COMPUTING PROJECT 1

NPRE 247

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Part 1

Theory

1.1) Show differential equations you are solving

The differential equations we are solving are the following:

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

Eq.1

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

Eq.2

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

Eq.3

These equations (Eq.1-3) are the general guesses for when N_1 and N_2 have relatively short half-lives compared to the half life of N_3. This assumption allows us to say that N_3 is stable and N_1 and N_2 are decaying with decay constants of λ_1 and λ_2 respectively.

1.2) Show analytic solutions of the differential equations

The following equations (Eq.4-6) are the solutions to the differential equations (Eq.1-3).

$$N_1(t) = N_{1,0} * \exp\left(-\lambda_1 * t\right)$$

Eq.4

$$N_2(t) = \frac{\lambda_1}{\lambda_2 - \lambda_1} * N_{1,0}[\exp(-\lambda_1 * \mathrm{t}) - \exp(\lambda_2 * \mathrm{t})]$$

Eq.5

$$N_3(t) = \frac{N_{1,0}}{\lambda_2 - \lambda_1} * [\lambda_2 * (1 - \exp(-\lambda_1 * \mathrm{t})) - \lambda_1 * (1 - \exp(\lambda_2 * \mathrm{t}))]$$

Eq.6

1.3) Show the complete derivation of numerical solution

The following equations (Eq.7-13) are the being done to generate the numerical solutions to the differential equations of decay (Eq.1-3).

$$\frac{df(x)}{dt} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

Eq.7

We can then apply this to the each differential equation (Eq.1-3) to generate the numerical integration technique.

Starting with $N_1(t)$ (Eq.1) and equating each expression (Eq.1 & Eq.7) we have for the rate of change of $N_1(t)$ we will get the following expression.

$$\frac{dN_1(t)}{dt} = \frac{N_1(t + dt) - N_1(t)}{dt} = -\lambda_1 * N_1(t)$$

Eq.8

We can then rearrange this equation (Eq.8) for $N_1(t + dt)$ to find the abundance of N_1 at the next dt in time.

$$N_1(t + dt) = -\lambda_1 * N_1(t) * dt + N_1(t)$$

Eq.9

Moving on to the expression for $N_2(t)$ (Eq.2), we can apply the same procedure as we did in Eq.8 to get the following.

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

Eq.10

Solving for $N_2(t + dt)$, we get the following.

$$N_2(t+dt) = \lambda_1 * N_1(t) * dt - \lambda_2 * N_2(t) * dt + N_2(t)$$

Eq.11

Finally, we can solve for $N_3(t)$ (Eq.3) by once again applying the same method as in Eq.8 to get the following.

$$\frac{dN_3(t)}{dt} = \frac{N_3(t+dt) - N_3(t)}{dt} = \lambda_2 * N_2(t)$$

Eq.12

Once again, solving this for $N_3(t + dt)$, we get the following solution to the next time step.

$$N_3(t+dt) = \lambda_2 * N_2(t) * dt + N_3(t)$$

Eq.13

The previous equations (Eq.8-13), lead us to find the solutions to the numerical integration to be Eq.9 for $N_1(t + dt)$, Eq.11 for $N_2(t + dt)$, and Eq.13 for $N_3(t + dt)$. These equations are easily implemented in code by applying the given initial conditions.

1.4) Show complete derivation for a time of maximum N_b.

We know that the maximum of a function is when the derivative is equal to 0. Using this information, we know that to find a maximum for N_b, we set Eq.2 equal to 0. The following equation is the application of this.

$$\frac{dN_2}{dt} = 0 = \lambda_1 * N_1(t) - \lambda_2 * N_2(t)$$

Eq.14

$$\lambda_1 * N_1(t) = \lambda_2 * N_2(t)$$

Eq.15

We can then substitute Eq.4 in for $N_1(t)$ and Eq.5 in for $N_2(t)$, which gives the following.

$$\lambda_1(N_{1,0} * \exp(-\lambda_1 * t)) = \lambda_2 \left(\frac{\lambda_1}{\lambda_2 - \lambda_1} * N_{1,0}[\exp(-\lambda_1 * \mathrm{t}) - \exp(\lambda_2 * \mathrm{t})]\right)$$

Eq.16

Dividing each side by λ_1 and $N_{1,0}$ gives...

$$\exp(-\lambda_1 * t) = \frac{\lambda_2}{\lambda_2 - \lambda_1}[\exp(-\lambda_1 * \mathrm{t}) - \exp(\lambda_2 * \mathrm{t})]$$

Grouping each term with a time dependence on one side.

$$\frac{\exp(-\lambda_1 * t)}{\exp(-\lambda_1 * \mathrm{t}) - \exp(\lambda_2 * \mathrm{t})} = \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

Eq.17

Factoring out an exp(-λ_1 * t) from the denominator allows us to simplify.

$$\frac{\exp(-\lambda_1 * t)}{\exp(-\lambda_1 * \mathrm{t})(1 - \frac{\exp(\lambda_2 * \mathrm{t})}{\exp(-\lambda_1 * \mathrm{t})})} = \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

Eq.18

$$\frac{1}{1 - \frac{\exp(\lambda_2 * \mathrm{t})}{\exp(-\lambda_1 * \mathrm{t})}} = \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

Eq.19

Applying exponent rules allows us to simplify.

$$\frac{1}{1 - \exp((\lambda_1 + \lambda_2) * \mathrm{t})} = \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

Eq.20

Solving this for (1 – exp((λ_1 + λ_2)*t).

$$1 - \exp((\lambda_1 + \lambda_2) * \mathrm{t}) = \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

Eq.21

Further solving this for $\exp((\lambda_1 + \lambda_2)*t)$.

$$\exp((\lambda_1 + \lambda_2) * \mathrm{t}) = 1 - \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

Eq.22

Combining the right side to give us a single fraction.

$$\exp((\lambda_1 + \lambda_2) * \mathrm{t}) = \frac{\lambda_2 - \lambda_1}{\lambda_2 - \lambda_1} - \frac{\lambda_2}{\lambda_2 - \lambda_1}$$

Eq.23

Simplifying.

$$\exp((\lambda_1 + \lambda_2) * \mathrm{t}) = \frac{-\lambda_1}{\lambda_2 - \lambda_1}$$

Eq.24

Taking the natural log of both sides.

$$(\lambda_1 + \lambda_2) * t = \ln\left(\frac{-\lambda_1}{\lambda_2 - \lambda_1}\right)$$

Eq.25

Solving for t.

$$t = \frac{\ln\left(\frac{-\lambda_1}{\lambda_2 - \lambda_1}\right)}{(\lambda_1 + \lambda_2)}$$

Eq.26

This answer for time in Eq.26 gives us the expression for the maximum abundance of N_b.

Part 2

Results

Given Parameters:

$T_{A,1/2}$ = 2.53 hours

$T_{B,1/2}$ = 11.05 hours

$T_{C,1/2}$ = ∞ hours

$N_{A,0}$ = 100

$N_{B,0}$ = 0

$N_{C,0}$ = 0

T_{final} = 60 hours

2.1) Plot the numerical solution for $N_b(t)$ vs. time for 3 different values of Δt (coarse, medium, fine), all of them on the same graph. Add the analytical solution on the same graph.

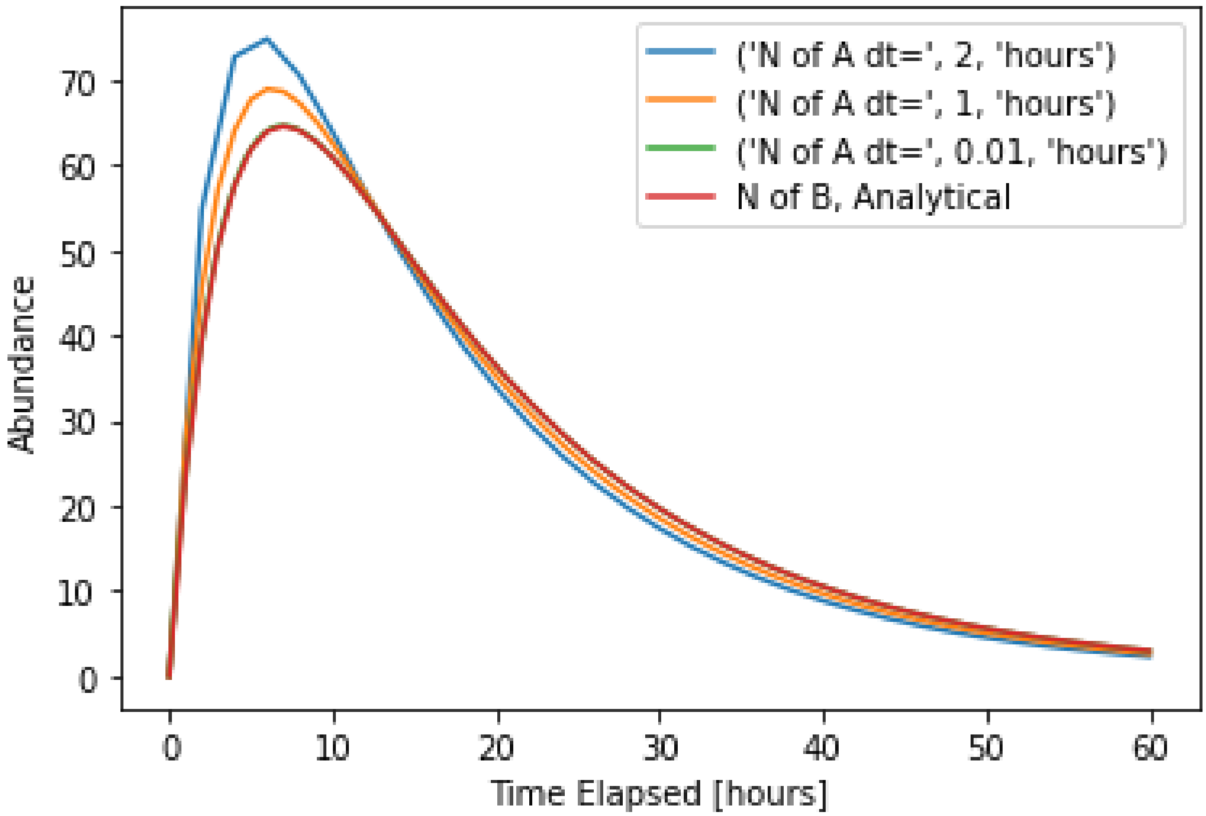

Figure 1: Graph of fine, medium, and coarse time steps for the numerical solution for N_b.

The results for Figure 1 are:

Abundance of NB after 60 hours with time step of 2 hours : 2.3246903954844282

Abundance of NB after 60 hours with time step of 1 hours : 2.6598318332152235

Abundance of NB after 60 hours with time step of 0.01 hours : 3.0050829379983575

Abundance of NB using the analytical solution : 3.008633669657686

Figure 1 has the fine, medium, and coarse dt time steps corresponding to .01 hours, 1 hour(initial dt), and 2 hours respectively. As can be seen on the graph, you cannot see where the line representing the fine dt time step (.01 hours). The time steps are so fine that the graph of the numerical solution is almost the same as the analytical solution.

It also makes sense that the highest point of the coarser time steps are higher than the analytical because they carry a higher slope for longer. This logic also applies to the lowest points where the higher negative slopes are carried for longer.

2.2) Plot numerical $N_A(t)$, $N_B(t)$, $N_C(t)$, and $N_A(t) + N_B(t) + N_C(t)$ as a function of time, all on the same graph, use a Δt that gives reliable solution.

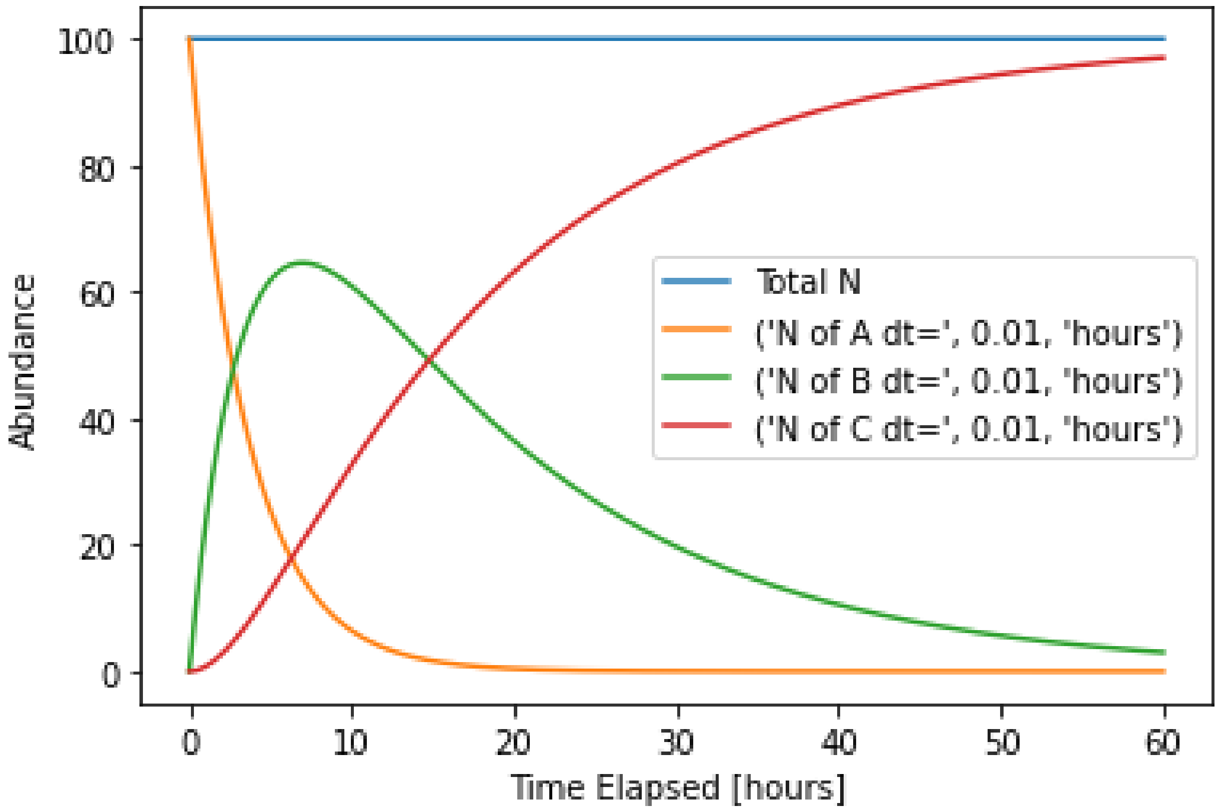

Figure 2: Graph of $N_A(t)$, $N_B(t)$, $N_C(t)$, and $N_A(t) + N_B(t) + N_C(t)$ vs. the elapsed time.

The results for Figure 2 are:

Abundance of NA after 60 hours with time step of 0.01 hours : 7.09825092701182e-06

Abundance of NB after 60 hours with time step of 0.01 hours : 3.0050829379983575

Abundance of NC after 60 hours with time step of 0.01 hours : 96.99490996375067

Abundance of NT after 60 hours with time step of 0.01 hours : 99.99999999999996

This is close to the analytical solution of:

Abundance of A after 60 hours has passed: 7.26020225449677e-6

Abundance of B after 60 hours has passed: 3.00863366965769

Abundance of C after 60 hours has passed: 96.9913590701401

Abundance of total after 60 hours has passed: 100

Figure 2 shows how each of the products decay as a function of time. Something notable is that the total N(t) is the same over time, which makes sense because one N_A decays to one N_B which decays to one N_C. Thus, the total over time is constant.

2.3) Using the numerical solution, plot the time of maximum NB vs. 1 Δt for several different Δt. Use the analytical solution to determine time of maximum NB, and add that value to the graph.

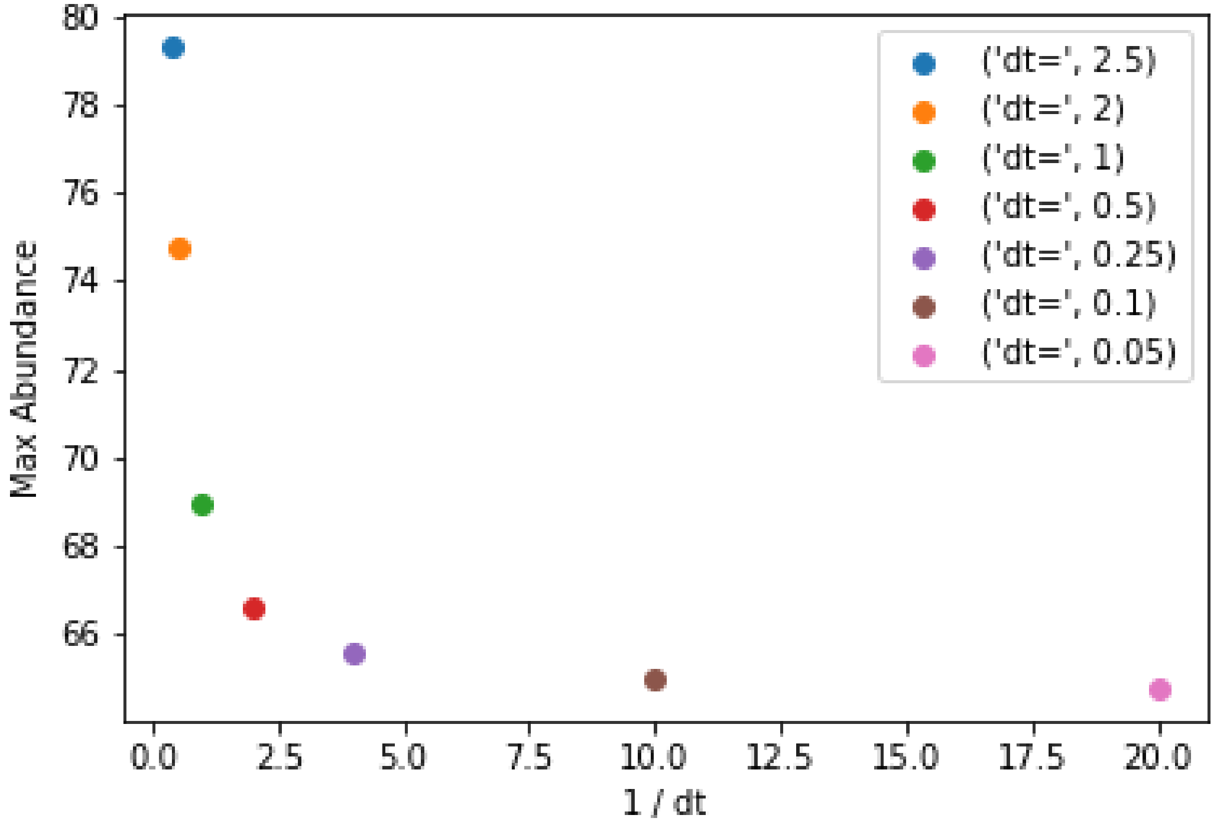

Figure 3: Plot of Max Abundance of N_B vs 1 / dt with varyingly fine dts.

Figure 3 shows that the graph of Max Abundance vs 1 / dt exponential decays to an asymptote of the analytical max abundance of N_b.