Simulations in Physics

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§ WEEK 1 §

Problem 1: Newton Raphson Method

Resource:

- https://www.geeksforgeeks.org/newton-raphson-method/

For a quantum mechanical problem, an electron in a symmetric square well potential governs the following transcendental equation for the quantized energies,

$$cos(\kappa L) = 0.226(\kappa L) \tag{1.1}$$

where $L = 0.2nm$ is the width of the well, $\kappa = \sqrt{\frac{2mE}{\hbar^2}}$, $m = 9.1 \times 10^{-31}$ Kg is the mass of the electron, $\hbar = 6.58 \times 10^{-16}$ eV.s. Solve the above transcendental equation using Newton Raphson method to calculate the ground state (lowest) energy (E) in eV.

Problem 2: Secant Method

Resources:

- https://www.tutorialspoint.com/fortran/fortran_arrays.htm
- https://www.tutorialspoint.com/fortran/fortran_file_input_output.htm
- https://www.geeksforgeeks.org/secant-method-of-numerical-analysis/

The file data.txt contains values of x and y for 100 data points. Read the values from the file into arrays. Use the secant method to find the roots of the function.

Problem 3: Euler Method

Resources:

- https://www.math.umd.edu/~petersd/460/html/euler_demo2.html

The Euler method can be used to solve second-order ODE by doing some variable changes. Using this technique, solve the following Damped-driven-harmonic oscillator.

$$y'' + 5y' + 6y = 10 \sin t \tag{3.1}$$

with the initial conditions $y(0) = 0$ and $y'(0) = 5$. The exact solution of this equation is

$$y(t) = -6e^{-3t} + 7e^{-2t} + \sin t - \cos t \tag{3.2}$$

Plot the Euler method solution and the exact solution on the same graph and compare your results. *Choose h = 0.1 & h = 0.01*

Problem 4: Runge Kutta 4th order method

Resources:

- https://math.libretexts.org/Courses/Monroe_Community_College/MTH_225_Differential_Equations/03%3A_Numerical_Methods/3.03%3A_The_Runge-Kutta_Method

Solve the above equation using the RK4 method. Plot the RK4 solution and the exact solution and compare your results. *Choose* $h = 0.1$

Problem 5: Lorenz Attractor / Chaos

Resources:

- https://en.wikipedia.org/wiki/Lorenz_system

We are going to solve a system of three ordinary differential equations now known as the Lorenz equations given as

$$\frac{dx}{dt} = \sigma(y - x) \tag{5.1}$$

$$\frac{dy}{dt} = x(\rho - z) - y \tag{5.2}$$

$$\frac{dz}{dt} = xy - \beta z \tag{5.3}$$

Choose $\rho = 28, \sigma = 10, \beta = \frac{8}{3}$. Plot this system of equations for two initial conditions sufficiently close to each other.

Make all plots using **GNUPLOT**. For installation http://www.gnuplot.info/download.html. Tutorial https://people.duke.edu/~hpgavin/gnuplot.html.