Simulation of Radioactive Decay

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1 Introduction

This report presents a numerical simulation of a three-state radioactive decay chain. The physical problem involves a parent nucleus (type 0) decaying into a daughter nucleus (type 1), which in turn decays into a stable nucleus (type 2). The decay processes are governed by first-order kinetics, characterized by decay constants λ_0 and λ_1. The system of differential equations describing the populations of the three types of nuclei ($N_0(t)$, $N_1(t)$, $N_2(t)$) is given by:

$$\frac{dN_0}{dt} = -\lambda_0 N_0 \tag{1}$$

$$\frac{dN_1}{dt} = \lambda_0 N_0 - \lambda_1 N_1 \tag{2}$$

$$\frac{dN_2}{dt} = \lambda_1 N_1 - \lambda_2 N_2 \tag{3}$$

We will solve this system numerically using an adaptive trapezoid method and compare the results with the analytical solution. We will also investigate the behavior of the numerical method for a stiff system, where the decay constants have vastly different magnitudes.

2 Numerical Method

The system of ODEs can be written in a vector form $\frac{d\mathbf{N}}{dt} = f(t, \mathbf{N})$, where $\mathbf{N} = [N_0, N_1, N_2]^T$. We use the trapezoid method. For a single step from t_n to $t_{n+1} = t_n + \Delta t$, the formula is:

$$\mathbf{N}_{n+1} = \mathbf{N}_n + \frac{\Delta t}{2}\left(f(t_n, \mathbf{N}_n) + f(t_{n+1}, \mathbf{N}_{n+1})\right) \tag{4}$$

Since the method is implicit, we need to solve a system of equations for $\mathbf{N}_{n+1}$ at each time step. In our implementation, we use Newton's method to solve this system iteratively.

To control the time step h, we use an adaptive algorithm. We perform one step of size Δt to get $\mathbf{N}_1$, and two steps of size $\Delta t/2$ to get $\mathbf{N}_2$. The difference between these two results gives an estimate of the local error:

$$\boldsymbol{\epsilon} = \frac{\mathbf{N}_2 - \mathbf{N}_1}{2^p - 1} \tag{5}$$

where $p = 2$ is the order of the trapezoid method. We then adjust the time step h to keep the maximum component of the error, ϵ_{max}, below a given tolerance TOL:

$$\Delta t_{new} = S \cdot h \left(\frac{TOL}{\epsilon_{max}}\right)^{\frac{1}{p+1}} \tag{6}$$

where S is a safety factor (typically close to 1).

3 Results

3.1 Non-stiff case

For the first simulation, we used the decay constants $\lambda_0 = 1$, $\lambda_1 = 5$, and $\lambda_2 = 50$. The initial conditions were $N_0(0) = 1$, $N_1(0) = 0$, $N_2(0) = 0$. The results are shown in Figure 1. The numerical solution shows excellent agreement with the analytical solution. Figure 2 shows how the time step changes during the simulation.

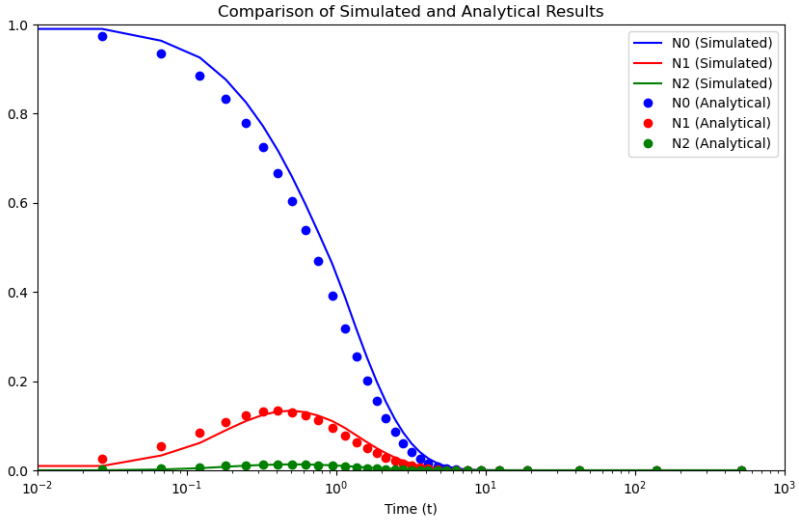

Figure 1: Comparison of simulated and analytical results for the non-stiff case.

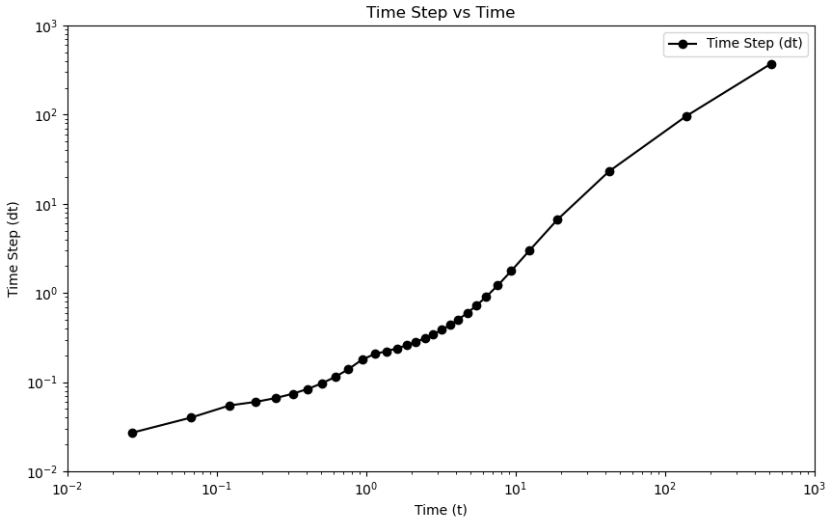

Figure 2: Time step as a function of time for the non-stiff case.

3.2 Stiff case

For the second simulation, we used a stiff set of decay constants: $\lambda_0 = 100$, $\lambda_1 = 1$, and $\lambda_2 = 0.01$. We ran the simulation with two different tolerances, $TOL = 10^{-6}$ and $TOL = 10^{-3}$. The results are shown in Figure 3.

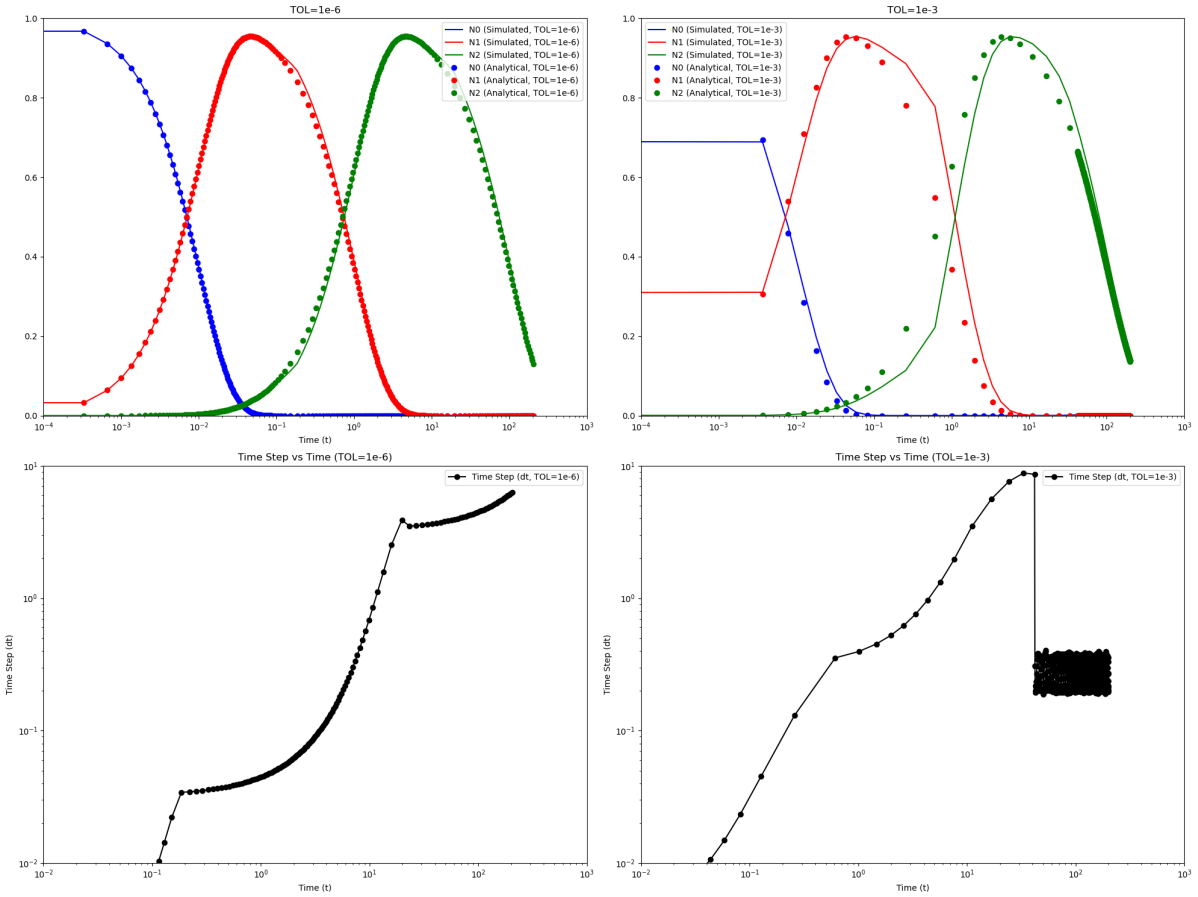

Figure 3: Comparison of simulated and analytical results for the stiff case with two different tolerances.

A striking discrepancy is observed between the time steps for the two tolerances. For $TOL = 10^{-6}$, the time step is initially very small and then increases. For $TOL = 10^{-3}$, the time step is larger. This is because of the stiffness of the system. The fast decay of N_0 (with $\lambda_0 = 100$) requires a very small time step at the beginning to accurately capture the dynamics.

To understand this better, let's analyze the behavior of $N_2(t)$. The analytical solution for $N_2(t)$ is a sum of three exponentials with different time scales. The initial rapid changes in N_0 and N_1 influence the initial value of dN_2/dt. Although N_2 itself changes slowly, the numerical method needs to resolve the fast dynamics of the other components to maintain the desired accuracy. With a stricter tolerance (10^{-6}), the adaptive algorithm is forced to use a very small time step to resolve the fastest time scale in the system, which is of the order of $1/\lambda_0 = 0.01$. With a looser tolerance (10^{-3}), the algorithm can take larger steps, effectively averaging over the fast oscillations.

4 Conclusions

In this project, we have successfully implemented an adaptive trapezoid method to solve the system of ODEs for a radioactive decay chain. The method proved to be accurate and efficient for both non-stiff and stiff systems.

The investigation of the stiff system highlighted the importance of adaptive time-stepping. The large disparity in decay constants leads to dynamics on very different time scales. An adaptive method can automatically adjust the time step to be small when the solution is changing rapidly and large when the solution is smooth. This allows for efficient and accurate simulations of stiff systems, which would be computationally expensive with a fixed-step method.

The comparison between the two tolerances for the stiff case showed that the choice of tolerance is crucial. A stricter tolerance forces the method to resolve all time scales, leading to a very small time step in the initial phase. A looser tolerance allows the method to step over the fast dynamics, which might be acceptable depending on the desired accuracy for the slowly varying components.

Overall, this project provided valuable insights into the numerical solution of ODEs, particularly the challenges and solutions for stiff systems. The implemented adaptive trapezoid method is a powerful tool for such problems.