

COMPUTING PROJECT 1

NPRE 247

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# Part 1 Theory

## Show differential equations you are solving

The differential equations we are solving are the following:

𝑑𝑁1

= −λ

∗ 𝑁 (𝑡)

𝑑𝑡

1 1

Eq.1

𝑑𝑁2

= λ

∗ 𝑁 (𝑡) − λ

∗ 𝑁 (𝑡)

𝑑𝑡

1 1 2 2

Eq.2

𝑑𝑁3

= λ2

𝑑𝑡

∗ 𝑁2(𝑡)

Eq.3

These equations (Eq.1-3) are the general guesses for when N1 and N2 have relatively short half-lives compared to the half life of N3. This assumption allows us to say that N3 is stable and N1 and N2 are decaying with decay constants of λ1 and λ2 respectively.

## Show analytic solutions of the differential equations

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

𝑁1(𝑡) = 𝑁1,0 ∗ exp (−λ1 ∗ 𝑡)

Eq.4

λ1

𝑁 (𝑡) = ∗ 𝑁

[exp(−λ

∗ t) − exp(λ

∗ t)]

2 λ2 − λ1

1,0 1 2

Eq.5

𝑁1,0

𝑁 (𝑡) = ∗ [λ

∗ (1 − exp(−λ ∗ t)) − λ ∗ (1 − exp(λ

∗ t))]

3 λ2 − λ1 2

1 1 2

Eq.6

## 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).

𝑑𝑓(𝑥)

𝑑𝑡

= lim

∆𝑥→0

𝑓(𝑥 + ∆𝑥) − 𝑓(𝑥)

∆𝑥

Eq.7

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

Starting with N1(t) (Eq.1) and equating each expression (Eq.1 & Eq.7) we have for the rate of change of N1(t) we will get the following expression.

𝑑𝑁1(𝑡)

=

𝑑𝑡

𝑁1(𝑡 + 𝑑𝑡) − 𝑁1(𝑡)

𝑑𝑡 = −λ1 ∗ 𝑁1(𝑡)

Eq.8

We can then rearrange this equation (Eq.8) for N1(t + dt) to find the abundance of N1 at the next dt in time.

𝑁1(𝑡 + 𝑑𝑡) = −λ1 ∗ 𝑁1(𝑡) ∗ 𝑑𝑡 + 𝑁1(𝑡)

Eq.9

Moving on to the expression for N2(t) (Eq.2), we can apply the same procedure as we did in Eq.8 to get the following.

𝑑𝑁2(𝑡) 𝑁2(𝑡 + 𝑑𝑡) − 𝑁2(𝑡)

= = λ

∗ 𝑁 (𝑡) − λ

∗ 𝑁 (𝑡)

𝑑𝑡

𝑑𝑡

1 1 2 2

Eq.10

Solving for N2(t + dt), we get the following.

𝑁2(𝑡 + 𝑑𝑡) = λ1 ∗ 𝑁1(𝑡) ∗ 𝑑𝑡 − λ2 ∗ 𝑁2(𝑡) ∗ 𝑑𝑡 + 𝑁2(𝑡)

Eq.11

Finally, we can solve for N3(t) (Eq.3) by once again applying the same method as in Eq.8 to get the following.

𝑑𝑁3(𝑡)

=

𝑑𝑡

𝑁3(𝑡 + 𝑑𝑡) − 𝑁3(𝑡)

𝑑𝑡 = λ2 ∗ 𝑁2(𝑡)

Eq.12

Once again, solving this for N3(t + dt), we get the following solution to the next time step.

𝑁3(𝑡 + 𝑑𝑡) = λ2 ∗ 𝑁2(𝑡) ∗ 𝑑𝑡 + 𝑁3(𝑡)

Eq.13

The previous equations (Eq.8-13), lead us to find the solutions to the numerical integration to be Eq.9 for N1(t + dt), Eq.11 for N2(t + dt), and Eq.13 for N3(t + dt). These equations are easily implemented in code by applying the given initial conditions.

## Show complete derivation for a time of maximum Nb.

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 Nb, we set Eq.2 equal to 0. The following equation is the application of this.

𝑑𝑁2

= 0 = λ

∗ 𝑁 (𝑡) − λ

∗ 𝑁 (𝑡)

𝑑𝑡

1 1 2 2

Eq.14

λ1 ∗ 𝑁1(𝑡) = λ2 ∗ 𝑁2(𝑡)

Eq.15

We can then substitute Eq.4 in for N1(t) and Eq.5 in for N2(t), which gives the following.

λ (𝑁

∗ exp(−λ

∗ 𝑡)) = λ

λ1

( ∗ 𝑁

[exp(−λ

∗ t) − exp(λ

∗ t)])

1 1,0

1 2 λ2 − λ1

1,0 1 2

Eq.16

Dividing each side by λ1 and N1,0 gives...

exp(−λ

λ2

∗ 𝑡) = [exp(−λ

∗ t) − exp(λ

∗ t)]

1 λ2 − λ1 1 2

Grouping each term with a time dependence on one side.

exp(−λ1 ∗ 𝑡) λ2

=

exp(−λ1 ∗ t) − exp(λ2 ∗ t) λ − λ1

2

Eq.17

Factoring out an exp(-λ1 \* t) from the denominator allows us to simplify.

exp(−λ1 ∗ 𝑡)

exp(λ ∗ t)

λ2

=

λ − λ

exp(−λ1 ∗ t)(1 −

exp(

2 ) 2 1

−λ1 ∗ t)

Eq.18

1 λ2

exp(λ ∗ t) = λ − λ

1 − ( 2 ) 2 1

exp −λ1 ∗ t

Eq.19

Applying exponent rules allows us to simplify.

1

1 − exp((λ1

+ λ2

) ∗ t) = λ

λ2

− λ1

2

Eq.20

Solving this for (1 – exp((λ1 + λ2)\*t).

1 − exp((λ1

+ λ2

λ2

) ∗ t) =

λ2 − λ1

Eq.21

Further solving this for exp((λ1 + λ2)\*t).

exp((λ1

+ λ2

λ2

) ∗ t) = 1 −

λ2 − λ1

Eq.22

Combining the right side to give us a single fraction.

exp((λ

λ2 − λ1 λ2

+ λ ) ∗ t) = −

1 2 λ2 − λ1

λ2 − λ1

Eq.23

Simplifying.

exp((λ1

+ λ2

−λ1

) ∗ t) =

λ2 − λ1

Eq.24

Taking the natural log of both sides.

(λ1

+ λ2

−λ1

) ∗ 𝑡 = ln ( ) λ2 − λ1

Eq.25

Solving for t.

−λln )

1

(

𝑡 = λ2 − λ1

(λ1 + λ2)

Eq.26

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

# Part 2 Results

## Given Parameters:

TA,1/2 = 2.53 hours TB,1/2 = 11.05 hours TC,1/2 = ∞ hours

NA,0 = 100

NB,0 = 0

NC,0 = 0

Tfinal = 60 hours

## Plot the numerical solution for Nb(t) vs. time for 3 different values of ∆t (coarse, medium, fine), all of them on the same graph. Add the analytical solution on the same graph.

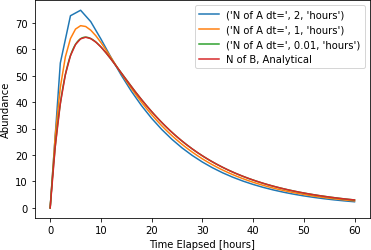


Figure 1: Graph of fine, medium, and coarse time steps for the numerical solution for Nb.

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.

## Plot numerical NA(t), NB(t), NC(t), and NA(t) + NB(t) + NC(t) as a function of time, all on the same graph, use a ∆t that gives reliable solution.

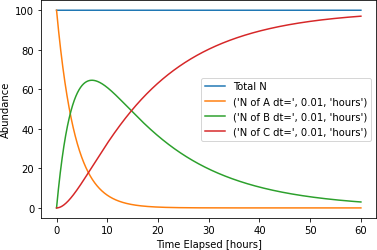


Figure 2: Graph of NA(t), NB(t), NC(t), and NA(t) + NB(t) + NC(t) vs. the elapsed time.

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 NA decays to one NB which decays to one NC. Thus, the total over time is constant.

## Using the numerical solution, plot the time of maximum NB vs. 1

∆t for several different ∆t. Use the analytical solution to determine time of maximum NB, and add that value to the graph.

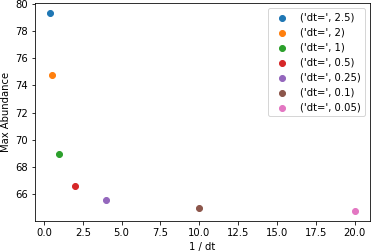


Figure 3: Plot of Max Abundance of NB vs 1 / dt with varyingly fine dts.

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