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. DYNAMICS OF EPIDEMICS

You will be examining the properties of the Susceptible-Infectious-Recovered (SIR) model of the dynamics of epidemics. The SIR dynamics of epidemics comprise a system of ordinary differential equations that ingores birth and death (this is called vital dynamics). This is a good approximation in some cases. The SIR equations are a triplet of first-order non-linear ordinary differential equations given by

$$\begin{aligned}\frac{dS}{dt} =& -\beta\frac{IS}{N},\\ \frac{dI}{dt} =& \beta\frac{IS}{N} - \gamma I \\ \frac{dR}{dt} =& \gamma I.\end{aligned} \tag{1}$$

where S is the number of Susceptible people, I the number of infected people, and R the number of recovered people. N is the total number of people which is conserved. Introduce properly rescaled rescaled variables such that instead of the total numbers of people we have a system of ODEs for the fractions of people who are S, I, R. Show your work in the term paper. The constants β, γ are positive real parameters describing the rate at which the number of susceptible people decrease, the rate at which the number of infected people decrease. One of the useful properties of Eq. (1) is that it admits the following integral of the motion which must be constant

$$C = S + I + R \tag{2}$$

The value of the constant C is determined by the initial conditions (think of this constant as the analogue of energy conservation). In the properly normalized version of the system with N not in the system, the constant C is always equal to unity ($C = 1$). The existence of this integral of the motion will help you assess the validity of the numerical solutions of Eq. (1).

The system of equations has multiple timescales involved, so it cannot be cast in pure dimensionless form independent of β, γ. But, the dynamics depends only on the dimensionless ratio $R_0 = \beta/\gamma$. Introduce R_0 in the equations of motion and then introduce a properly dimensionless time variable (call it $\tilde{t}$ so that the eventual system of ODEs depends only on R_0 which is called the basic reproduction number. It turns out that whether there will be an epidemic or not depends on R_0 and the initial fraction of susceptible people. In particular, we have the following cases

- If $R_0 > R_{\rm crit} = \frac{1}{S(0)}$ then there will be an epidemic outbreak.
- If $R_0 < R_{\rm crit} = \frac{1}{S(0)}$ then the disease cannot cause a an epidemic outbreak.

You will be studying these cases.

1. Use RK4 to integrate numerically the system of ODEs (1) from $t = 0$ and for sufficiently long times until either solution settles or an epidemic outbreak takes place. You will need to be plotting S, I, R vs t to determine when to stop the integration. You will need initial conditions to integrate the equations. Let us fix these to $S(0) = 0.6$, $I(0) = 0.3$ and $R(0) = 0.1$. Therefore, the critical basic reproduction number is $R_{\rm crit} = 1/0.6 = 5/3$. You will be experimenting with R_0.

   - First test what happens when $R_0 = R_{\rm crit}$. Does the fraction of infected people stay the same or does it increase/decrease? What about the fractions of recovered and susceptible people? What does this imply about the evolution when basic reproduction number is equal to the critical value? Make a plot showing the evolution of S, I, R vs time and discuss it in your term paper.
   - Now test the case $R_0 < R_{\rm crit}$. Set $R_0 = 0.5R_{\rm crit}$. Does the fraction of infected people stay the same or does it increase/decrease? What about the fractions of recovered and susceptible people? What does this imply about the evolution when basic reproduction number is less than the critical value? Make a plot showing the evolution of S, I, R vs time and discuss it in your term paper.
   - Finally test the case $R_0 > R_{\rm crit}$. Set $R_0 = 1.5R_{\rm crit}$. Does the fraction of infected people stay the same or does it increase/decrease? What about the fractions of recovered and susceptible people? What does this imply about the evolution when basic reproduction number is greater than the critical value? Make a plot showing the evolution of S, I, R vs time and discuss it in your term paper.

     In addition, set Set $R_0 = 2.0R_{\rm crit}$. How is the evolution different from the case Set $R_0 = 1.5R_{\rm crit}$? What happens when the basic reproduction number increases in this case?

   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 the constant of the motion Eq. (2) to determine how small the step size has to be. If $|C(t) - C(0)|/|C(t)| < 10^{-3}$, you have decent accuracy.

2. **Convergence**: The quantity $|C(t) - C(0)|/|C(t)|$ must be zero at all times. Choose one set of initial conditions integrate to some final time of your choise t_f; Solve the system (1) using a number of step sizes and make a plot to demonstrate that $|C(t_f) - C(0)|/|C(t)|$ at the final time converges to 0. Does the order of convergence match your expectation? If not, try to explain why.

3. **Self-convergence**: Use a number of step sizes and make a plot to demonstrate that the code solution for S, I, R at the final time self-converges. 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 $S(t)$ at a time t of your choosing.