NE 301
Fall 2018

**Project #1**
**Numerical Solution to the Decay Equations**

Due Date: Friday, September 21, 2018 at 11:55 PM

## Assignment

Write a computer program that will solve the radioactive decay equations numerically using the Euler method discussed in class. The program should be able to solve for an arbitrary number of coupled nuclides.

The computer program can be written in any standard language (e.g. Fortran, Maple, Mathematica, Java, Python), but the instructor may only be able to answer any programming questions in Fortran. All of the difference equations must be solved explicitly (e.g. you cannot use a pre-built library or built-in function to solve the equations).

The program shall read the following values from input: (i.e. no hard-coded values in the code)

1. Number of nuclides
2. Half-lives for each nuclide
3. Initial values of each nuclide
4. Starting time, ending time, and number of time steps
5. Source strength for first isotope and duration

The output shall be a text file of number densities vs. time which can be used to create plots.

The results shall be documented in a memo written to the instructor.

The memo shall be in a standard memo format (Date, To, From, Subject, etc.) and written so that any instructor in the NE department can read it and clearly understand the assignment (why are you writing this memo?), how you are solving it, and what the results are. More information and requirements on how to write a memo are included on the Moodle website.

The memo and computer program shall be submitted to the Moodle website before the due date. The memo should be in "pdf" format. The name of the program and memo should start with your last name. For example, the program should have a name like "palmtag_proj1.f90" and the memo should have a name like "palmtag_memo1.pdf".

## Part 1:

The purpose of Part 1 is to compare your program results to an analytic solution so you can show that the program is working properly. This is known as "solution verification".

Solve the numerical decay equations for the following problem:

- 2 nuclides, labeled "A" and "B"
- The half-lives of A and B are 1.0 min, and 2.0 min, respectively
- The initial values of A and B are zero.
- Nuclide A is being produced at a rate of 1 atom/min
- Solve for the time interval 0 to 20 min.

Include the following in your memo:

a) Calculate the saturated number densities of A and B
b) Plot the nuclides A and B as a function of time as calculated by your program. Include lines with the saturated values.
c) What is the analytic solution for this problem? (refer to HW 2). What is the nuclide concentrations from the analytic solution at 5 minutes?
d) Run the problem with at least six time step sizes and plot the absolute error between the calculated solution and analytic solution at time 5 minutes. The plot should show the absolute error vs. the time step size. Choose at least one time step size so the absolute error is less than 0.0001. What relationship between the error and time step size is observed? (e.g. generate a curve fit for error vs. time step size.)
e) What time step is necessary to obtain a maximum absolute error less than 0.0001?

The absolute error is defined as the absolute value of the calculated values minus the analytic solution.

## Part 2:

The purpose of Part 2 is to solve a problem where the analytic solution is not known.

Solve the decay equations for the following problem:

- 4 isotopes
- The half-lives are 6.7, 9.2, 2.6, and 3.1 months, respectively
- The initial values of all nuclides are zero.
- Nuclide A is being produced at a rate of 1 million atoms/month for the first 20 months, then the production rate drops to zero.
- Solve for the time interval 0 to 40 months.

In the same memo as Part 1, provide the following results:

f) Plot the nuclide concentrations as a function of time.
g) What are the values of all the nuclides at 30 months? All of the values should have an absolute error less than 0.0001.
h) What time step size was necessary to obtain this error level? How did you arrive at this conclusion? (Hint: you need to do an error analysis)

## Discussion and Hints

When writing a computer program, it is often better to start small and work your way up to the final program. Break the program down into manageable steps and solve them one at a time. For example, you may want to start by solving the decay equations for a single nuclide. Then add a second nuclide, and then figure out how to generalize the problem to an arbitrary number of nuclides.

Let the computer do as much of the work for you as possible. For example, let the program determine what the maximum nuclide concentrations are, and when they occur. Do not try to post-process this information manually. Manual post-processing is tedious, and is also error prone.

The program should check to make sure that the problem is stable. What criteria ensures that the equations will converge?

Write the output file so that it is easy to post-process. If you are using Excel to make your plots, then write your output to a comma-separated-value (csv) file that Excel can import easily. If you are using a different program to create your plots, make the output easy to import into that program.

This program will be expanded in a later class project, so you should include as many comments as necessary to make the program easy to modify in the future.

Use double precision in your program. If you don't understand what this means, refer to the document on Moodle to find out more.

Finally, turn on as many compiler warnings as possible. Compiler warnings are your friend and will help you catch mistakes early. Example warning messages include checking for arrays that are out of bounds, or if variables are used before they are initialized. Always use "implicit none" in Fortran programs!

Do not wait until the last minute to start this project!