PHY407 Lab7

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Oct 2020

Question 1

a)

We repeat the RK4 method from Lab 06 but with adaptive time stepping. We use have an initial h of 0.01. We obtain the orbit as shown below in Fig 1, superimposed onto our previously obtained orbit with a fixed time step for N = 10000 points, or h =0.001s. The two methods should have a similar accuracy. We solve over 10 seconds.

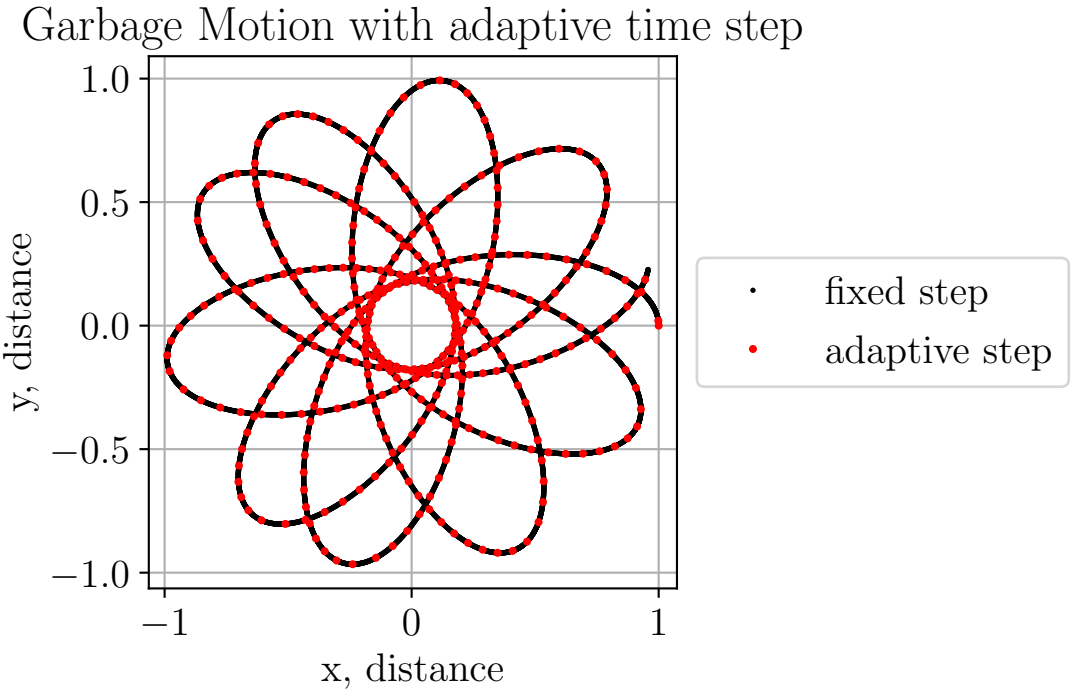

Figure 1: We obtain the above orbit with a fixed step of h = 0.001 for the fixed step method, and an initial step of h = 0.01 for the adaptive method.

We see that the adaptive step method uses fewer points to obtain the shape of the orbit, despite a same initial step size. Essentially, we get the same information on orbit shape and size at a lower point resolution.

b)

We are instructed to consider the time of the two solutions, one with a fixed time step and the other with the adaptive time step. We use the time() before and after each solver loop to call for the time and took the difference. We printed the time it took for both methods, our output can be seen below for one run can be seen below (the times are expected to be within ±0.1s of the below values should the reader run it). In our last particular run, the adaptive step method took 0.173s while fixed terms took 0.775s, the latter being significantly slower.

This is expected: we can see in Fig 1 the adaptive step method requires far fewer steps to achieve a similar accuracy and thus takes less computational time.

Output

```
Time required for adaptive steps with RK4 0.192 seconds
Time required for fixed steps with RK4 0.815 seconds
```

c)

We want to explore the relationship between step size and point in time in the integration in the adaptive time step method. We plotted the step size against the time point using the method, as shown in Fig 2. We can see a oscillatory sawtooth pattern reflective of the somewhat oscillatory nature of the x , y coordinates in the orbit.

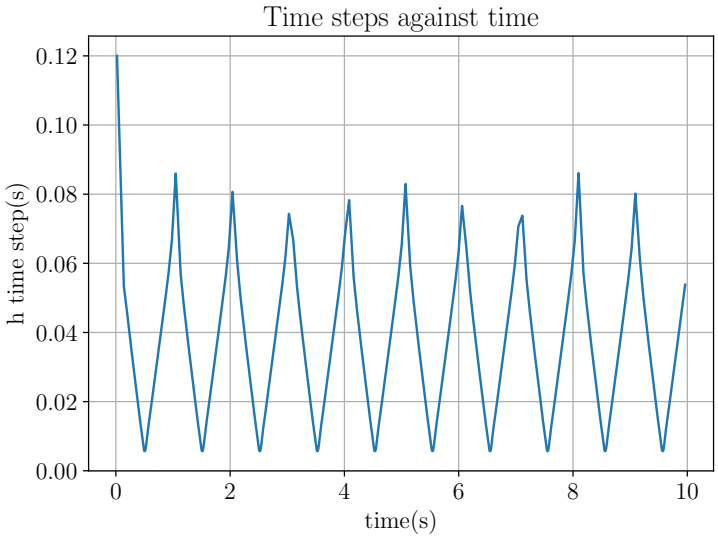

Figure 2: We plot the time steps h against time for the adaptive time step method.

We can see that the size of h depends on the radial distance – the way we compute the error functions with $\epsilon_x^2 + \epsilon_y^2$ heavily eludes to that. We plot $r = x^2 + y^2$ against time, seen in Fig 3. Maxima in h rougly correspond to the peaks in r, and similarly with its minima.

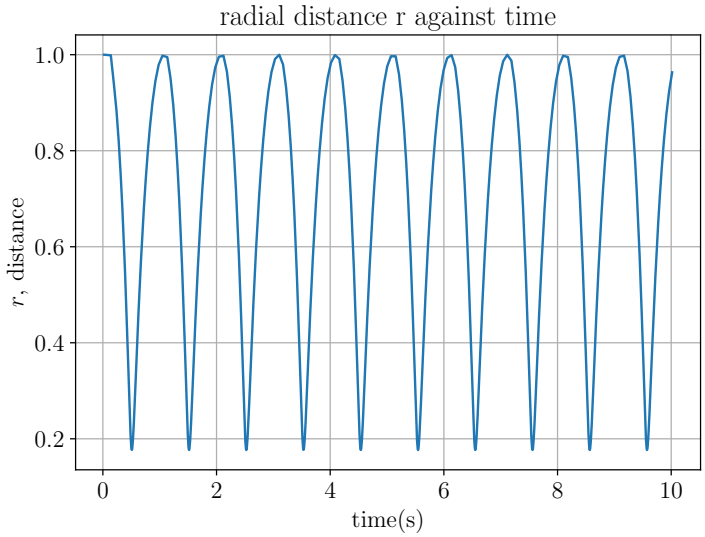

Figure 3: We plot r against time for the adaptive time step method.

Question 2

a)

We want to solve the second order ODEs

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -GM\frac{x}{r^3} \tag{1}$$

$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} = -GM\frac{y}{r^3} \tag{2}$$

We solve this simulatenously as a system of 4 single order ODEs:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = vx \tag{3}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = vy \tag{4}$$

$$\frac{\mathrm{d}v_x}{\mathrm{d}t} = -GM\frac{x}{r^3} \tag{5}$$

$$\frac{\mathrm{d}v_y}{\mathrm{d}t} = -GM\frac{y}{r^3} \tag{6}$$

with the initial values (in SI units):

$$x = 1.4710 \times 10^{11} \qquad y = 0 \tag{7}$$

$$v_x = 0 \qquad v_y = 3.0287 \times 10^4 \tag{8}$$

And M = Mass of the sun as provided in the text.

We adapted `burlisch.py` as well as the solution for 8.12 provided from the Professor as provided to solve this system using the Burlirsch-Stoer method. We do this to a positional accuracy of 1Km/Hr and a step of $H = 1$week, over an integration time of 5 years (5 revolutions). We obtain the plot as seen in Fig 4.

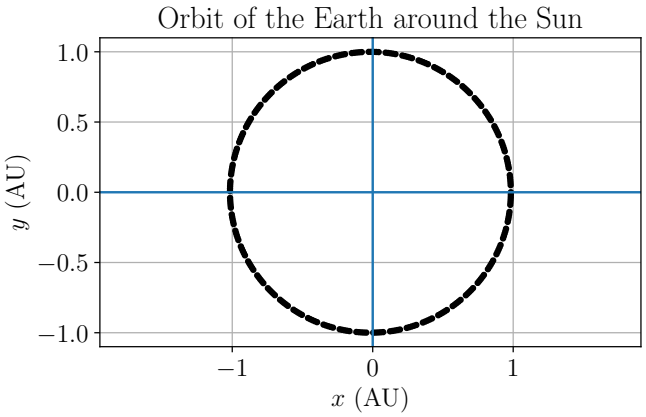

Figure 4: Orbit of the earth for 5 revolutions with a time step of $H = 1$week

b)

We do this again for Pluto. This time our initial values are:

$$x = 4.4368 \times 10^{12} \qquad y = 0 \tag{9}$$

$$v_x = 0 \qquad v_y = 6.1218 \times 10^{3} \tag{10}$$

We went for $H = 200$ weeks (we will explain the reasoning in the next paragraph). We obtain the plot as seen in Fig 5. We can see the asymmetric nature elliptic orbit in the figure.

We are asked to choose a time step that ensures the code runs fast. We assume that means it runs as at the same speed as the previous part when we resolved the earth orbit for 5 years with a time step of a week We experimented with the time steps - the orbit of pluto is ≈ 250 years and thus we wanted to choose a time step that is roughly the same proportion as our previous integration. $H = 200$ weeks roughly does the trick. We confirmed this by timing it and printing the times it took to resolve both ode systems and found that the their speed was of the same order of magnitude. We can see the printed output below. We can see we obtained roughly the same computational speed.

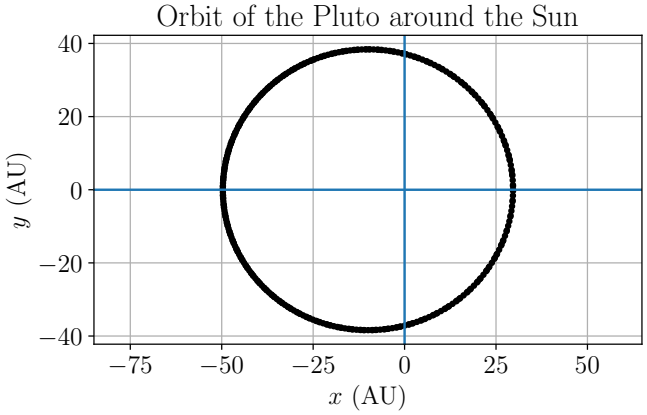

Figure 5: Orbit of Pluto

Output

Output Question 2a

The time it takes to run the loop is, 0.15s with h step of 1 weeks

Output Question 2b

The time it takes to run the loop is, 0.12s with h step of 200 weeks

Question 3

b)

We rewrite equation 2 from the lab manual to be a system of 2, first order differential equations.

$$\frac{dR}{dr} = S$$
$$\frac{dS}{dr} = (l(l+1)R + \frac{2mr^2}{\hbar^2}(V(r) - E) - 2rS)/r^2$$

We references to Newman's code `squarewell.py` and the secant method. We use the RK4 method in the `solve` function to find the value of the wave function at out boundary condition at r_∞, we then adjust the energy using the secant method until we have our boundary condition satisfied within our desired target value.

State	Numerically Computed Energy
Ground state, n = 1, l = 0	-13.5521359476493457 eV
First excited state, n = 2 , l = 0	-3.394360103961082 eV
First excited state, n = 2 , l = 1	-3.401276518385415 eV

Table 1: The eigenvalues energy print outs, for $h = 0.001a$, $r_\infty = 20a$ where a is the bohr radius

State	Numerically Computed Energy
Ground state, n = 1, l = 0	-13.000000306107804 eV
First excited state, n = 2 , l = 0	-3.2501006733496487 eV
First excited state, n = 2 , l = 1	-3.2501003303829203 eV

Table 2: The eigenvalues energy print outs, for $h = 0.001a$, $r_\infty = 200a$ where a is the bohr radius

Known solutions to for the hydrogen atom predict that the energy level is $\frac{-13.5eV}{n^2}$, we notice that there is a slight energy difference in the excited state between the systems where l = 0 and l = 1. We see a bigger difference in energy numbers with with a 10 fold increase in the $r = 200a$, table 2 than with a 10 fold decrease to our step size h, table 3. make h 10x smaller

d)

We compute the wave functions by using the energies found in part b, and using RK4 on the differential equations. We commute the integral of the absolute wave function squared to find the normalization factor. We then plot the normalized analytical solution as found on hyperphysics. We see in figure 6 that the computational solutions are perfectly overlayed by the analytical solutions. We see with the computational solution that there is an additional zero crossing close to the center of the atom which is a result of the divergence in the computational solutions. The computational solutions are additionally plotted in figure 7.

State	Numerically Computed Energy
Ground state, n = 1, l = 0	-13.552142107679513 eV
First excited state, n = 2 , l = 0	-3.394360920991721 eV
First excited state, n = 2 , l = 1	-3.401276759466438 eV

Table 3: The eigenvalues energy print outs, for $h = 0.0001a$, $r_\infty = 20a$ where a is the bohr radius

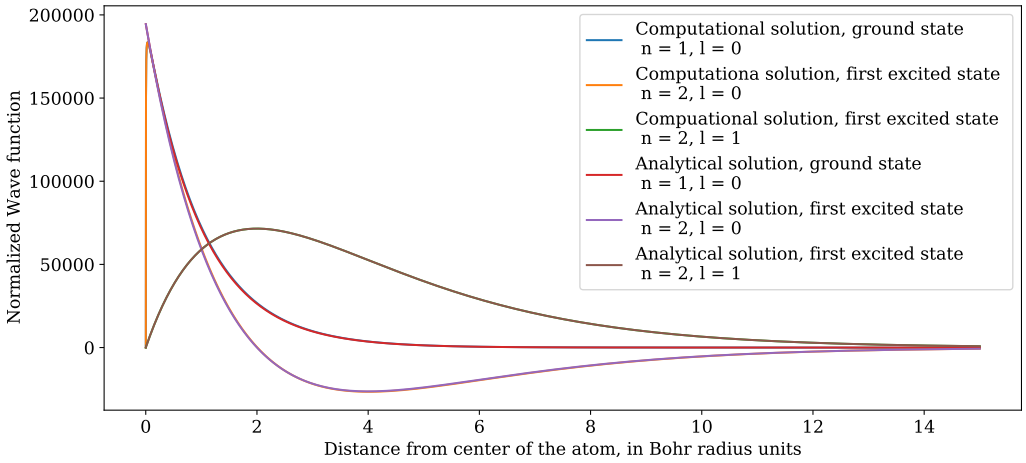

Figure 6: We plot the wave function solutions for the computational and analytical solutions

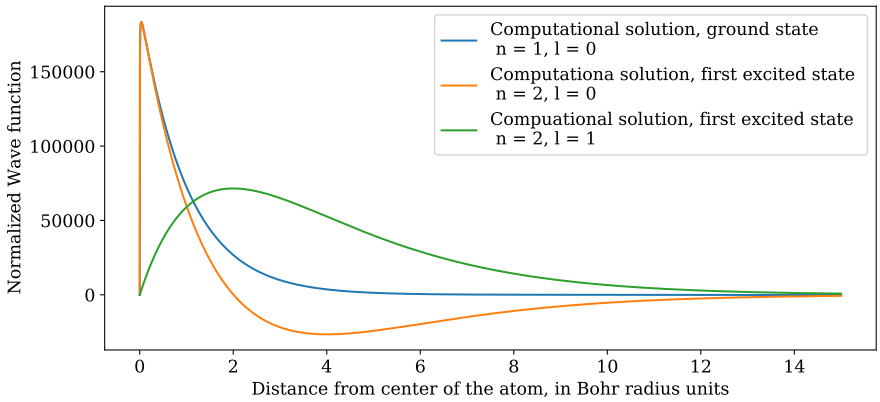

Figure 7: We plot the wave function solutions for the analytical solutions