PHY407 Lab 7: ODEs Part II

Work Distribution:
Emma Jarvis: Q3
Lisa Nasu-Yu: Q1, Q2

September 24, 2023

1 Space Garbage

1.a

We simulate the trajectory of a ball around a space rod to an accuracy of order -6, using adaptive steps and the 4th order Runge Kutta method. The uniform time-step simulation code was provided. We can see from Fig. 1 that the points for the adaptive step are slightly closer, indicating a shorter time-step, on the tighter curves of the trajectory.

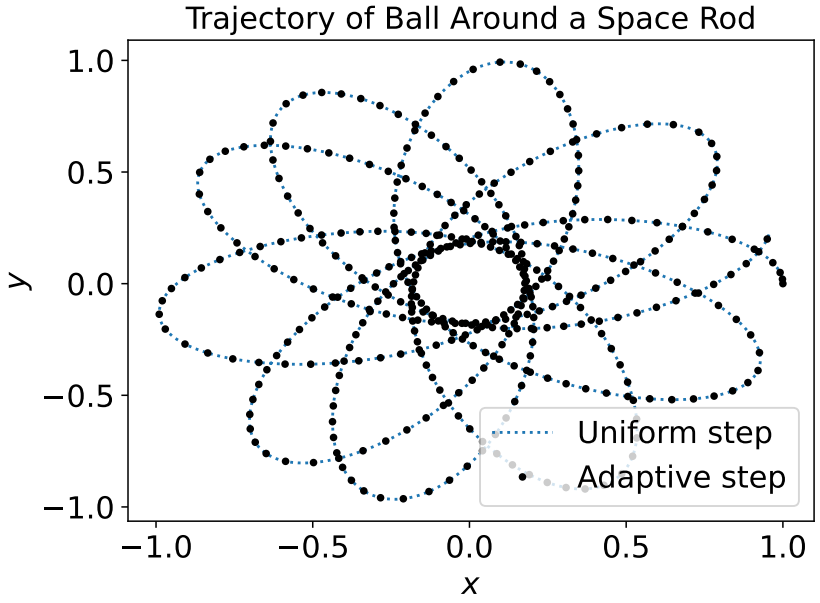


Figure 1: Trajectory of a ball around a space rod using adaptive steps and the 4th order Runge Kutta method.

1.b

The adaptive time-step simulation with an initial step of h=0.01s and target accuracy of order -6 took 0.07945466041564941 s. The uniform step simulation with a step size of h=0.001s took 0.4124011993408203 s. We see that the adaptive time-step method is indeed faster.

1.c

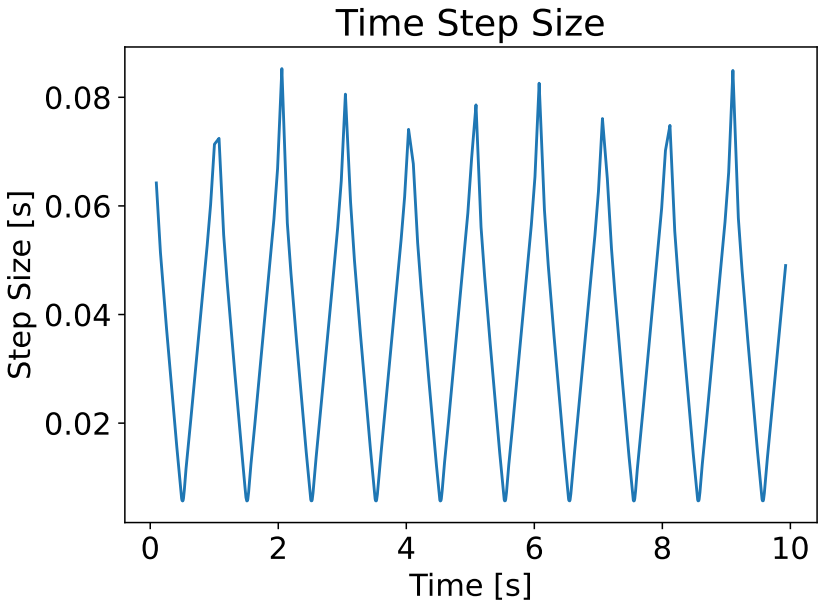


Figure 2: Time-step sizes for the adaptive time-step RK4 method.

Fig. 2 shows that the time step size oscillates for the adative time-step RK4 simulation of the trajectory of the ball. This is reflective of the ellipsoidal orbital motion of the ball, disregarding precession. While the motion of ball is in the relatively flat portion of the orbit, the time-step size is large. While the motion of of the ball is in the tightly curved portions of the orbit, the time-step size is small.

2 Quantum Oscillators

2.a

Using the secant method with RK4, we compute the energy levels of the first 3 states for a time-independent wave with harmonic potential $V(x) = V_0 x^2/a^2$, where we took $V_0 = 50\text{eV}$ and $a = 10^{-11}\text{m}$.

State	Energy [eV]
0	138.02397131916698
1	414.07191653946415
2	690.1198621106303

Table 1: Energy levels of the first 3 states for $V(x) = V_0 x^2/a^2$

The 3 energy levels are evenly spaced to an accuracy on the order of e^{-7}, which is indeed lower than our target accuracy of e^{-3}. Here, e is the elementary charge.

2.b

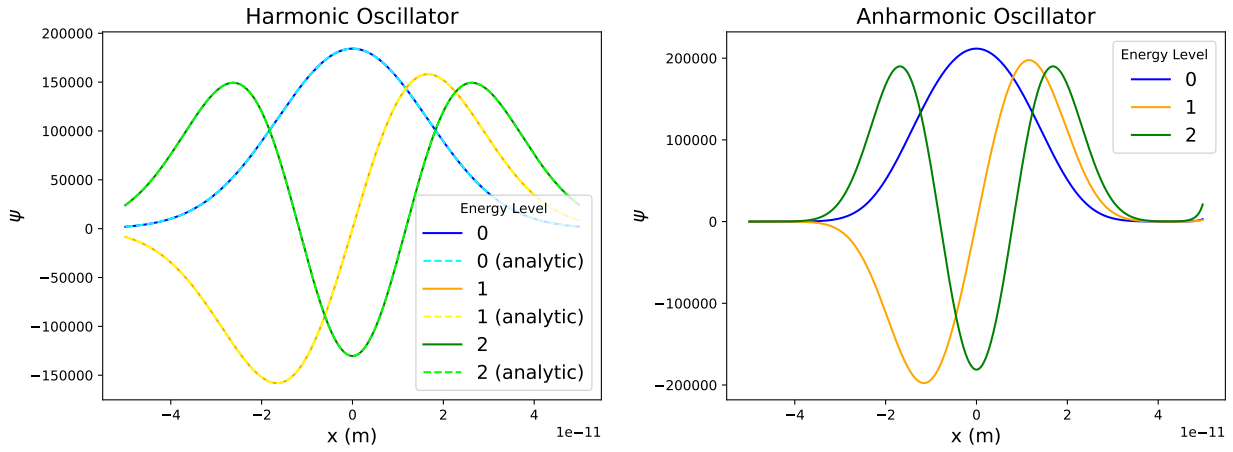
We repeat part a), this time for a potential $V(x) = V_0 x^4/a^4$

State	Energy [eV]
0	205.30690346934986
1	735.6912470402124
2	1443.5694214051407

Table 2: Energy levels of the first 3 states for $V(x) = V_0 x^4/a^4$

2.c

ψ was normalized using the equations given in the link provided in the lab assignment. In each state, we computed $w = \frac{2}{2n+1} E_n/\hbar$.



(a) Harmonic

(b) Anharmonic

Figure 3: Normalized probability amplitudes of the first 3 states for a harmonic and anharmonic oscillator. For the harmonic oscillator (Figure a), the analytic solution is plotted in dotted lines to show our solution indeed matches.

3 Oscillating Chemical Reactions

We then created a program that solves the equations for the Brusselator given by 1 and 2 using an adaptive Bulirsch-Stoer method. In this equation we set $a = 1$ and $b = 3$ as specified in the question and we set the the initial conditions to be $x = y = 0$. The accuracy was set to be of order -10. To create the adaptive Bulirsch-Stoer method, we started with the uniform step Bulirsch-Stoer method code provided in `bulirsch.py`. We then modified this code so that if n (the number of modified midpoint steps) is bigger than 8 when the error converges, we set H to $H/2$ and redid the calculation. We started with a single time interval of size $H = 20$. The pseudocode for this method is provided. Using this, we obtained solutions for x and y and plotted them as a function of t (the adaptive time steps) and this can be seen in Fig. 4. This shows that the points are closer together where the variables are changing rapidly.

$$\frac{dx}{dt} = 1 - (b+1)x + ax^2y \tag{1}$$

$$\frac{dy}{dt} = bx - ax^2y \tag{2}$$

```
"""
Pseudocode: Adaptive Bulirsch-Stoer Method

    Author: Emma Jarvis, October 2021

    Goal:
        Write a program that solves the B-Z reacion equations using adapive
        Bulirsh-Stoer method from t = 0 to t = 20. Allow maximum for n = 8
        modified midpoint steps before dividing interval in half and trying again.
        Then plot x and y as functions of time (on same plot) and add dots to show
        boundaries of the time intervals.

    1. Write function f(r) to compute the function that returns x and y

    2. Set initial conditions x0 = 0, y0=0 and empty lists for x and y points
       and array r with initial conditions. And array of t points from 0 to 20.

    3. Set initial H = 20

    4. Carry out the operations of B-S method on each interval as normal,
       subdividing each one into n modified midpoint steps and then
       extrapolating the results as we increase the value of n. For each n,
       calculate the error and if the error meets the required accuracy we are
       done.

    5. If n reaches 8 and we have not met the accuracy goal, abandon
       calculation and subdivide current time interval of size H into two
       smaller intervals of size 0.5H. Then apply B-S to each of these
       intervals in turn. Do this with recursion:
           - Write a function step(r, t, H) that takes arguments r(x,y),
             initial time t, interval length H and returns r at t+H. This
             function performs the B-S calculation until either the error is
             met of n reaches 8.
           - Then if it fails, it calculates seperately the solution for the
             1st and 2nd halves of the interval seperately from t to t + H:
                 r1 = step(r, t, H/2)
                 r2 = step(r1, t + H/2, H/s)
           - Then these functions call themselves until subdividing as manu\y
             times as needed to meet the required accuracy


    6. Continue subdividing intervals until the required accuracy is reached.
```

```
        Any interval that fails to meet the accuracy before n = 8 will be
        subdivided into 2 parts.

        Note: intervals may be subdivided different number of times. So the
        ultimate size of the intervals used for different parts may be
        different.
"""
```

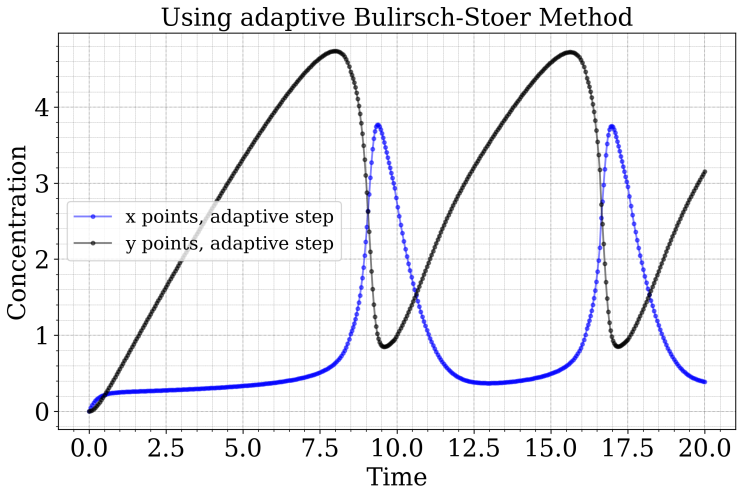


Figure 4: Solution to Brusseltator equaions using an adaptive Bulirsch-Stoer method. method.