Adaptive Trapezoidal Integration of Radioactive Decay Chain

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1 Introduction

The purpose of this work was to implement an adaptive implicit trapezoidal method to solve a stiff system describing a radioactive decay chain. The model consists of three isotopes that decay sequentially:

$$\frac{dN_0}{dt} = -\lambda_0 N_0,$$
$$\frac{dN_1}{dt} = \lambda_0 N_0 - \lambda_1 N_1,$$
$$\frac{dN_2}{dt} = \lambda_1 N_1 - \lambda_2 N_2.$$

The parameters λ_i are decay constants. Because some of them differ by several orders of magnitude, the system becomes *stiff*, requiring an implicit integration method for stability.

The adaptive time step adjusts Δt according to an error estimate based on step doubling, maintaining the local truncation error near a user-specified tolerance (TOL).

2 Numerical method

The implicit trapezoidal rule is given by

$$N_{k+1} = N_k + \frac{\Delta t}{2}\left[f(t_k, N_k) + f(t_{k+1}, N_{k+1})\right],$$

which is solved iteratively using Newton's method. The adaptive step-size controller compares one full step (Δt) with two half steps ($\Delta t/2$) and scales Δt by

$$\Delta t_{\text{new}} = \Delta t \cdot 0.9 \left(\frac{\text{TOL}}{\text{err}}\right)^{1/3},$$

where *err* is the estimated local error. Initial conditions were $N_0(0) = 1$, $N_1(0) = N_2(0) = 0$, $\Delta t_0 = 10^{-2}$, $t_{\max} = 200$.

3 Results

Case 1: $\lambda_0 = 1$**,** $\lambda_1 = 5$**,** $\lambda_2 = 50$**, TOL=**10^{-4}

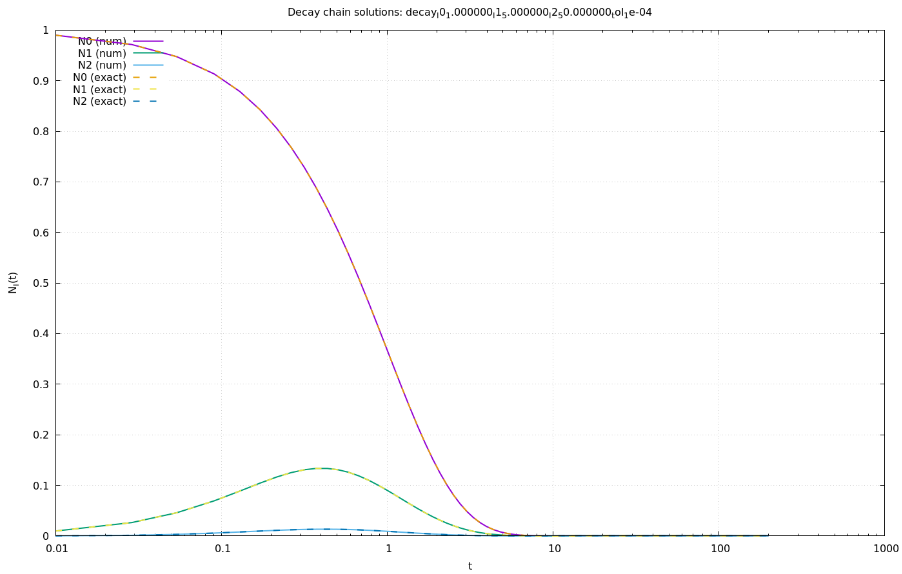

Figure 1: Numerical and analytical solutions $N_i(t)$ for $\lambda_0 = 1$, $\lambda_1 = 5$, $\lambda_2 = 50$, TOL=10^{-4}.

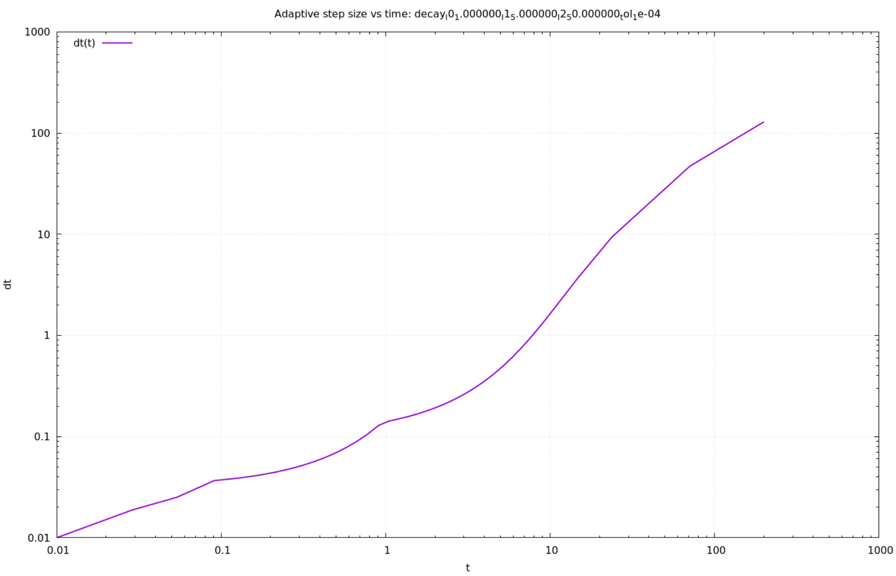

Figure 2: Adaptive time step $\Delta t(t)$ for the same parameters.

The numerical curves overlap the analytical ones almost perfectly, confirming high accuracy. The adaptive step begins small ($\Delta t \approx 10^{-2}$) while the fastest decay ($\lambda_2 = 50$) dominates, then increases as the rapid components vanish. This confirms that the adaptive scheme automatically chooses stable and efficient time steps.

Case 2: $\lambda_0 = 100$, $\lambda_1 = 1$, $\lambda_2 = 0.01$, **TOL**=10^{-6}

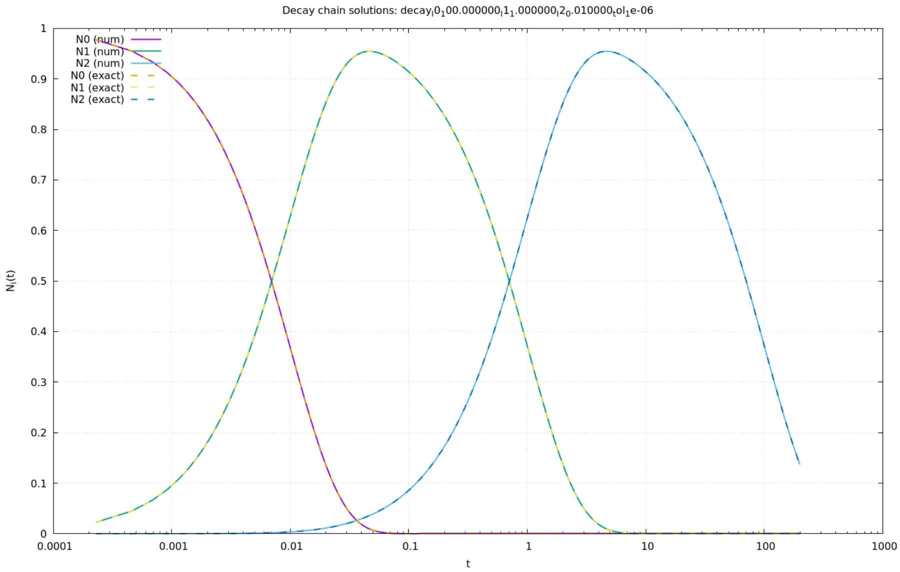

Figure 3: Solutions $N_i(t)$ for the stiff case with TOL=10^{-6}.

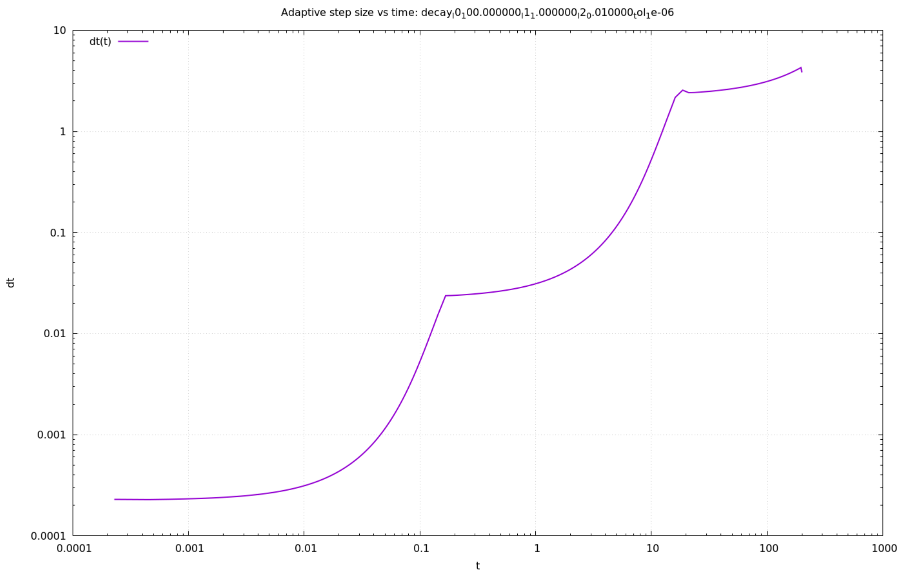

Figure 4: Adaptive time step history for TOL=10^{-6}.

The tighter tolerance maintains small Δt throughout the fast transient caused by $\lambda_0 = 100$, and again later when the slow decay of N_2 begins. The smallest step sizes ($\Delta t < 10^{-3}$) appear near $t \approx 10^{-2}$, when multiple decay rates interact.

Case 3: $\lambda_0 = 100$**,** $\lambda_1 = 1$**,** $\lambda_2 = 0.01$**, TOL=**10^{-3}

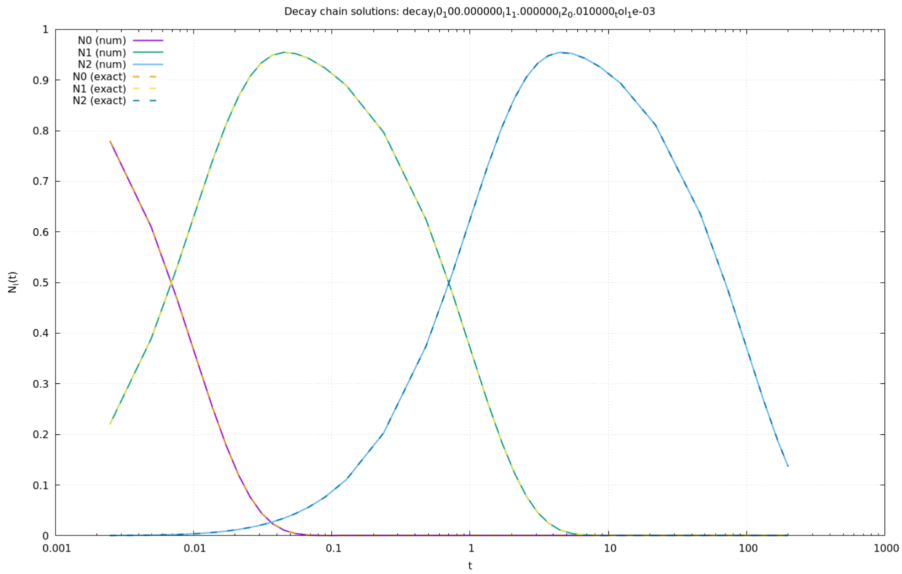

Figure 5: Solutions $N_i(t)$ for the stiff case with TOL=10^{-3}.

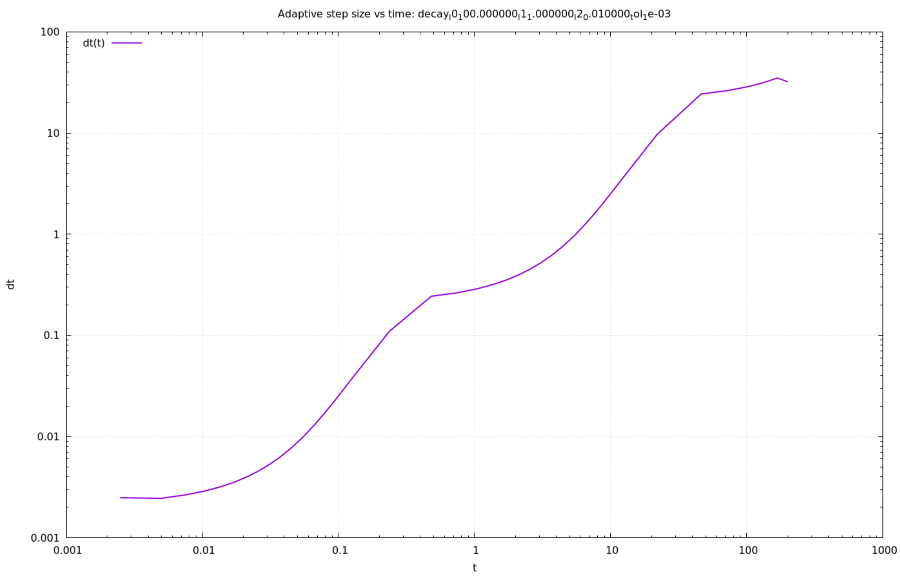

Figure 6: Adaptive time step history for TOL=10^{-3}.

The looser tolerance allows Δt to grow by nearly two orders of magnitude. While the main profiles of N_0 and N_1 remain accurate, $N_2(t)$ begins to deviate slightly for small magnitudes ($N_2 < 10^{-6}$). This demonstrates how the solver relaxes accuracy when local changes fall below the tolerance level.

4 Discussion

For the base case ($\lambda_0 = 1, \lambda_1 = 5, \lambda_2 = 50$) the adaptive method behaves smoothly and the computed Δt grows monotonically with time. In the stiff systems ($\lambda_0 = 100, \lambda_1 = 1, \lambda_2 = 0.01$), the step-size controller responds to strong stiffness: for TOL=10^{-6}, it keeps Δt very small during rapid transients and again reduces it when $N_2(t)$ becomes extremely small but nonzero. For TOL=10^{-3}, the solver allows much larger steps, skipping over those tiny changes.

The striking discrepancy between both $\Delta t(t)$ curves is linked to $N_2(t)$ values: when N_2 is close to zero, its derivative is still nonzero, making the local error estimator sensitive to tolerance. With tighter TOL, the solver resolves even the slow tail of N_2, while with loose TOL, it effectively ignores it. Hence, the adaptive method correctly balances efficiency and accuracy based on the requested precision.

5 Conclusion

The adaptive implicit trapezoidal integrator successfully handled both non-stiff and stiff decay chains. For $\lambda_0 = 1, \lambda_1 = 5, \lambda_2 = 50$, the numerical results perfectly matched the analytical ones. For the highly stiff case, the step-size controller automatically adjusted to the rapid and slow phases of the system. Comparison between TOL=10^{-6} and TOL=10^{-3} clearly showed that smaller tolerance enforces finer time resolution, especially when the last isotope $N_2(t)$ has very small values. Overall, the method demonstrated accuracy, stability, and automatic step-size control suitable for stiff ODEs.