PHY407 Lab 07

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The workload was distributed as followings:

- **Jianbang Lin did question 3**
- **Sang Bum Yi did question 1 and 2**

Question 1

Part a)

In Question 1 of lab 6, the Runge-Kutta method with the fixed step size h was used to model the space garbage. However, the results of the same model would have been better if the step size could be allowed to vary. This method of varying the step size is called an "adaptive step size" method and has been applied to the space garbage.

In summary, the adaptive step size method compares two estimates of x(t + 2h). The first estimate is denoted as x_1 made by taking two steps of the same size 'h' from x(t), whereas the second estimate is denoted as x_2 and made by taking one step of size '2h' from the same point. Then, it computes the ratio of the target accuracy to the actual accuracy and checks if it exceeds 1. If it does, it means the actual accuracy is better than the target accuracy and the method continues the procedure at the new point x(t + 2h) with the new step size h' as defined in Equation 1.1. On the other hand, if p < 1, the actual accuracy is poorer than the target accuracy. In this case, the method repeats the procedure at the same point x(t) with the new step size h' also as defined in Equation 1.1.

$$h' = h\rho^{1/4} \quad \text{[Eq 1.1]}$$

where ρ, ϵ_x, and ϵ_y are defined as followings:

$$\rho = \frac{h\delta}{\sqrt{\epsilon_x^2+\epsilon_y^2}} \quad \text{[Eq 1.2]}$$

$$\epsilon_x = \frac{1}{30}(x_1 - x_2) \quad \text{[Eq 1.3]}$$

$$\epsilon_y = \frac{1}{30}(y_1 - y_2) \quad \text{[Eq 1.4]}$$

Starting from h = 0.01 and the error-per-second $\delta = 10^{-6}\ m/s$, the space garbage was applied the Runge-Kutta algorithm with the adaptive step size method and its trajectory was plotted and overlayed on top of the trajectory by the non-adaptive step size method in Figure 1.1

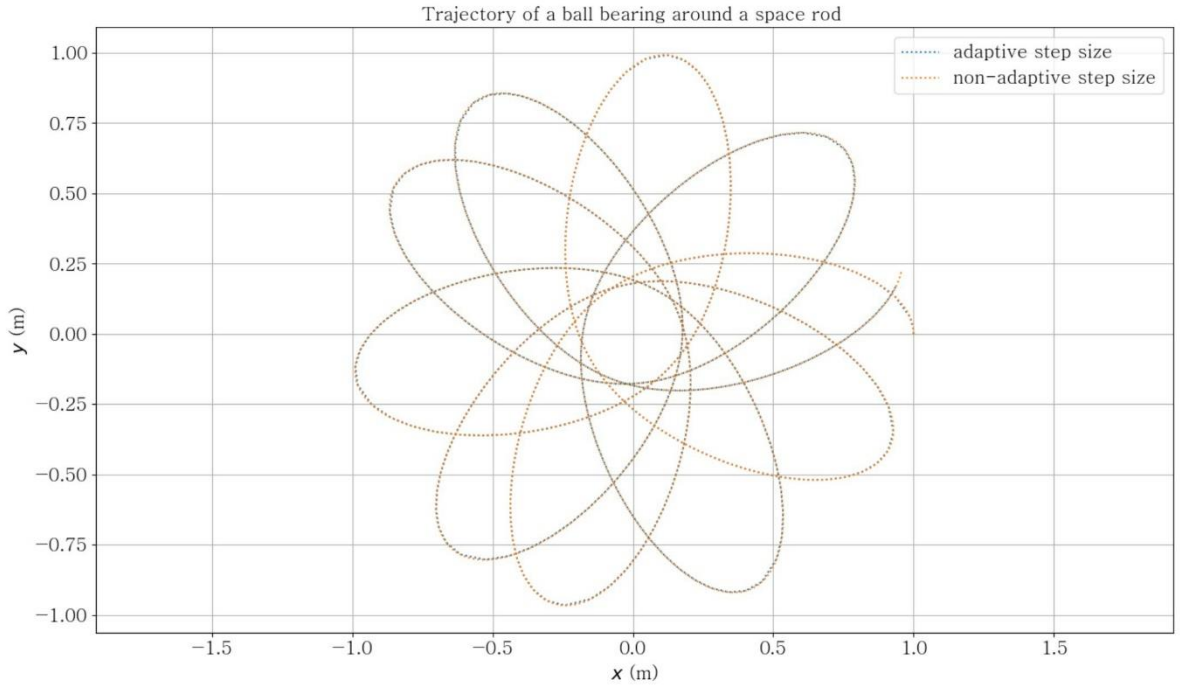

Figure 1.1: The Trajectory of a ball bearing around a space rod with the Adaptive Step Size and Non-Adaptive Step Size method, at h = 0.01 for the adaptive method and N = 10,000 for the non-adaptive method.

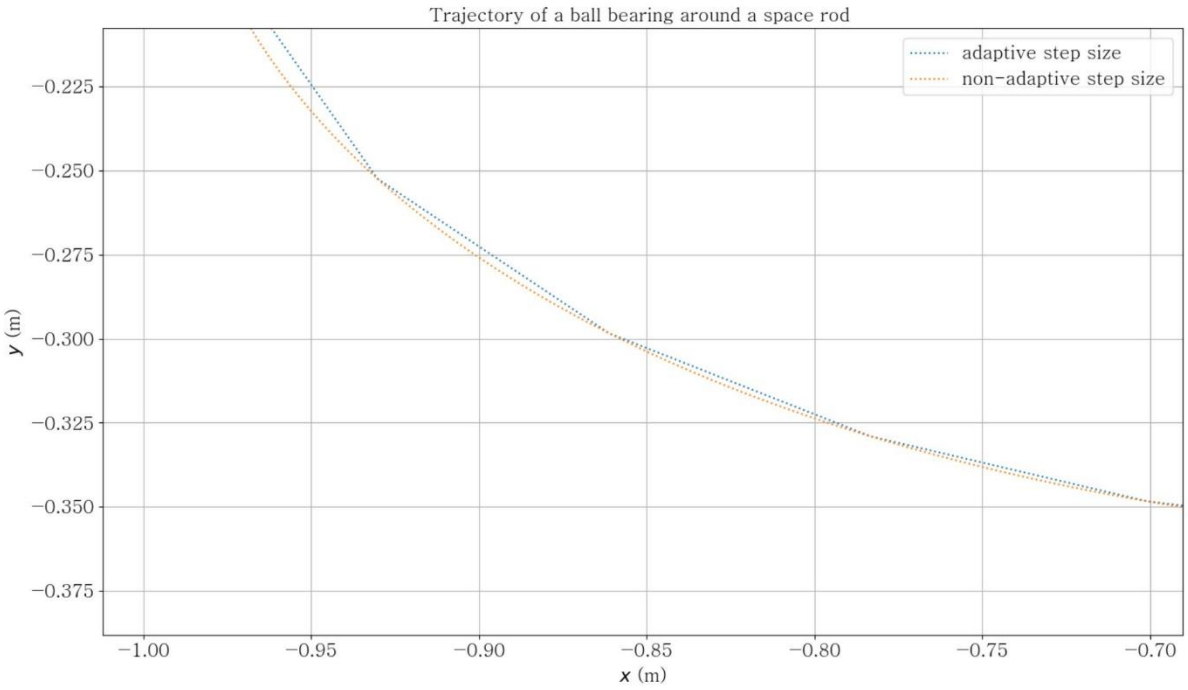

Figure 1.2: The close-up of the trajectory in Figure 1.1

Figure 1.1 shows that the trajectories generated by adaptive step size method and non-adaptive step size method are in fact similar, following the same path. However, the closer look at the overlay of two trajectories reveals the difference, which is the gap between blue and orange lines in Figure 1.2.

Part b)

The run-times for the adaptive and non-adaptive step size methods were compared with the error-per-second $\delta = 10^{-6}\ m/s$ for the adaptive step size and h = 0.001 (N = 10,000) for the non-adaptive step size. The printed outputs for the adaptive and non-adaptive method are shown in Figure 1.3 and Figure 1.4, respectively.

```
C:\Users\paran\PycharmProjects\PHY407\venv\Scripts\python.exe C:/Users/paran/PycharmProjects/PHY407/Lab07/Lab07_Q1.py
Q1 Part b - The run time of the adaptive step size method is  0.14154791831970215
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Figure 1.3: The printed output of the run-time for the adaptive step size with $\delta = 10^{-6}\ m/s$

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C:\Users\paran\PycharmProjects\PHY407\venv\Scripts\python.exe C:/Users/paran/PycharmProjects/PHY407/Lab07/Q1_sample.py
Q1 Part b - The run time of the nonadaptive step size method is  0.4969336986541748
```

Figure 1.4: The printed output of the run-time for the non-adaptive step size with h = 0.001

Obviously, the run-time of the adaptive step size was a lot faster than that of the non-adaptive step size, the former being 0.142s and the latter being 0.497s (*three sig. fig*). This was predicted in the textbook on page 355 and page 359, which said “we can calculated the whole solution faster (because we need fewer points overall) but still very accurately” and “In the end the program almost always take less time to run, and usually much less” respectively. Indeed, the run-time for the non-adaptive step size method used in this exercise was approximately 3.5 times greater than that for the adaptive step size method.

Part c)

Since the adaptive step size method uses large time steps for slowly varying regions of the function and small time steps for rapidly varying regions of the function, the size of the time step varies throughout the iterations. Then, the sizes of the time steps between t=0 and t=10 were plotted in Figure 1.5 below.

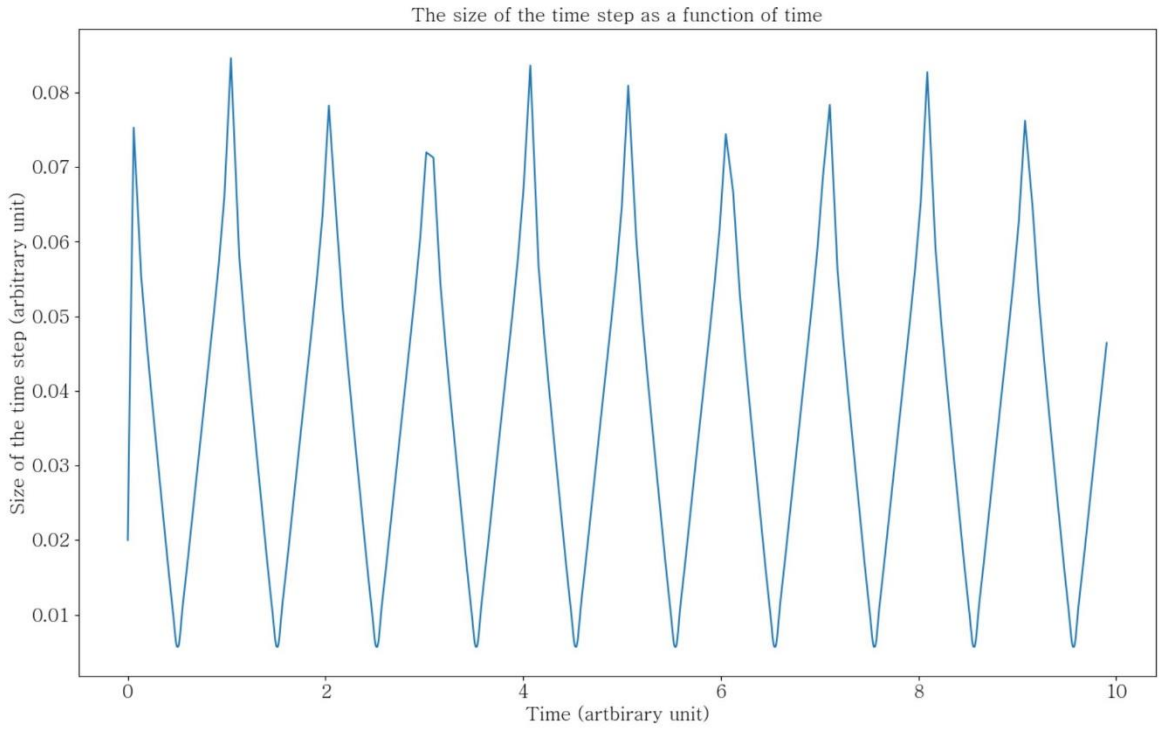

Figure 1.5: The size of the time step as a function of time. Note that the time is in an arbitrary unit.

Figure 1.5 shows a predictable behaviour, as expected. The size of the time step is oscillating, which matches with the oscillating ellipses of the trajectory in Figure 1.1. In other words, the time steps tend to be relatively short when the change in position is more rapid, and relatively long when the change in position is slower, which is the principle of the adaptive step size method.

The complete time steps can be found in Appendix A. Note that the second time step is 0.02, which equals to t + 2h = 0.0 + 2 * 0.01. Likewise, the third time step is 0.06, which equals to t + 2h = 0.02 + 2 * 0.02. However, the later time steps are shown to vary more flexibly depending on the value of ρ.

Question 2

Part a) Exercise 8.13 Part a

The Earth's orbit around the Sun was plotted using the Bulirsch-Stoer method. The equations of motion for an orbit of a planet is given by Equation 2.1 and 2.2 below.

$$\frac{d^2x}{dt^2} = -GM\frac{x}{r^3} \qquad \text{[Eq 2.1]}$$

$$\frac{d^2y}{dt^2} = -GM\frac{y}{r^3} \quad \text{[Eq 2.2]}$$

where G = 6.6738 * 10^{-11} $m^3kg^{-1}s^{-2}$, M = 1.9891 * 10^{30} kg, and r = $\sqrt{x^2 + y^2}$

The Bulirsch-Stoer combines the modified midpoint method and Richardson extrapolation. The modified midpoint makes an estimate of x(t + H) with equations 2.3, 2.4, and 2.5 below.

$$y_{m+1} = y_m + hf(x_m, t + mh) \quad \text{[Eq 2.3]}$$

$$x_{m+1} = x_m + hf(y_{m+1}, t + \left(m + \frac{1}{2}\right)h) \quad \text{[Eq 2.4]}$$

$$x(t + H) = \frac{1}{2}[x_n + y_n + \frac{1}{2}hf(x_n, t + H)] \quad \text{[Eq 2.5]}$$

Denoting the first estimate of x(t + H) as $R_{1,1}$, the Richardson extrapolation uses Equation 2.6 to make subsequent estimates of x(t + H) with the step size of h = H/n.

$$R_{n,m+1} = R_{n,m} + \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m}-1} \quad \text{[Eq 2.6]}$$

Therefore, the estimate of the error is given by Equation 2.7

$$c_m h_n^{2m} = \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m}-1} \quad \text{[Eq 2.7]}$$

After calculating $R_{n,m}$, the error given by Equation 2.7 is compared to the target accuracy Hδ. If the error is larger than the target accuracy, the number of steps 'n' gets increased by one and a new modified midpoint estimate $R_{n,1}$ is calculated as well as the subsequent $R_{n,m}$. However, the iteration proceeds to the next time interval H if the error is smaller than the target accuracy.

Applying the Bulirsch-Stoer method with Equation 2.1 and 2.2, the orbit of the Earth was plotted with a positional accuracy of δ = 1 km/year. The initial position and velocity in x-direction were 1.4710 * 10^{11} m and 0 m/s, whereas the initial position and velocity in y-direction were 0 m and 3.0287 * 10^4 m/s. The interval was H = 1 week = 1/52 year.

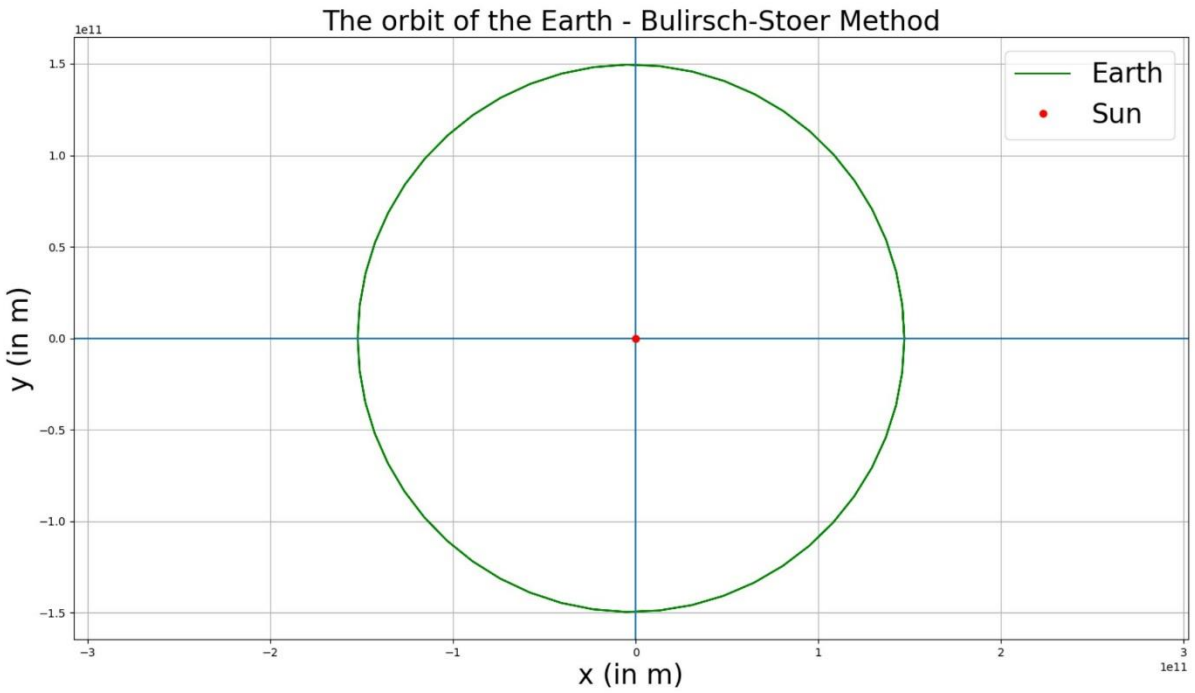

Figure 2.1: The orbit of the Earth plotted by Bulirsch-Stoer method. Note that the red dot at (0,0) represents the Sun, whereas the green line represents the orbit of the Earth. The scales of x-axis and y-axis were set to equal.

The following figure 2.2 shows the orbit of the earth plotted using the Verlet method, which is generated by the sample code provided by the professor.

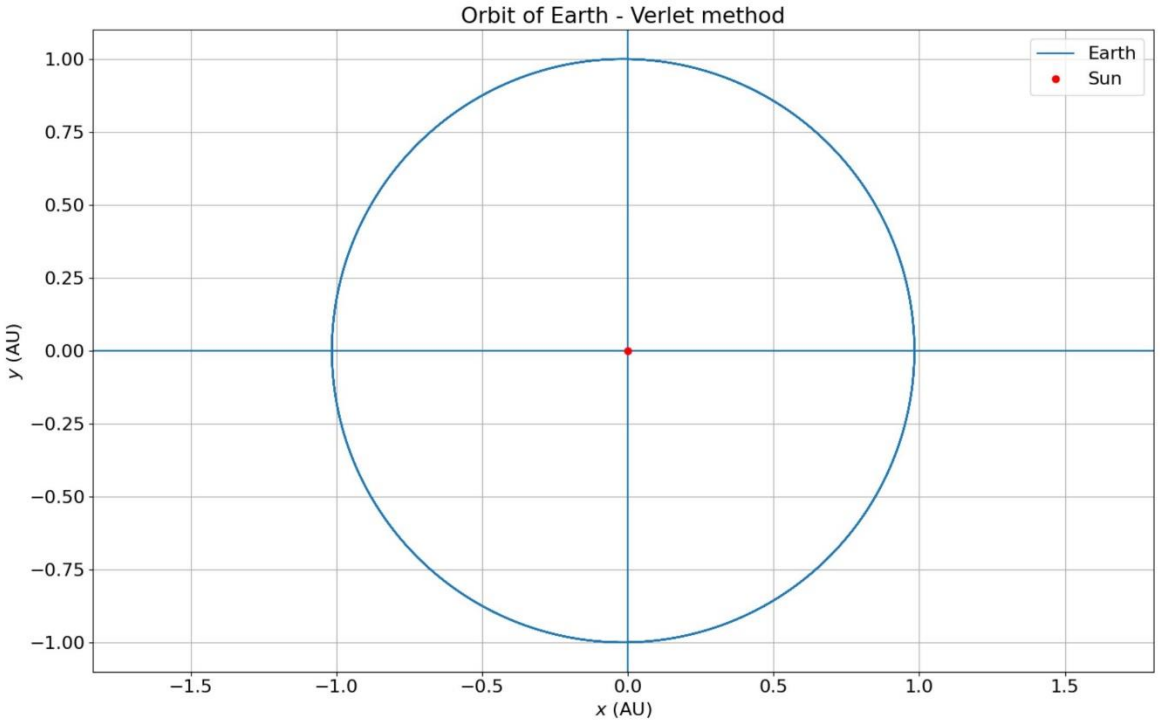

Figure 2.2*: The orbit of the Earth plotted by Verlet method. Note that the red dot at (0,0) represents the Sun, whereas the blue line represents the orbit of the Earth. The scales of x-axis and y-axis were set to equal.*

Although they are in different units for x and y positions, figure 2.1 and 2.2 shows the similar orbit for the Earth around the Sun, as expected.

Part b)

Using the same Bulirsch-Stoer method, the orbit of the Pluto was plotted with a positional accuracy of δ = 1 km/year, as shown in Figure 2.3. The initial position and velocity in x-direction were 4.4368 * 10^{12} m and 0 m/s, whereas the initial position and velocity in y-direction were 0 m and 6.1218 * 10^{3} m/s. The interval was set to H = 1 year so that one complete revolution about the Sun could be displayed.

Knowing the orbits of both planets, the orbits of the Earth and the Pluto were put together in Figure 2.4 with the Sun at (0,0)

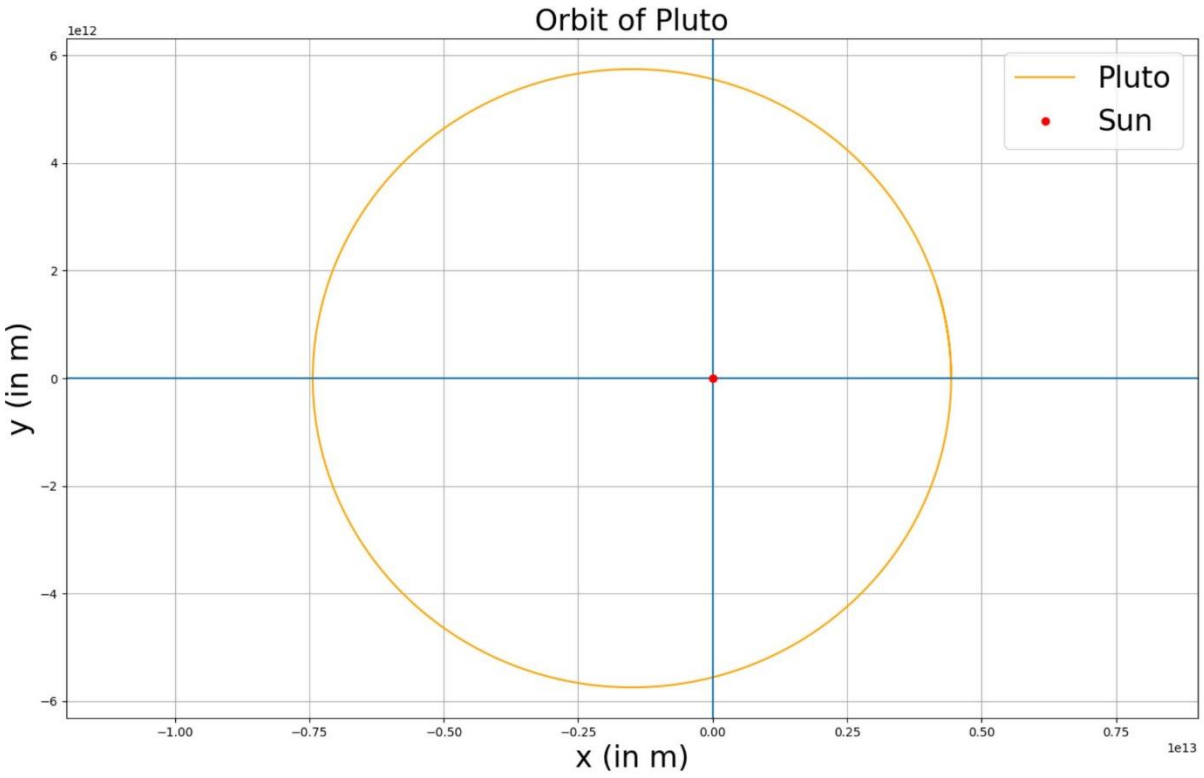

Figure 2.3: The orbit of the Pluto by Bulirsch-Stoer method. *Note that the red dot at (0,0) represents the Sun, where the orange line represents the orbit of the Pluto. The scales of x-axis and y-axis were set to equal.*

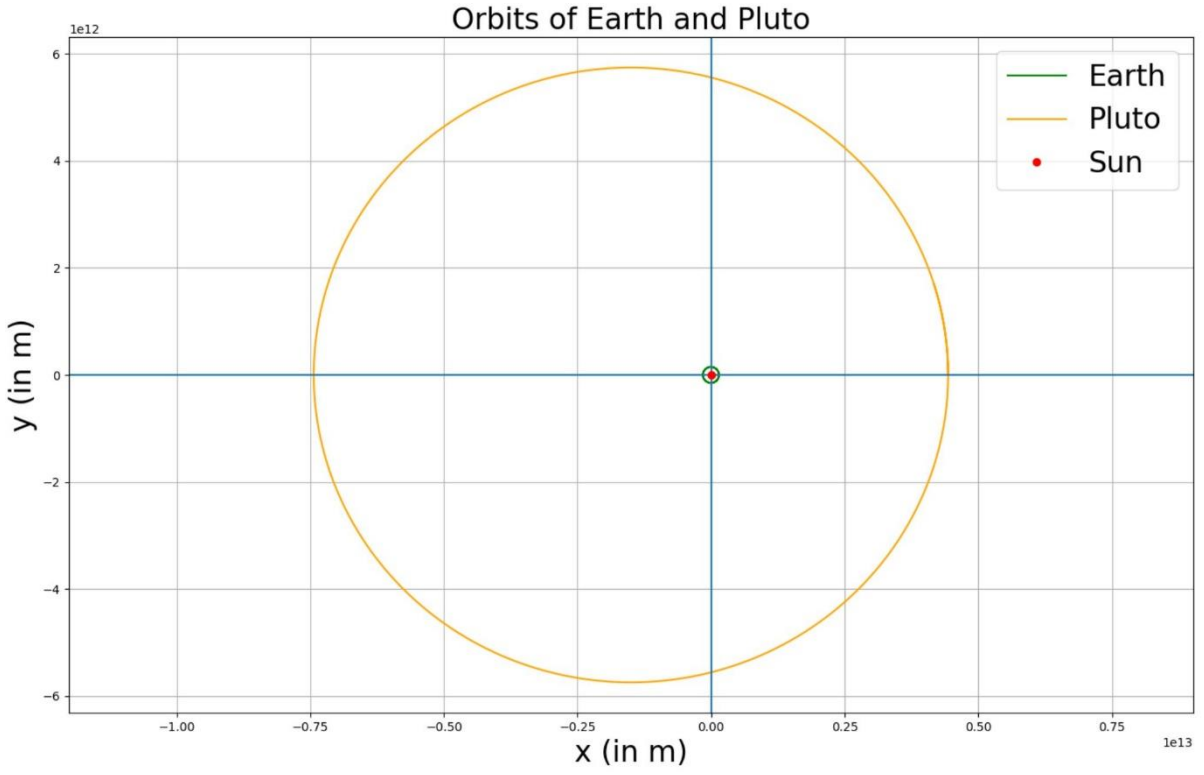

Figure 2.4: The orbits of the Earth and Pluto by Bulirsch-Stoer method. *Note that the red dot at (0,0) represents the Sun, where the green and orange lines represent the orbit of the Earth and the Pluto, respectively. The scales of x-axis and y-axis were set to equal.*

Note that the orbit of Pluto has much larger distance to the Sun that that of the Earth does, as expected by the initial position of Pluto being approximately 30 times greater than that of the Earth. Also, the Sun is located slightly off from the center of the orbit for Pluto.

Question 3

Part a)

The time-independent Schrodinger equation is given by following:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + V(x)\,\psi(x) = E\psi(x) \qquad \text{[eq 3.1]}$$

Using method of separation of variable, write the wave function as following:

$$\psi(x) = R(r)\,Y_l^m(\theta,\ \phi) \qquad \text{[eq 3.2]}$$

Where m and l are spherical harmonic degree and order. Then the time-independent Schrodinger equation can be solved as:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r) - E)\,R = l(l+1)\,R \qquad \text{[eq 3.3]}$$

In this question, the behaviour of the bound states of hydrogen are being studied, so the potential energy is given as following:

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r} \qquad \text{[eq 3.4]}$$

The time-independent schrodinger equation can also be written a pair of coupled first order ODEs:

$$S = \frac{dR}{dr} \qquad \text{[eq 3.5]}$$

$$\frac{dS}{dr} = \frac{l(l+1)\,R}{r^2} + \frac{2m(V(x) - E)\,R}{\hbar^2} - \frac{2S}{r} \qquad \text{[eq 3.6]}$$

Part b)

The energy level of a hydrogen atom can be obtained using following formula:

$$E = -\frac{E_0}{n^2} \qquad \text{[eq 3.7]}$$

Where E_0 is 13.6 eV, and n is the energy level. Therefore E_1 is -13.6 eV and E_2 is -3.4 eV. By the equation above, energy of hydrogen is independent of order l, therefore E_2 is -3.4 eV when l=1 or 0. These energies are the eigen energies, they are the energies that converge and can be obtained using secant method. The results are E_1 = -13.494 eV and E_2 = -3.387 eV when l = 0, and E_2 = -3.401 eV when l = 1. The theory predicts that eigen energies will not differ by changing l, and numerical value shows that they differ slightly.

By making the value of target energy smaller, the eigen energy obtained will be closer to the theoretical value. The numerical value can also be more accurate by making step size smaller or making total length larger.

Part c)

The normalized eigenfunction R for cases when n=1 and l=0, n=2 and l = 0, n=2 and l = 1 are plotted as following:

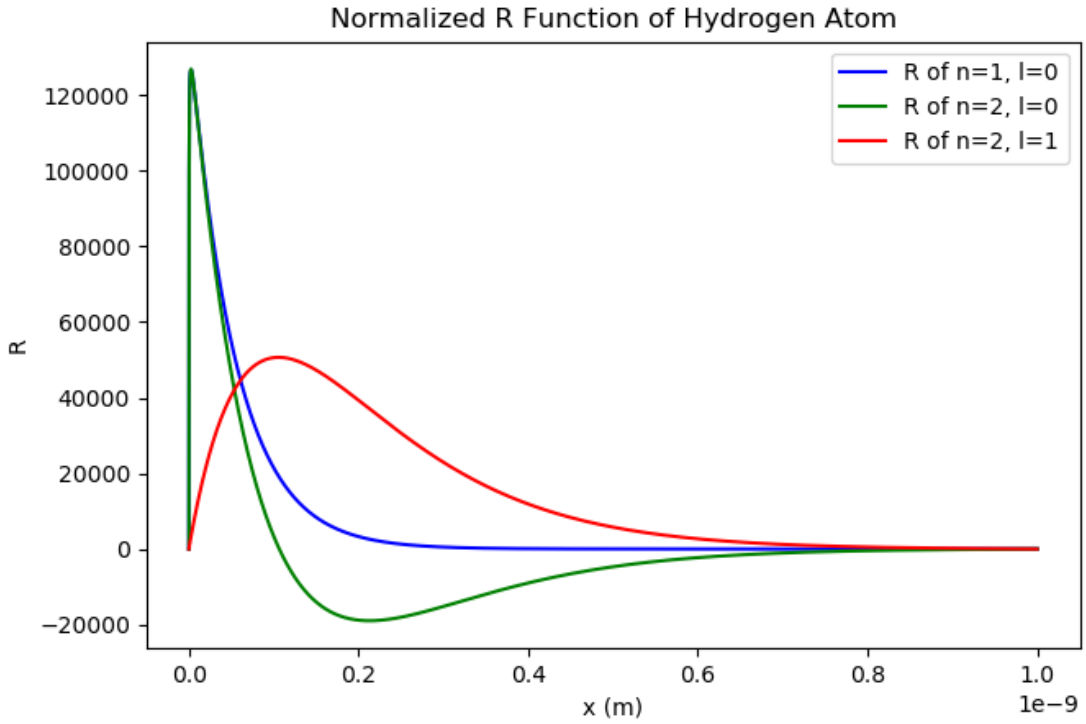

Figure 3.1: Normalized R function of three different cases; R of n=1, l=0, R of n=2, l=0, and R of n=2, l=1

This graph shows the normalized R function of hydrogen atom with various energy levels n and order l, All three functions converge to 0 as r increases approaches infinity. Noticeably, the R function crosses 0 once if n=2, and it does not cross 0 if n=1.

The probability density function R^2can be plotted and they are shown as following:

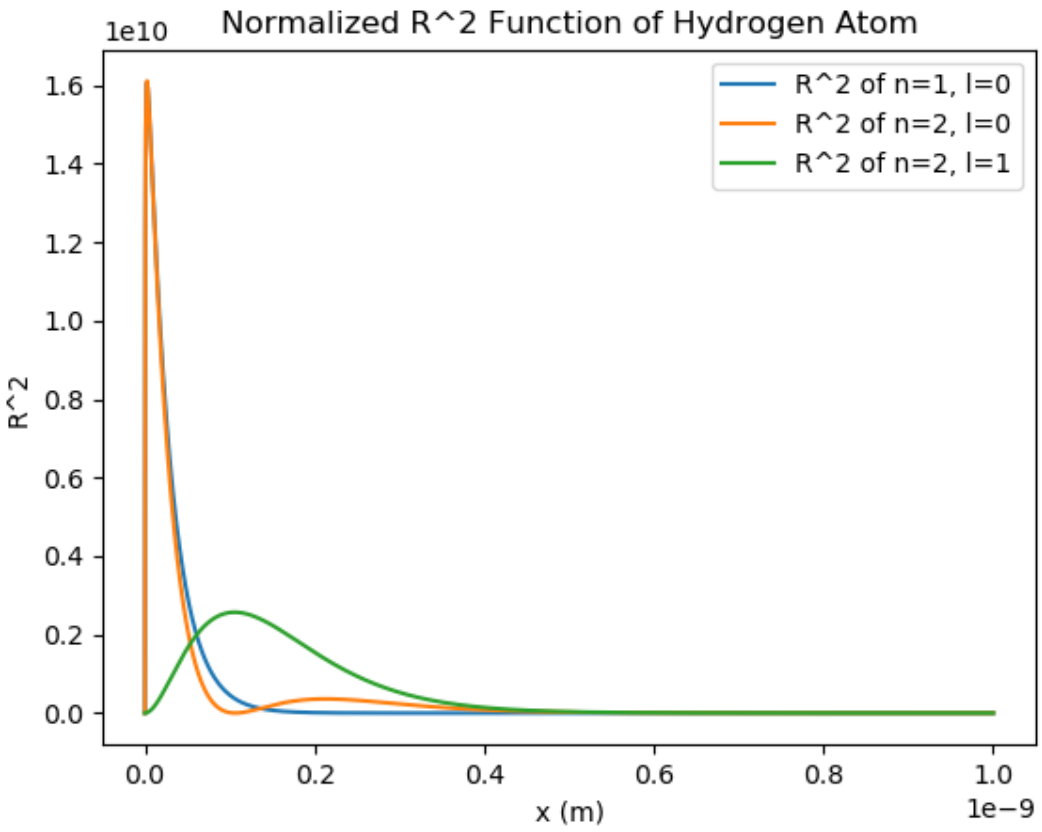

Figure 3.2: Normalized R^2 function of three different cases; R of n=1, l=0, R of n=2, l=0, and R of n=2, l=1

R^2 functions have similar shape as R functions, and they are the functions used for normalization, therefore the integration is 1 for all three functions.

Part d)

Theoretical curves for R function are not normalized, their values are extremely large compared with numerical curve, therefore they are scale down, so that their shapes can be compared:

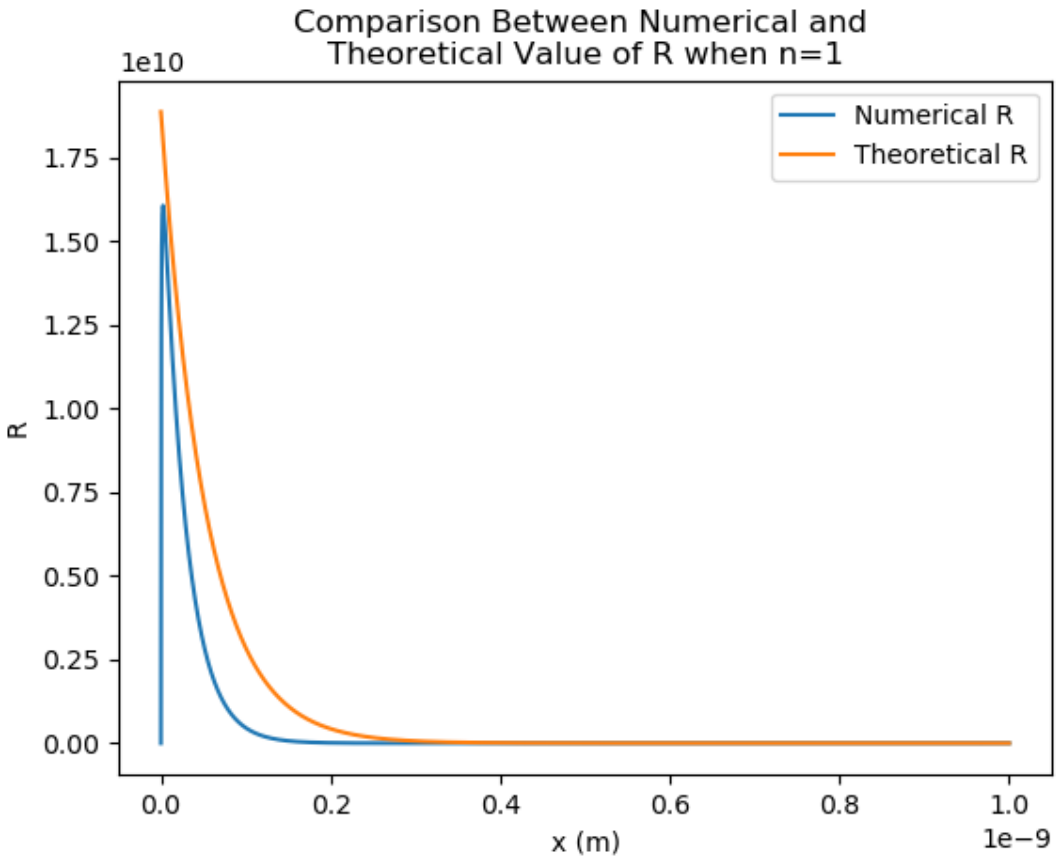

Figure 3.3: Comparison between numerical and theoretical curves of function R when n=1

This graph shows that when n=1, numerical and theoretical value for R have similar shape, However, the theoretical curve approaches infinity as x approaches 0, but the numerical curve approaches 0 as x approaches 0. This inaccuracy is caused by boundary condition initially set, the numerical curve is set to be zero when x=0. When n=2, the curves comparison is following:

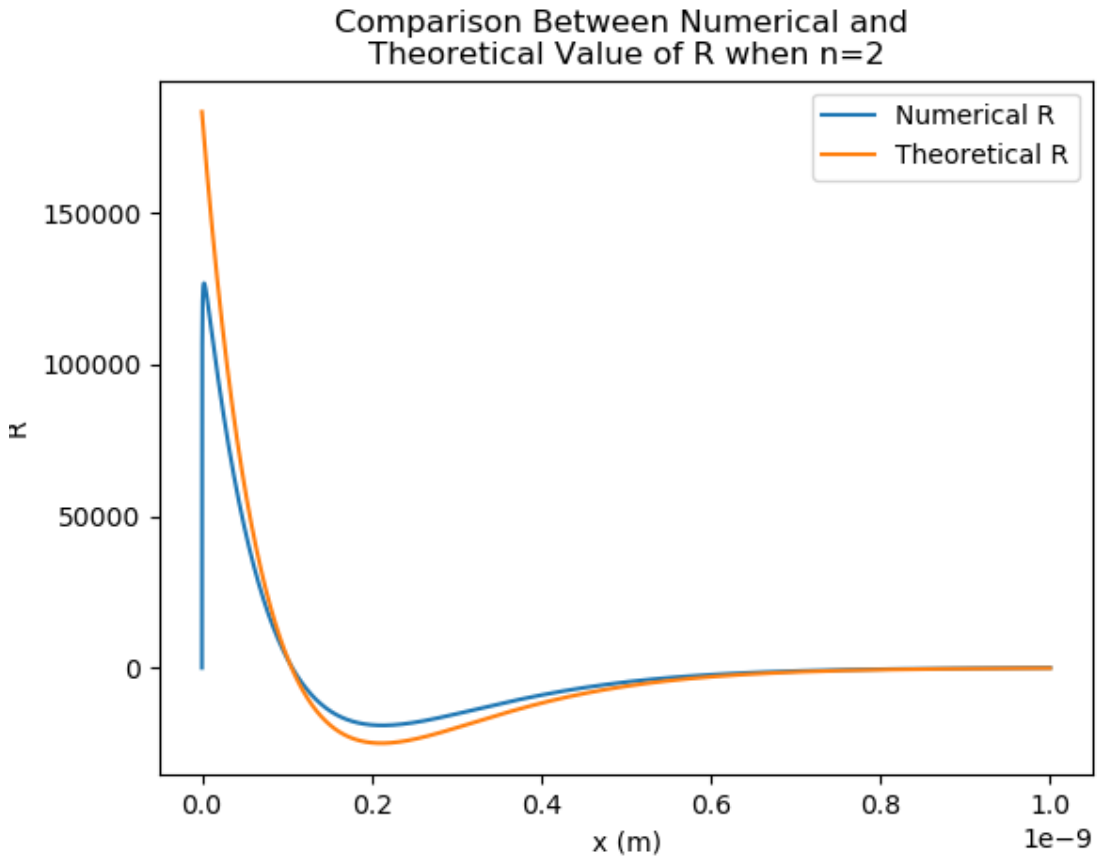

Figure 3.4: Comparison between numerical and theoretical curves of function R when n=2

This graph shows the comparison between numerical and theoretical values of R when n=2, their shapes are similar, they both pass zero once, and they both have a global minima. However, just like graph for n=1, they differ when x approaches 0, and this difference is again caused by the boundary condition.

Appendix A – Complete time steps for Question 1 Part c

[0.0, 0.02, 0.06, 0.13528079863550196, 0.19073809550105747, 0.23728125510028336,
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