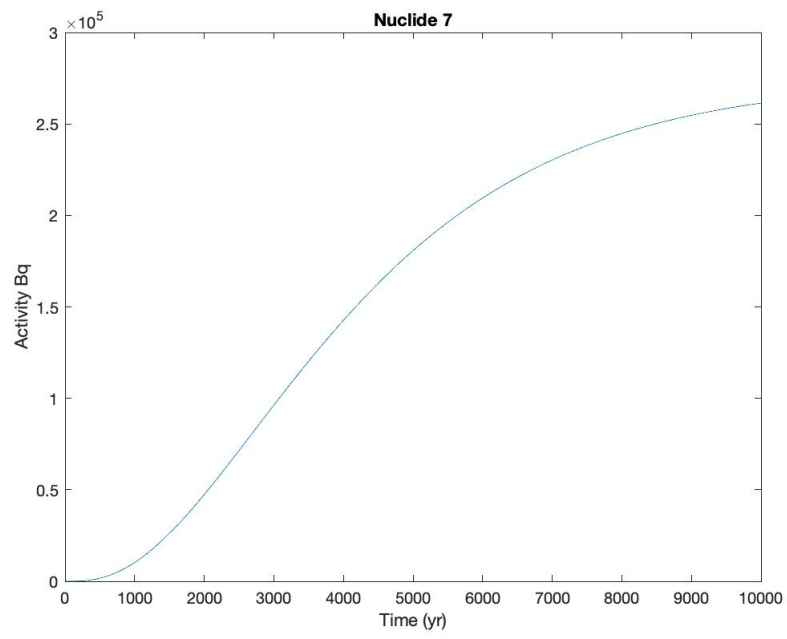Figure 13: Plot of the activity of N5

Figure 14: Plot of the activity of N6

Figure 15: Plot of the activity of N7