Physics 305 – Computational Physics, Fall 2020
Term Project
Full project submission Due Date: Tuesday December 15, 5pm
Presentation Phase: November 30 - December 11

The program in your term project can be either submitted as a python program or ipython notebook, where the latter is preferred. The program, an explanation of what the program does, along with answers to **all** questions asked should be uploaded to d2l.

You are expected to write a term paper (in word or Latex) on your project that discusses the problem you are trying to solve, the basic equations that govern the problem, includes plots that show the solutions, and describes the solution and the numerical method involved. In addition, you must demonstrate that your solution is correct by showing that the code converges at the expected order. If your code does not converge at the expected order you should try to identify potential reasons for why this is the case. You are expected to work on your term project by yourself..

Your term project will receive full credit **only** if: (a) the program runs successfully without errors using python 3, (b) the programs have explanatory comments and variable names that identify with the problem equations you are trying to solve, (c) give the correct output, and (d) demonstrate the validity of the solution through convergence plots. No credit will be given to late term projects.

The term paper is as important as the code (50% of the term project credit will go to the code and the other 50% to the paper). Answers to the questions and analysis requested below should be elaborated in the report. Plots should be clearly labeled and be properly described in the report, and not just shown. You will need to explain what each and every plot demonstrates. A polished paper written in word or LaTex (preferred, e.g. please try overleaf) is expected to get full credit.

Note: Before you present results from numerical integrations that answer the questions in the project, it is critical to *first* perform the convergence tests for one case, and to estimate errors. This will tell you how small a step size is necessary for accurate solutions. Only after errors are estimated, does it make sense to run your code for producing results that help you learn more about the system you study.

I. BATEMAN'S EQUATIONS: CHAIN OF DECAYS OF 3 NUCLEAR SPECIES

You will be examining properties of the Bateman equations that govern the decay of multiple nuclear species. While the problem is exactly solvable in iterative form we will consider it as a coupled system of equations, to determine the co-evolution of all species. It is well known that if there is only one nuclear species A the number of radioactive decays is proportional to the number of radioactive nuclei, N_A, i.e., the species evolves according to the ordinary differential equation (ODE)

$$\frac{dN_A}{dt} = -\lambda_A N_A, \tag{1}$$

where λ_A is related to the half-life of the species A $t_{1/2,A} = \ln 2/\lambda_A$.

Now consider the case of a chain of two decays: one nucleus A decays into another B by one process, then B decays into another C by a new process. The previous equation cannot be applied to the decay chain. Since A decays into B, and B decays into C, the activity of A adds to the total number of B nuclei. Therefore, the number of second generation nuclei B increases as a result of the decay of first generation A nuclei, and decreases as a result of its own decay into the third generation nuclei C, thus, the B species evolves as

$$\frac{dN_B}{dt} = -\lambda_B N_B + \lambda_A N_A. \tag{2}$$

We will now treat a more interesting possibility, where we have 3 radioactive species, the first generation A decays into second generation B and C. For example, ^{40}K has a 89.3% probability of decaying to ^{40}Ca, and 10.7% to ^{40}Ar. To make the problem more fun we will add the possibility that species B can, too, decay into species C. We will also consider that C decays into stable nuclei D. Based on the above considerations we have:

$$\begin{aligned}
\frac{dN_A}{dt} =& -\lambda_A N_A, \\
\frac{dN_B}{dt} =& -\lambda_B N_B + \lambda_{A,B} N_A \\
\frac{dN_C}{dt} =& -\lambda_C N_C + \lambda_{A,C} N_A + \lambda_B N_B \\
\frac{dN_D}{dt} =& \lambda_C N_C
\end{aligned} \tag{3}$$

where $\lambda_{A,B} + \lambda_{A,c} = \lambda_A$, and $\lambda_{A,B}/\lambda_{A,c}$ must equal the ratio of the probability that A will decay into B to the probability that A will decay into C.

This system of equations has an integral (constant) of the motion,

$$N = N_A + N_B + N_C + N_D \tag{4}$$

which is the total number of nuclei and is determined by the initial conditions.

The system (3) has multiple timescales involved, and hence it is not possible to completely non-dimensionalize it. However, you can use λ_A to introduce a non-dimensionsal time (call it $\tilde{t}$), and in this time only the ratios λ_B/λ_A, λ_C/λ_A, $\lambda_{A,B}/\lambda_A$ and $\lambda_{A,c}/\lambda_A$ matter, with of course $\lambda_{A,B}/\lambda_A + \lambda_{A,c}/\lambda_A = 1$. We will be experimenting with these paramaters.

In addition, use N to introduce normalized species numbers $\tilde{N}_i = \frac{N_i}{N}, i =$ A,B,C,D, so that the final equations in dimensionless time describe the evolution of the fraction of each species in an initial sample. This way the constant of the motion becomes

$$\tilde{N}_A + \tilde{N}_B + \tilde{N}_C + \tilde{N}_D = \tilde{N} = 1. \tag{5}$$

This constant $\tilde{N}$ will allow you to validate the quality of the numerical integration of Eq. (3).

Show in your term paper the derivation of the the normalized and dimensionless version of (3). To solve this normalized and dimensionless version of (3) you will need to specify initial conditions. Do the following:

1. Use RK4 to integrate numerically the dimensionless and normalized version the ODE (3) from $t = 0$ forward in time and for sufficiently large t until the populations of each species settles. You will need to be plotting $\tilde{N}_i$ vs t to see if the solution is settling and to determine when to stop the integration. Run a couple of numerical experiments with different parameters to test the dynamics of the species populations.

    - First, consider the case where the A species decays very slowly and test whether it is possible to run out of B and C nuclei. For this experiment you will set λ_B/λ_A=5, $\lambda_C/\lambda_A = 10$, $\lambda_{A,B}/\lambda_A = 0.85$ and $\lambda_{A,C}/\lambda_A = 0.15$. Consider initial conditions $\tilde{N}_A = 0.5$, $\tilde{N}_B = 0.25$, $\tilde{N}_C = 0.1$, $\tilde{N}_D = 0.15$.

      Show plots of your solution for $\tilde{N}_i$ vs t. Does this evolution eliminate the species A and B completely?

    - Second, consider the case where the A species decays very rapidly. For this experiment you will set λ_B/λ_A=0.05, $\lambda_C/\lambda_A = 0.1$, $\lambda_{A,B}/\lambda_A = 0.85$ and $\lambda_{A,C}/\lambda_A = 0.15$. Consider initial conditions $\tilde{N}_A = 0.5$, $\tilde{N}_B = 0.25$, $\tilde{N}_C = 0.1$, $\tilde{N}_D = 0.15$.

      Show plots of your solution for $\tilde{N}_i$ vs $\tilde{t}$. How is this evolution different from the previous one?

    - Third, the system of equations has an "equilibrium" point for the B species, when $\lambda_B\tilde{N}_B/\lambda_A = \lambda_{A,B}\tilde{N}_A/\lambda_A$, because then $\frac{d\tilde{N}_B}{d\tilde{t}} = 0$, which implies that the number of B species remains constant, the B decay rate is balanced by the replenishment of B from the decay of A species. You can now study if this "equilibrium" is stable, by considering initial conditions that satisfy it. We will keep the same $\lambda_{A,B}/\lambda_A = 0.85$ and $\lambda_{A,C}/\lambda_A = 0.15$, and initial conditions $\tilde{N}_A = 0.5$, $\tilde{N}_B = 0.25$, $\tilde{N}_C = 0.1$, $\tilde{N}_D = 0.15$. The condition $\lambda_B\tilde{N}_B/\lambda_A = \lambda_{A,B}\tilde{N}_A/\lambda_A$ implies $\lambda_B/\lambda_A = 1.7$. And set again $\lambda_C/\lambda_A = 0.1$.

      Show plots of your solution for $\tilde{N}_i$ vs $\tilde{t}$. Does the population of B species remain constant?

   Use your judgement as to how small a step size you need to solve this system accurately. If you cannot figure this out from pure thought, experiment with different step sizes and use $\delta\tilde{N} = |(\tilde{N}(t) - \tilde{N}(t=0))/\tilde{N}(t=0)|$ to determine the accuracy. If $\delta\tilde{N}$ is smaller than 10^{-3} for all integration times, then you have decent accuracy.

2. **Convergence:** For one of the set of initial conditions and initial parameters, demonstrate that as you decrease the step size h, $\delta\tilde{N}(\tilde{t}=3)$ converges to 0. Make a plot to determine the order of convergence of $\delta\tilde{N}$, and discuss why or why not this matches your expectation.

3. **Self-convergence**: Use a number of step sizes and make a plot to demonstrate that the code solution for $\tilde{N}_C$ at $\tilde{t}=3$ self-converges for fixed initial conditions and initial parameters. Does the order of convergence match your expectation? If not, try to explain why.

4. Using the order of convergence you determined, employ Richardson extrapolation to determine an error for the solution for $\tilde{N}_C(\tilde{t})$ at a time of your choosing.