To: NE301 Class
From: NE301 Instructor
Date: September 21, 2018

Re: Solution to Project #1 Numerical Solution to the Decay Equations

Introduction

The memo should be written so that any instructor in the NE department can read it and clearly understand the assignment, how you are solving it, and what the results are. What are you trying to show, and why is it important to the reader?

The introduction should include a section describing the problem (sometimes called "Background" or "Theory"). This section should include a problem description and show the equations you are solving. (See class notes for more details.)

The format of the memo should match the instructions on how to write a memo. This includes:

- Use memo header.
- Use page numbers.
- Number all tables and figures, and include captions.
- Type all equations.
- Include a summary.

(25 points for Memo format)

Part 1: Two Isotope System (25 Points)

In Part 1, we are running the program for two nuclides, where nuclide A is being created by a fixed source. We are comparing our calculated results to an analytic solution to verify that the program is working correctly, and to determine the number of time steps needed to achieve a desired accuracy.

When radioactive nuclides are being calculated from a fixed source, they will reach a saturation activity where the activity of the nuclide is equal to the activity of the source.

$$A_{sat} = \lambda N_{sat} = A_0$$

Solving for the saturated number density

$$N_{sat} = A_0/\lambda$$

For our case, we were given A_0 =1 atom/minute and the following half-lives

Table 1: Saturation activities for Part 1

	T _{half} (min)	λ (per min)	N_{sat}
Α	1 min	0.69315	1.44270
В	2 min	0.34657	2.88539

A plot of the two nuclides as a function of time, along with the saturated values, is shown in Figure 1.

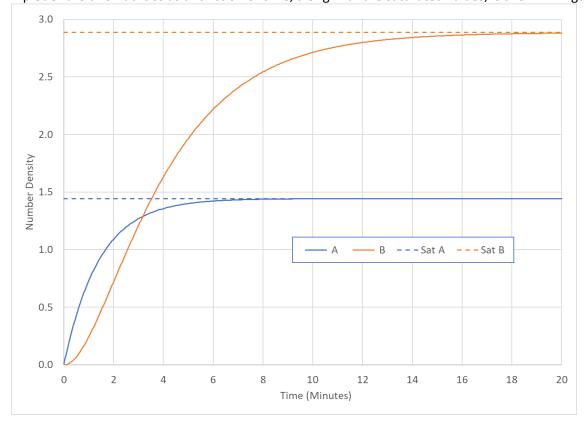


Figure 1: Nuclide Density for Part 1

The analytic solution for this problem was derived in Homework 2, Problem 3. The analytic solutions are:

$$N_A(t) = \frac{A_0}{\lambda_A} \left[1 - e^{-\lambda_A t} \right]$$

$$N_B(t) = \frac{A_0}{\lambda_B} \left[1 - e^{-\lambda_B t} \right] + \frac{A_0}{\lambda_B - \lambda_A} \left[e^{-\lambda_B t} - e^{-\lambda_A t} \right]$$

At a time of 5 minutes, the analytic solutions are shown in Table 2

Table 2: Analytic Solutions at 5 minutes

	N(5 min)
Α	1.397611
В	1.955419

The program was run with several different time steps and the calculated results were compared with the analytic solution. The results are plotted in Figure 2. Using Excel, a "Power Curve Fit" was applied to show that the error shows a nearly linear relationship to time (the exponent on the curve fit is nearly 1). This result shows the expected trend, and helps give confidence that the program is working correctly.

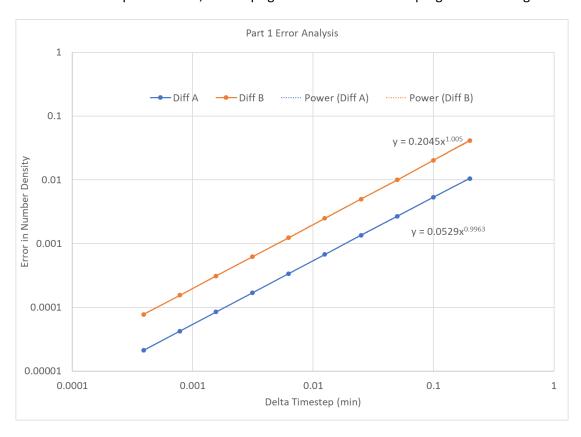


Figure 2: Error Analysis for Part 1

The next step is to determine the time step necessary to give results with an error less than 0.0001. This could be done by trial and error where you keep doubling the number of time steps (and cut the delta time step in half), and then find out when the error is less than the required tolerance (need to show work).

Another way is to use the Excel curvefit and solve for the required number of times. From the curvefit in Figure 2 for nuclide B (the one with the larger error), the "power fit" is

Error =
$$0.2045 (\Delta t)^{1.005}$$

Solving for a time step with an error of 0.0001 gives

$$\Delta t = \left(\frac{0.0001}{0.2045}\right)^{\frac{1}{1.005}}$$

$$\Delta t = 0.000508 \, min$$

or nstep = 20.0/0.000508 = 39,378 steps for a 20-minute calculation.

Students will get slightly different results depending on the fit parameters used, but the results should be close to 40,000 steps. It is also acceptable to find the necessary time step by trial and error, but they must show their work.

Several students used a linear fit. This will work for this particular case because the error is linear (first-order), but if the error is not linear, this will not work.

It is also strongly advised to use a log-log plot in order to see the relationship at small error values. If you do not use a log-log plot, the small error values are all "bunched together" and you can't tell where the fit crosses an error of 0.0001.

Note that we derived an analytic solution for the error in a single time step that was proportional to $(\lambda \Delta t)^2$ (i.e. second order). To get the error at a single point, you have to sum up all the errors from the individual time steps, which decrease the error about an order of magnitude (to first-order). This is what we observe in our results.

Just a note of interest, a higher-order method like Runge-Kutta can produce fourth-order results. To put this in perspective, a Runge-Kutta method only needs 400 steps to produce the same error as a 40,000 step Euler method.

Part 2: Five Isotope System (25 Points)

In Part 2, we are asked to plot four nuclides over a period of 40 months. A source is present in the first 20 months. The results are shown in Figure 3.

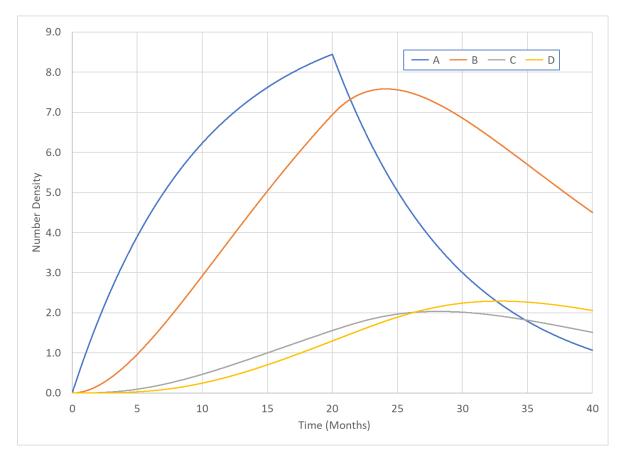


Figure 3: Nuclide Density for Part 2

Note that the initial value of all nuclides is zero, and the concentration of nuclide A drops off at 20 months when the source is removed.

The nuclide concentrations at 30 seconds are listed in Table 3. The absolute differences are less than 0.0001.

Table 3: Calculated Results at 30 months

N(30)
3.0013
6.8530
2.0147
2.2402

The student results need to agree to 0.0001

There are different ways of determining when the error is less then 0.0001. I started with 1000 steps, then kept doubling the number of steps (cutting the step size in half) until the difference between two steps was less than the desired accuracy for ALL nuclides. This occurred at **128,000 steps**, or a step size of **3.125e-4 months**. The hardest nuclide to converge was nuclide B.

Note that the doubling time study only works if you cut the timestep in half! This because we have a first-order method. Refer to class notes for more information.

The results of the doubling study are shown in Table 4.

Table 4: Nuclide differences when performing step doubling study

				0 1:	0 7
step	delta	Diff A	Diff B	Diff C	Diff D
2000	0.02	0.004835	0.012553	0.003626	0.003467
4000	0.01	0.002415	0.006268	0.001811	0.001733
8000	0.005	0.001207	0.003132	0.000905	0.000866
16000	0.0025	0.000603	0.001565	0.000452	0.000433
32000	0.00125	0.000302	0.000783	0.000226	0.000217
64000	0.000625	0.000151	0.000391	0.000113	0.000108
128000	0.0003125	0.000075	0.000196	0.000057	0.000054
256000	0.0001563	0.000038	0.000098	0.000028	0.000027
512000	7.813E-05	0.000019	0.000049	0.000014	0.000014

Alternatively, you could plot the differences and perform a curve fit.

Students must describe <u>how</u> they arrived at the time step they used.

Code Inspection (25 Points)

The code was inspected for this part of the grade. Students were required to allow an arbitrary number of nuclides (not hardwire solution to 2 or 4).

It is also suggested that programs use double precision numbers (see notes on Fortran double precision).

NE301 Project 1 Grade

Memo Format (to/from/date)	
Background or theory	
Summary	
Page numbers	
Figures and Tables numbered	
Equations Typed	

Part 1 (25 Points)

a) Calculate Saturated Values	
b) Plot Results with saturation	
c) Analytic Solution at 5 minutes	
d) Plot error with at least 6 times steps	
e) What time step is error less than	
0.0001? ~40,000	

Part 2 (25 points)

f) Plot Nuclides	
g) What are values at 30 months?	
Report to correct precision.	
h) Time step for error less than	
0.0001? ~128,000	

Program (25 points)

Read values from input	
Solver	

Notes:

Some comments after grading papers:

- There was quite a bit of confusion about calculating the saturation values. There is a formula for this, the saturation is not just the max values that you calculated in Part 1. The values in Part 2 did not approach the saturation values, and the saturation should not be plotted. No points taken off for this.
- Lots of missing page numbers!
- In the background section, it was very common to leave the source term out of the equations (either the differential equations and/or the discretized equations). The source term was in included in the programs. No points taken off for this.
- One suggestion I have is to put your results in tables. This makes it much easier to see the results without having to find the values in paragraphs.
- The error plots should use a log-log plot to accurately show values at small time steps.
- Lots of mistakes with inconsistent units! Part 1 used minutes and Part 2 used months. Seconds were not used anywhere. No points taken off for this.