Part C: Numerical Solution of Rate Equations

C1: Solution using a numerical solver

a) Starting from the numerical solution done in class as an example (in Mathematica, we used NDSolve, but feel free to use something else or your own numerical solver), solve the sequential first order reactions from **B6**

$$A \rightleftharpoons B \rightleftharpoons C.$$

using the same values of $k_1 = 1.0$, $k_{-1} = 0.05$, $k_2 = 0.1$, $k_{-2} = 0.1$.

C2: Solution using Euler's Method; a simple first order reaction

It is instructive to see how numerical methods for solving differential equations work. This way you will be able to write a program yourself for solving differential equations. Starting with the Euler algorithm we discussed and did in class, integrate the first order reaction

$$A \rightarrow B$$

with $k = 0.05$, and $A_0 = 1.0$. Use a finite difference step size of $h = 1.0$, and a total time of $t = 100$.

a) It is essential to check how small the step size, h, needs to be in order to get accurate enough results. Repeat the calculation above for a smaller step size of $h = 0.5$ and a larger step size of $h = 2$. Give the resulting arrays different names so that you can in the end plot all three results on the same graph. Also, note what value of the concentration of A is obtained at time $t = 100$ in each case. Let's assume that you are willing to accept an error of 0.001 in the concentration. Try using a very small step size, such as $h = 0.02$ and check what value of the concentration is obtained at $t = 100$. How small a step size do you need to use? Evaluate what concentration the analytical solution predicts at $t = 100$ and compare with your numerical results.

C3: Sequential first order reactions with no back-reactions

The numerical procedure above can rather easily be generalized to more complex reactions. For example, for the sequential first order reaction

$$A \rightarrow B \rightarrow C.$$

Repeat your calculation from **C2** for this reaction using $k_1 = 0.01$ and $k_2 = 0.2$

C4: Solution using Euler's Method; sequential reversible reactions

Extend your code from question **C3** to include back reactions. Calculate and plot the solution for a few different values of the back reaction rate constants.