Experiment 4: Problem set

The assignment is worth **20 marks**.

The final submission should be a PDF file uploaded in Moodle. No email submissions.

Unless otherwise specified there is no need to include the source code.

Submission deadline: September 16, 2021 (Thursday), 12 pm

1. Consider the following ODE

$$\frac{dy}{dt} = yt^3 - 1.5y$$

y(0) = 1 and the interval over which this ODE is to be considered is t = 0 to 2. Solve this ODE using the **fourth order Runge-Kutta method** with a step size, h, equal to 0.05. You can write a short code for doing this. Evaluate this ODE analytically as well, and plot y vs. x for the analytical and numerical solutions, on the same graph. Use appropriate legend to mark the curves.

2. The position of a body is given by the second order ODE

$$\frac{d^2x}{dt^2} + \frac{c}{m}\frac{dx}{dt} - g = 0$$

where c is a first order drag coefficient equal to 12.5 kg/s, m = 70 kg, and g is 9.8 m²/s. Use the shooting method to solve for the position and velocity of the body given the boundary conditions x(0) = 0 and x(12) = 500. Use an appropriate step size and plot both position and velocity as a function of time.

3. The following equations define the concentrations of three reactants:

$$\frac{dc_a}{dt} = 10 c_a c_c + c_b$$

$$\frac{dc_b}{dt} = 10 c_a c_c - c_b$$

$$\frac{dc_c}{dt} = -10 c_a c_c + c_b - 2c_c$$

If the initial conditions are $c_a = 50$, $c_b = 0$, and $c_c = 40$, find the concentrations for the times from 0 to 3 s.

4. A famous second order ODE is the 1D time-independent Schrodinger wave equation. Analytical solutions are available for simple systems, such as the particle in a potential well. Show that it is also possible to solve this system using a numerical approach and obtain the ground state solution. Take a well width of 0.5 nm for this problem. Compare the energy obtained with that from the analytical solution.