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Computational Physics Lab Report-6

Aim:

Q1.

*Define a function *Eul* ($f(x,y)$, x_0, y_0, h, N) that will return the the value of y after N steps of size h. Use this to solve the two problems below:

***ODE1: a)** Solve the ODE $(1+x)\frac{dy}{dx}-2y+18x=0 \; with \; y(0)=4$ and interval h=0.05 in the interval (0, 3) (*i.e.* 60 steps) by using Euler's method. Plot the analytical solution ($y=-5x^2+8x+4$) and the numerical solution in the same figure to visually inspect the outcome.

b) Plot the absolute error at each point for Euler's method as a function of *x*.

Q2.

***Coupled ODE 1:** While solving a set of *M* coupled ODEs the function '*Eul*' may be extended to return an array *Y= Eul* ($F(x,y)$, x_0, y_0, h, N,M), where *Y* is the *M*-dimensional array of solutions and *F* is a *M*-dimensional array of RHS functions for coupled ODEs. Using this modified function find the phase space trajectory of a particle of *unit mass* in a potential *V(x)*. You need to solve the Hamilton's equations of the system, given by:

$$\frac{dp}{dt}=\frac{-\partial H}{\partial x}$$

$$\frac{dx}{dt}=\frac{\partial H}{\partial p}$$

(a.) Start by taking simple harmonic oscillator potential $V(x)=\frac{1}{2}kx^2$, $k=1$ N/m. What is the period T of this oscillator? Use h=T/S with S=10, 100 and 1000 for the step size and follow the trajectory over a time 10 T considering the initial condition (x, p_x) = (1.0, 0.0). Fro all the cases, compare the following

(i) Show the trajectory i.e. x and p as functions of time and also the phase space . Compare these with the analytical solutions.

(ii) The energy E is expected to be conserved. Plot the relative change in energy dE/E=(E_n-E)/E as a function of time, here E_n and E are respectively the numerically calculated energy and the actual energy respectively.

b) Now consider a double well potential $V(x)=(x^2-1)^2$. Start by plotting this potential for x = [-2, 2]. Considering phase space, plot the contours corresponding to different values of energy E. Analyse these to discuss the various kinds of trajectories possible in this potential.
For this new potential, repeat the same exercises as in **(a)** for the initial conditions (x, p_x) = (1.0, 0.1), (-1.0, 0.1) and (1.0, 10.0).

Q3.

***R-K 2nd order:** Define a function 'RK2 =($f(x,y)$, x_0, y_0, h, N)' which will return the solution of a ODE of the form $\frac{dy}{dx}=f(x,y)$ for N steps of size h using 2nd order Runge-Kutta (R-K) method.

Solve the ODE $(1+x)\frac{dy}{dx}-2y+18x=0 \; with \; y(0)=4$ and increment h=0.05 in the interval (0, 3) by using function RK2. Compare this with the analytical solution and that from Euler's method. Compare the absolute error in Energy with the results from the Euler's method.

Q4.

***Coupled ODE 2:** Extend the function 'RK2' to generalize it for M coupled ODEs as Y= $RK2$ ($F(x,y)$, x_0, y_0, h, N,M), where Y is the array of solutions and F is a M-dimensional array of RHS functions for coupled ODEs. Solve the following coupled ODE by R-K 2nd order method for x = [0.0 0.5] with h=0.05. I.C. are $y(0)=0$, $z(0)=1$.

$$\frac{dy}{dx}=-x-yz$$

$$\frac{dz}{dx}=-y-xz$$

Plot the solutions $y(x)$ and $z(x)$.

Q5.

***Coupled ODE 4:** Write a program to follow the motion of an electron (*e*) in an electric field *E(x, t)* and a magnetic field *B(x, t)*. Numerically determine the trajectory of an electron for 1 micro second with 1 nano second of time resolution by solving Lorentz force equation:

$$m\frac{d\vec{v}}{dt}=q(\vec{E}+\vec{v}\vec{B}).$$

Assume that the particle starts at the origin with velocity v = (1.0, 1.0, 1.0) m/sec for the following field configurations:
(i) Uniform magnetic field 10^{-4} Tesla along the z-axis.
(ii) Uniform magnetic field 10^{-4} Tesla along the z-axis and a uniform electric field 1V/m along the y-axis.

Visualize these trajectories by plotting different two dimensional sections (x-y) (x,z) etc.

How will you ensure that your step size is small enough? You can possibly check conservation of energy i.e. Kinetic + Potential. Show the accuracy to which your trajectory conserves energy as the particle evolves.

[Use parameters q=-1.6×10^{-19}C, m_e=9.11×10^{-31} Kg]

[Hint: Write down the Lorentz force equation in component form. That will give three coupled equations in velocity components. Position equations are directly solvable from obtained velocity values.]

Tools Used: Jupyter Notebook, Python, NumPy, Pandas, Matplotlib.

Theory:

1. Euler's Method is a first-order numerical procedure for solving ordinary differential equations (ODEs) with a given initial value. It is the simplest Runge–Kutta method.
   Euler's Method -
   $$y_{n+1} = y_n + hf(t_n, y_n).$$
   where f is the derivation of the given ODE (dy/dx), h is the step size and the initial value of y is given.
2. The Euler method is a first-order method, which means that the local error (error per step) is proportional to the square of the step size, and the global error (error at a given time) is proportional to the step size.
3. Euler Method is more accurate if the step size is smaller.

4. In numerical analysis, the Runge–Kutta methods are a family of implicit and explicit iterative methods, which include the Euler method, used in temporal discretization for the approximate solutions of simultaneous nonlinear equations.

   Second Order Runge-Kutta Method (RK-2) Formula-

$$k_1 = h*f(x,y)$$
$$k_2 = h*f(x + h/2,\ y + k_1/2)$$
$$y_{n+1} = y_n + k_2$$

5. In mathematics, an ordinary differential equation (ODE) is a differential equation whose unknown(s) consist of one (or more) function(s) of one variable and involves the derivatives of those functions.
6. Typically a complex system will have several differential equations. The equations are said to be "coupled" if output variables (e.g., position or voltage) appear in more than one equation.

Observations:

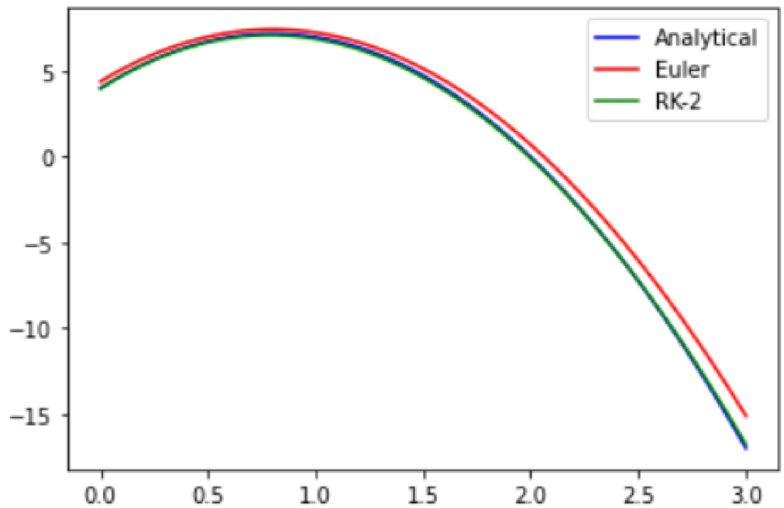
<u>For problems 1 and 3:</u>

From the graphs below, we see that Euler's Method overestimates the curve upon solving the ODE. We see that the curve estimated by Euler's Method is above that obtained by using an analytical function.

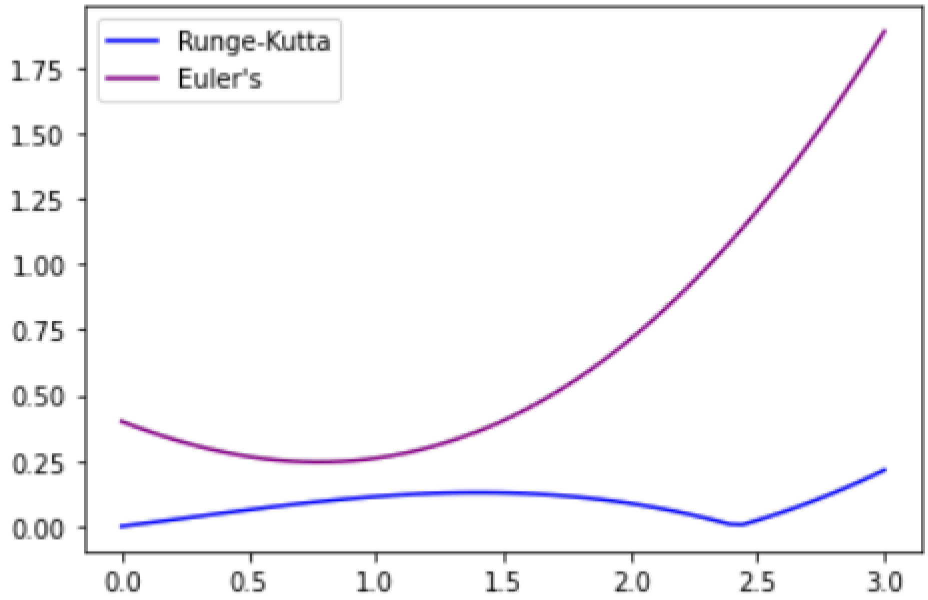
Runge-Kutta - second order method overlaps with the curve obtained using analytical function.

Graphs-

Numerical solution as a function of x
Analytical Solution as a function of x
Runge-Kutta Method as a function of x



Error in Euler's Method as a function of x
Error in Runge-Kutta second order method as a function of x



For problem-2:

Part - (a)
Part - (i)

The time period of the oscillation is given by $T = 2\Pi\sqrt{\frac{m}{k}}$, therefore the values of m and k are equal to 1, hence the time period is 2Π.

The time range goes from 0 to 10T.

On comparing the phase space graph with the analytical solution, we see that the plots overlap with each other as the step size becomes smaller, i.e, the numerical solution curves become elliptical, for the first case when h = T/10, we can get a spiral plot, and later for h = T/1000, we get an elliptical curve which matches with the analytical solution.

On comparing the x vs time and p vs time with the analytical solutions, we see that with a smaller step size, their graphs become sinusoidal and overlap with the analytical solutions.

Graphs-

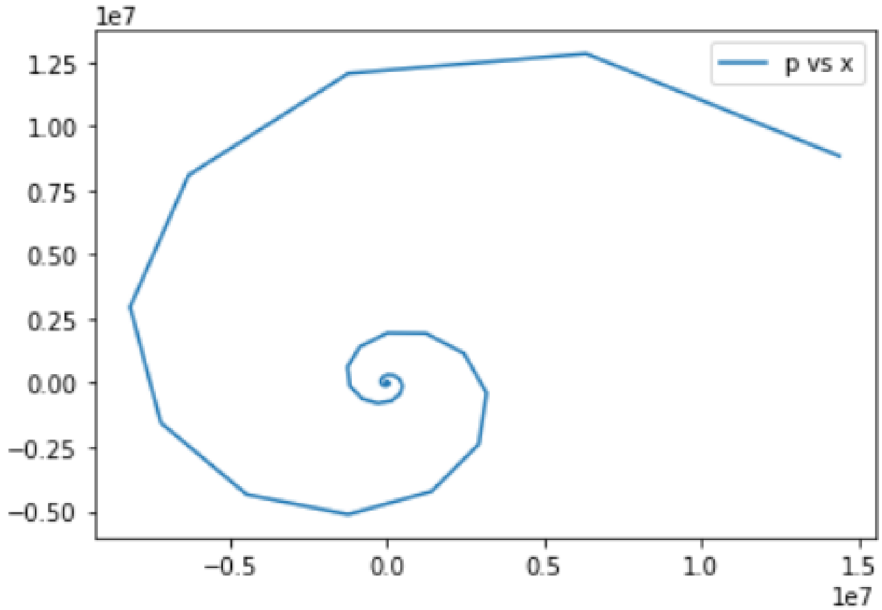
For h = T/10

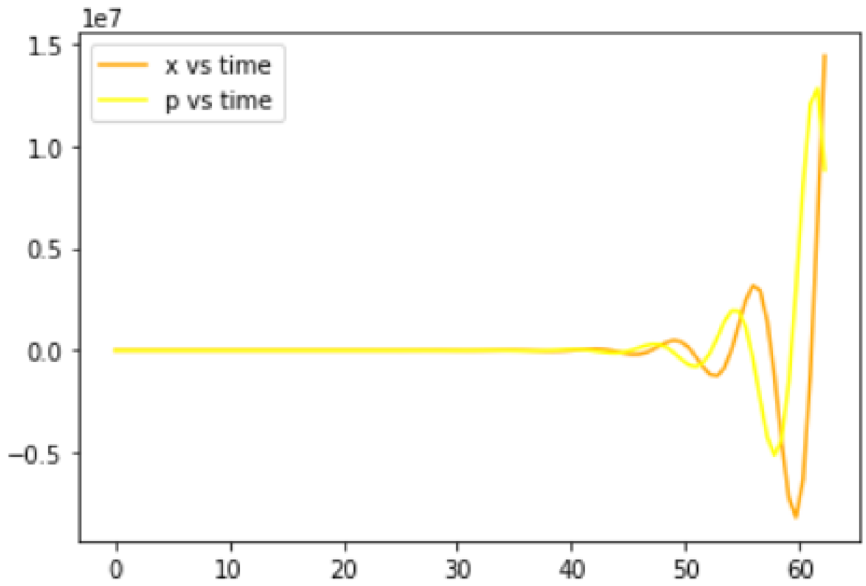
p vs x

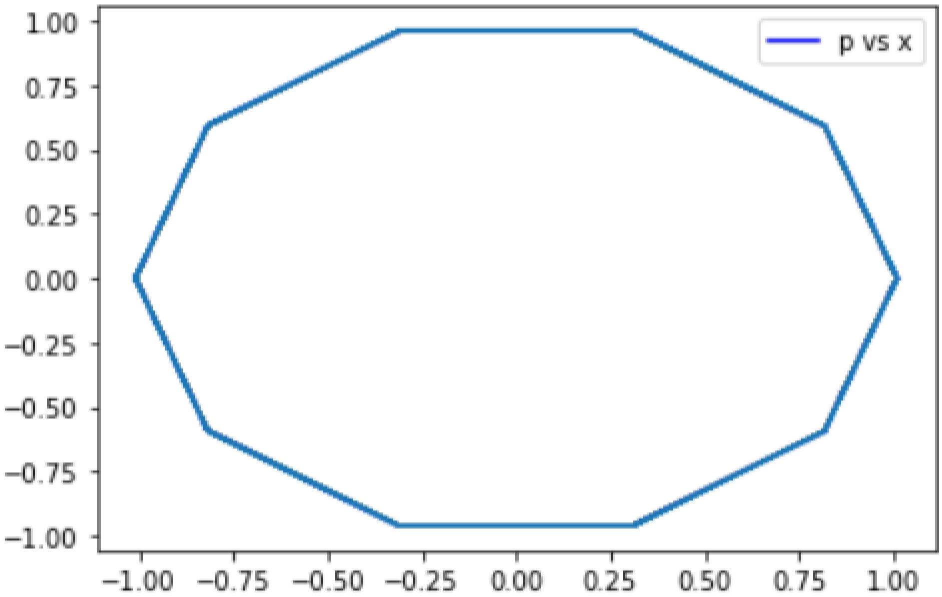
x vs time

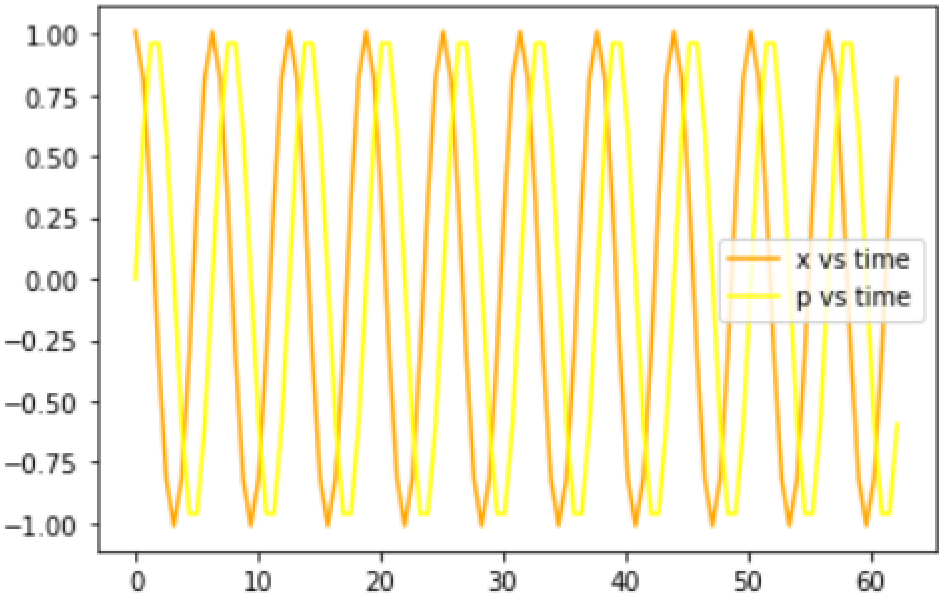
p vs time

Comparison of phase space, x vs time and p vs time with analytical solutions









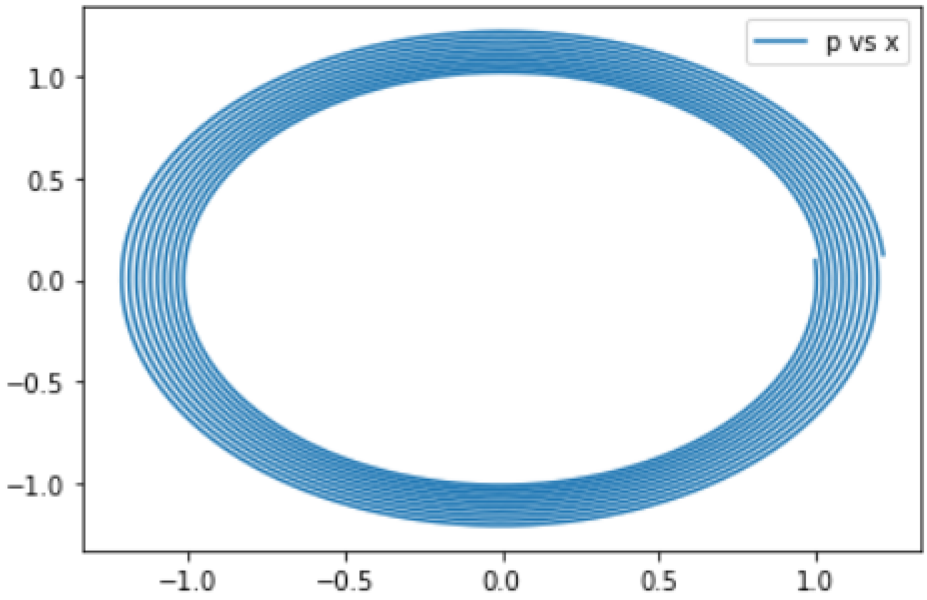
For h = T/100

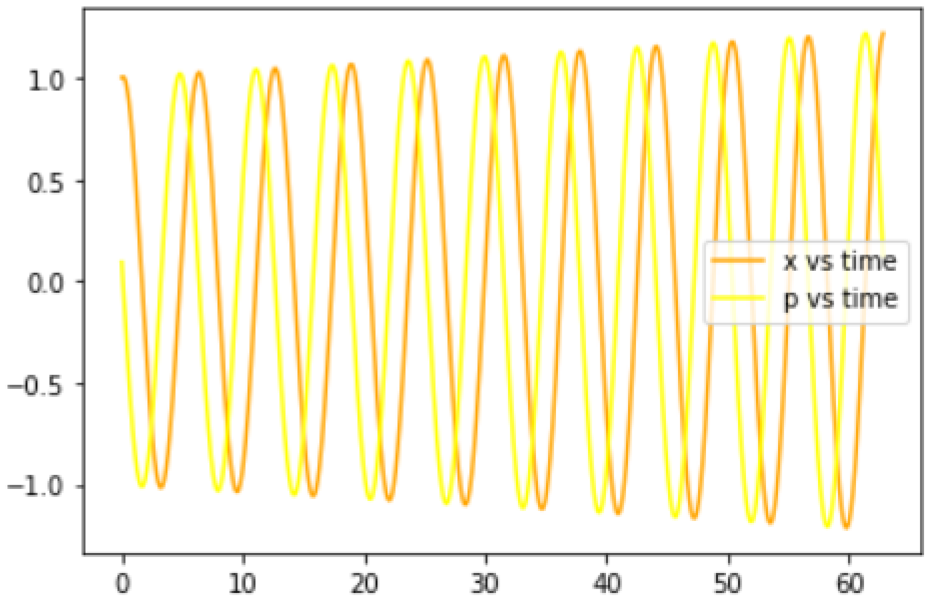
p vs x

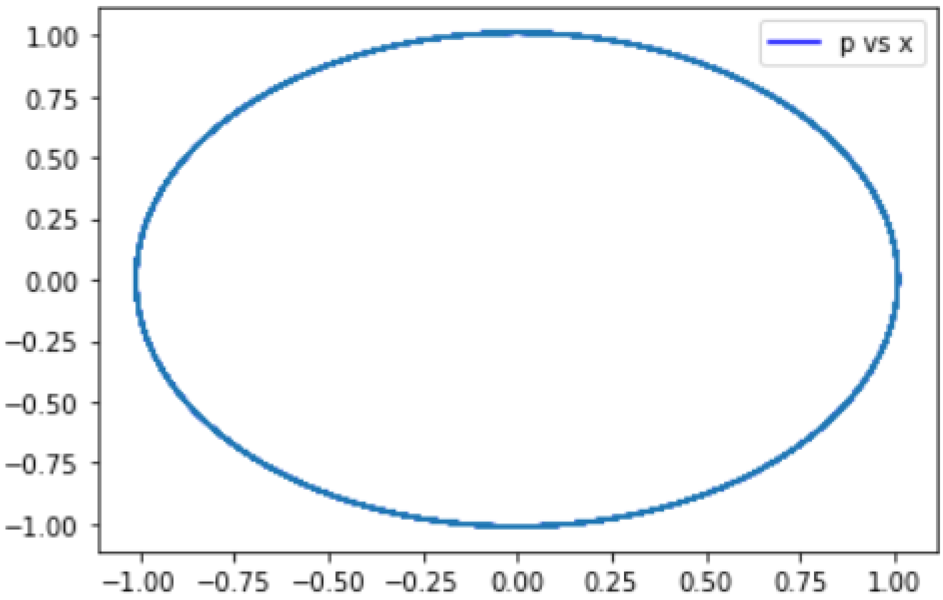
x vs time

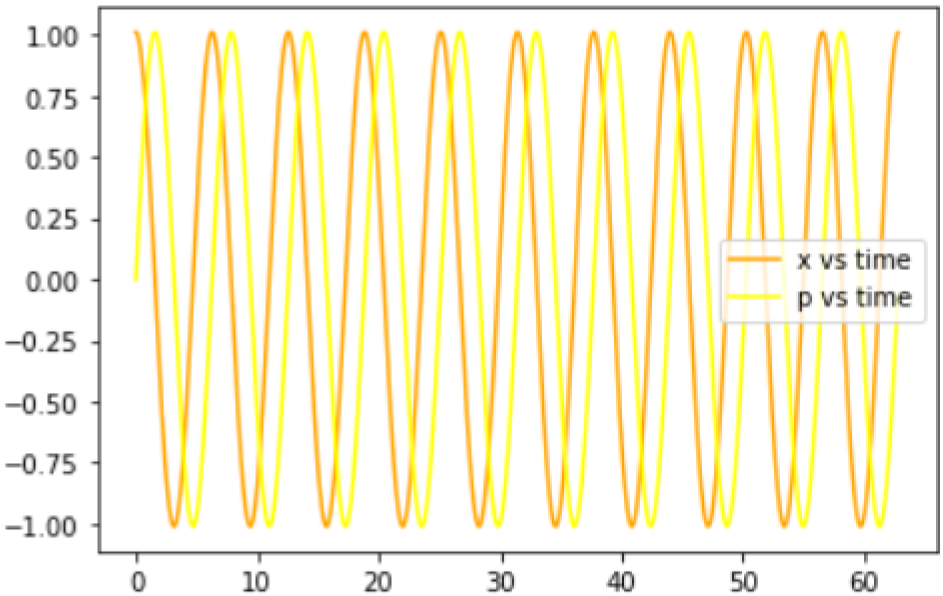
p vs time

Comparison of phase space, x vs time and p vs time with analytical solutions


p vs x
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0


x vs time
p vs time
1.0
0.5
0.0
−0.5
−1.0
0
10
20
30
40
50
60





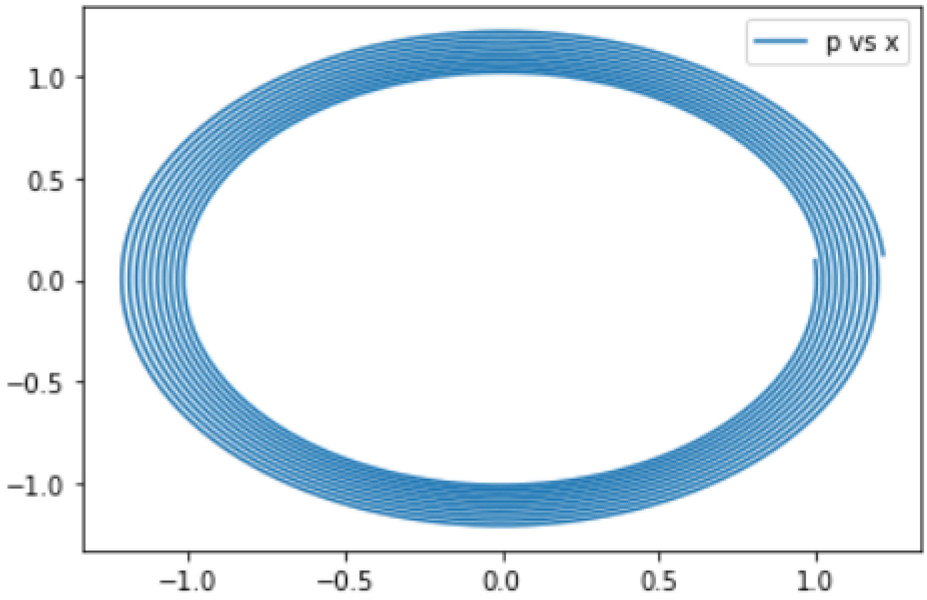
For h = T/1000

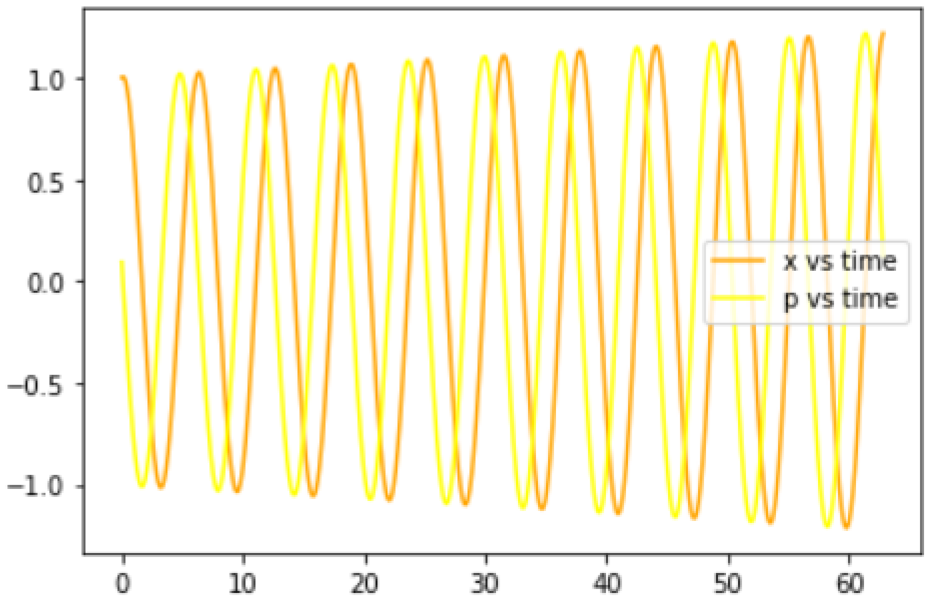
p vs x

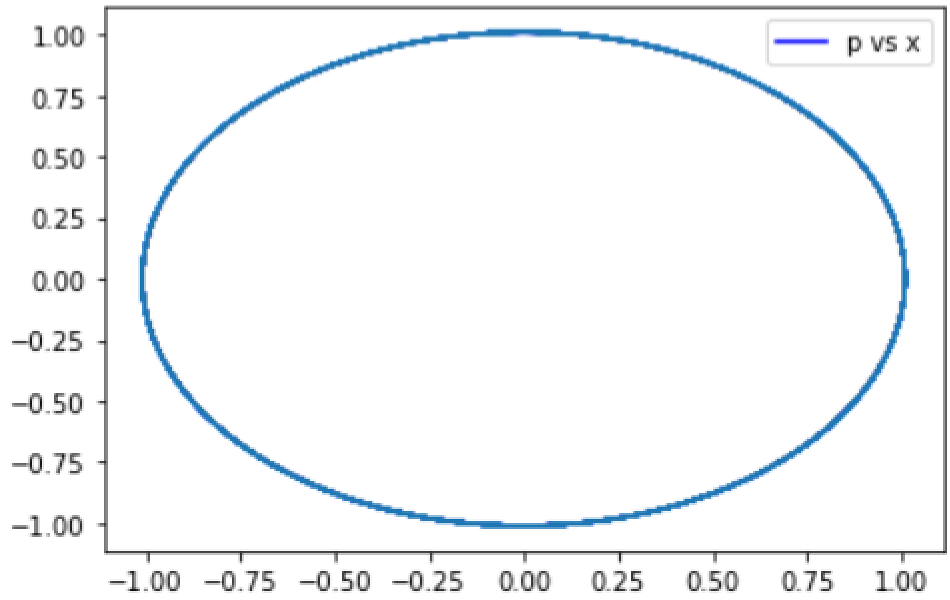
x vs time

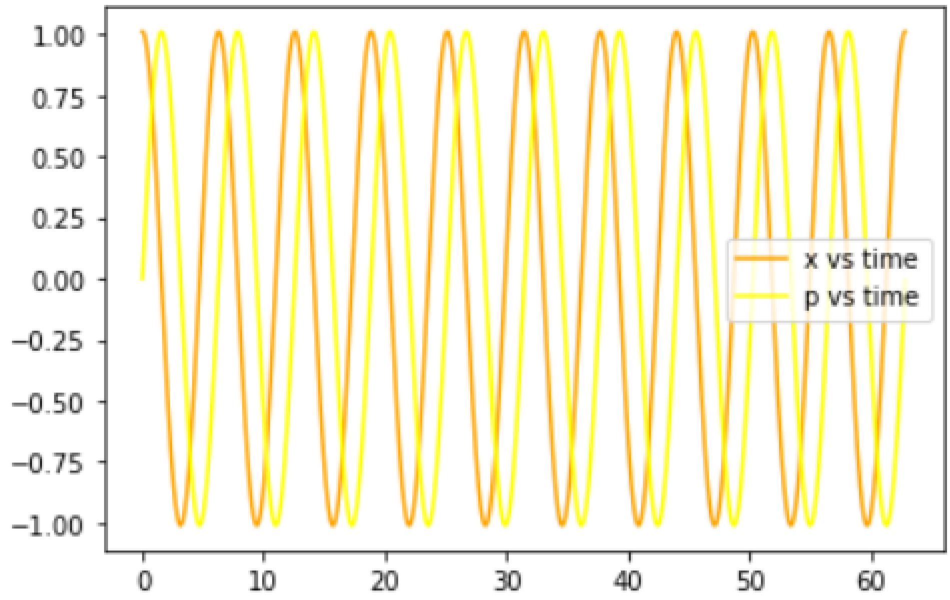
p vs time

Comparison of phase space, x vs time and p vs time with analytical solutions


p vs x
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0


x vs time
p vs time
1.0
0.5
0.0
−0.5
−1.0
0
10
20
30
40
50
60





Part - (ii)

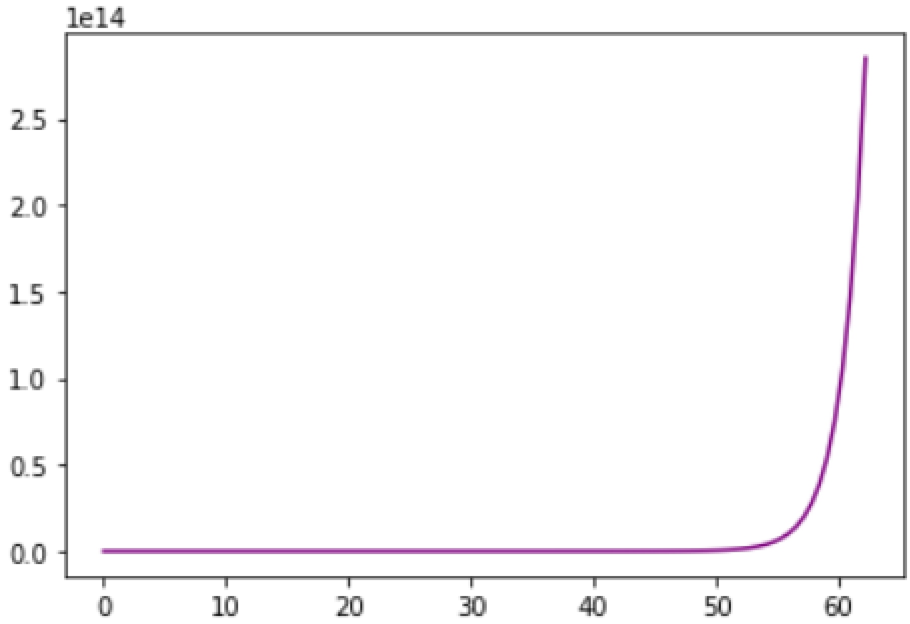
Analytical energy value for the given initial condition is 0.5.

On decreasing the step size, we see that the relative error between the analytical and numerical energy values as a function of time becomes a straight line.

Graphs-

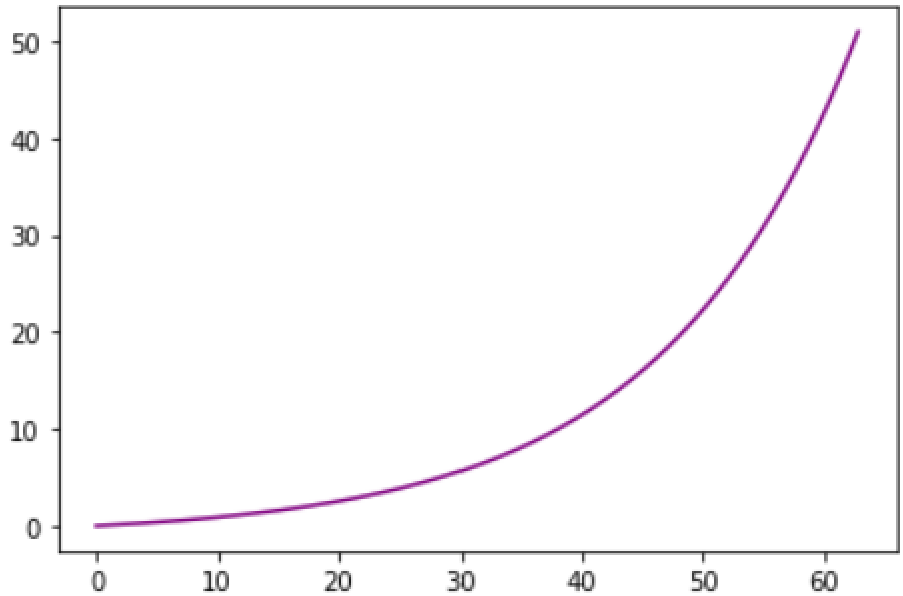
For h = T/10

$(E_n - E)/E$ vs time



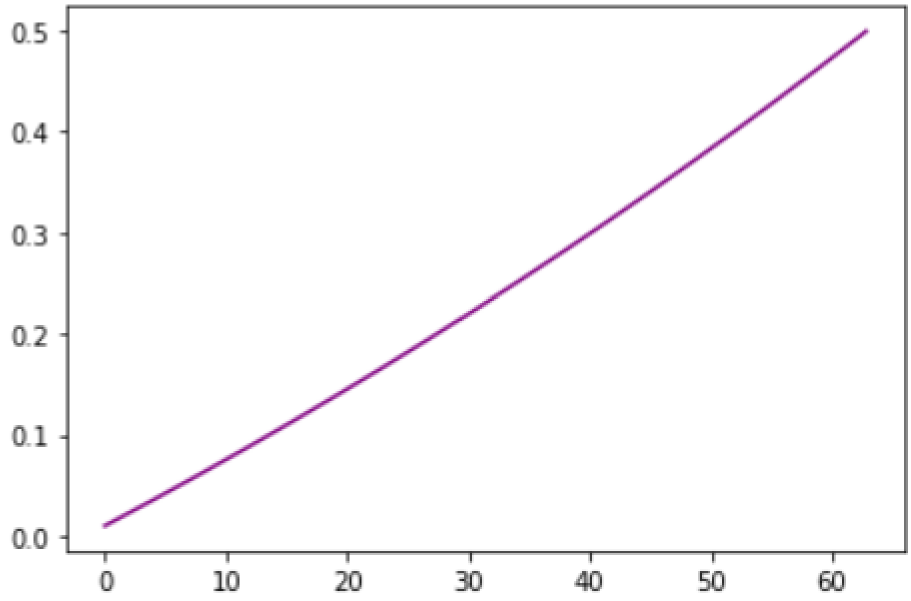
For h = T/100

$(E_n - E)/E$ vs time



For h = T/1000

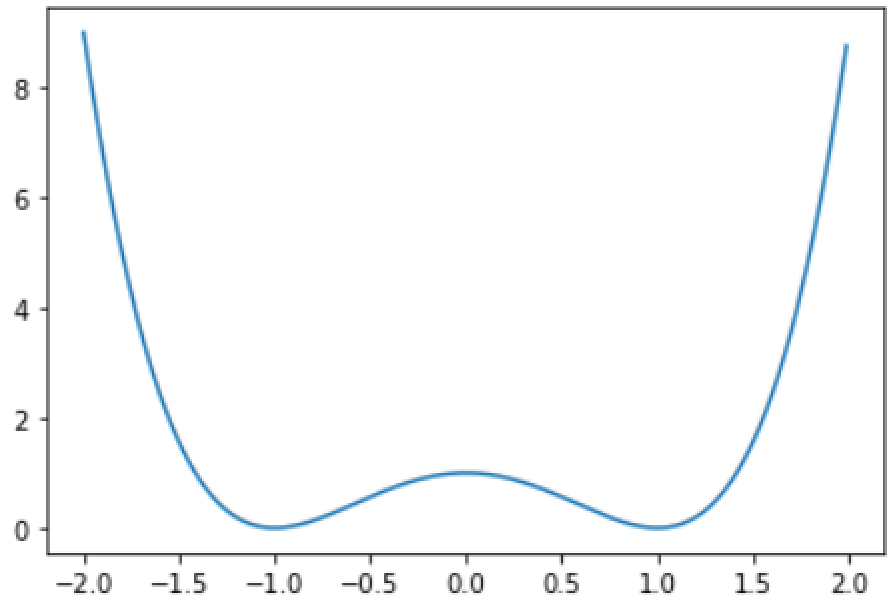
$(E_n - E)/E$ vs time



Part - (iii)

Graphs-

Plot of V vs time



Part - (b)

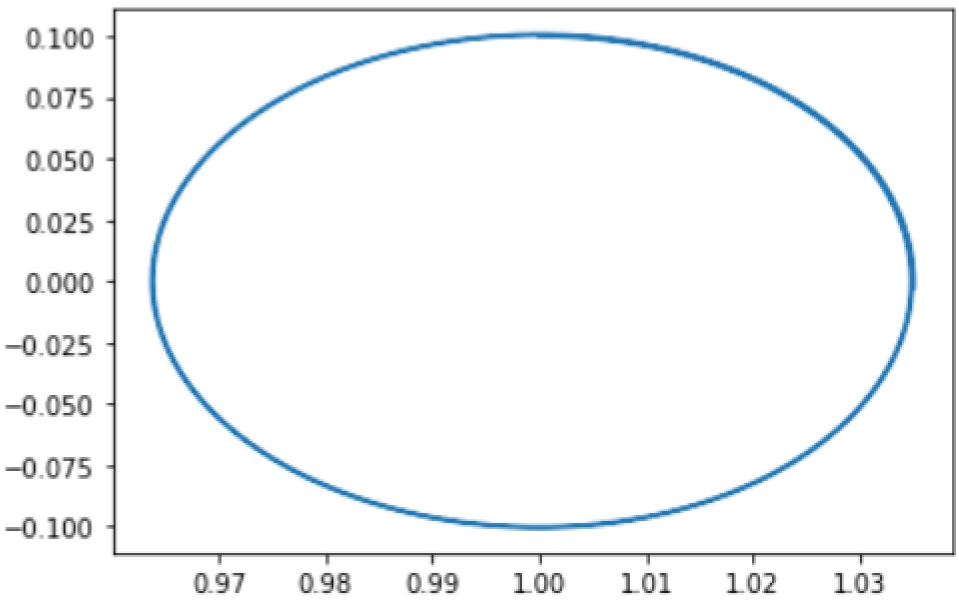
Part - (i)

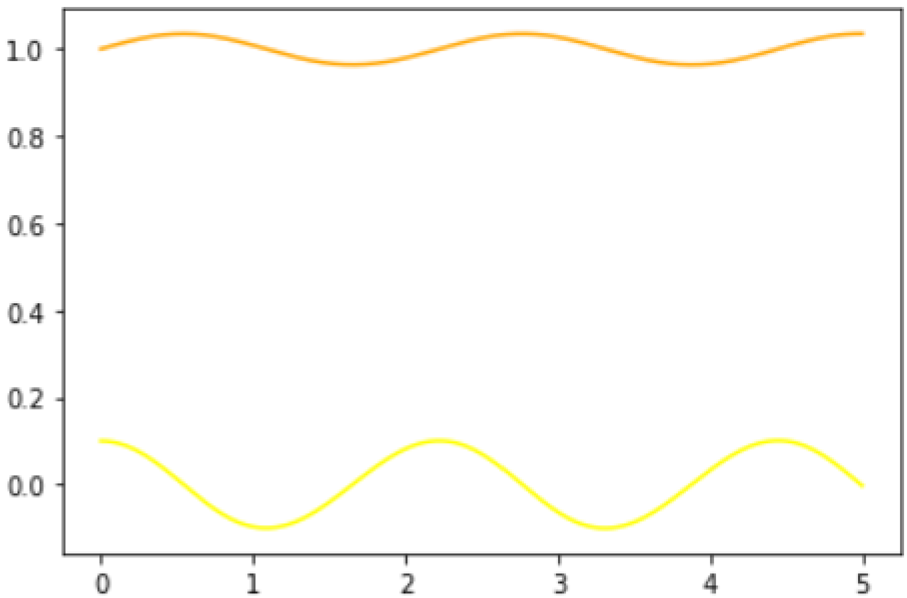
For X = (1, 0.1)

p vs x

x vs time

p vs time



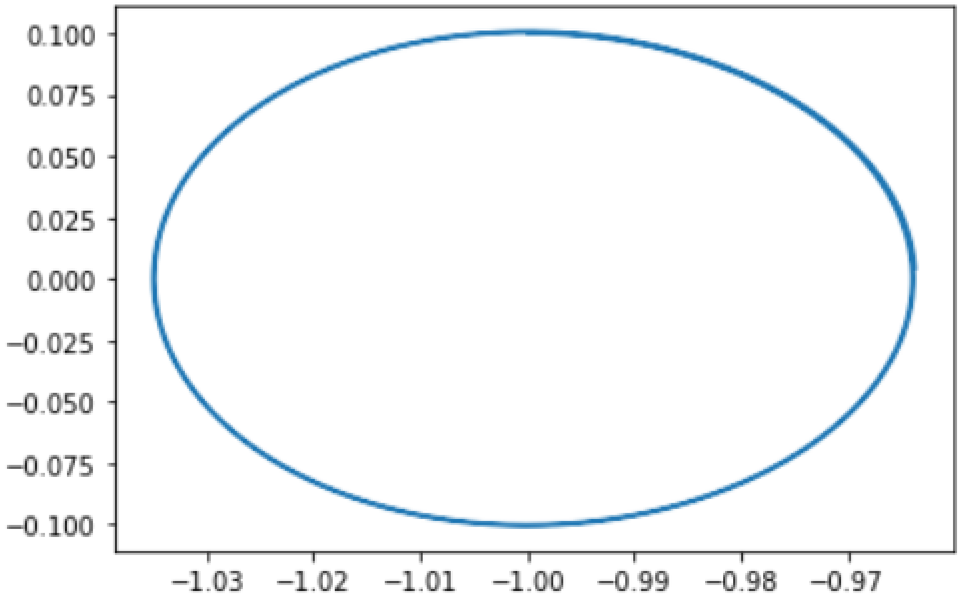


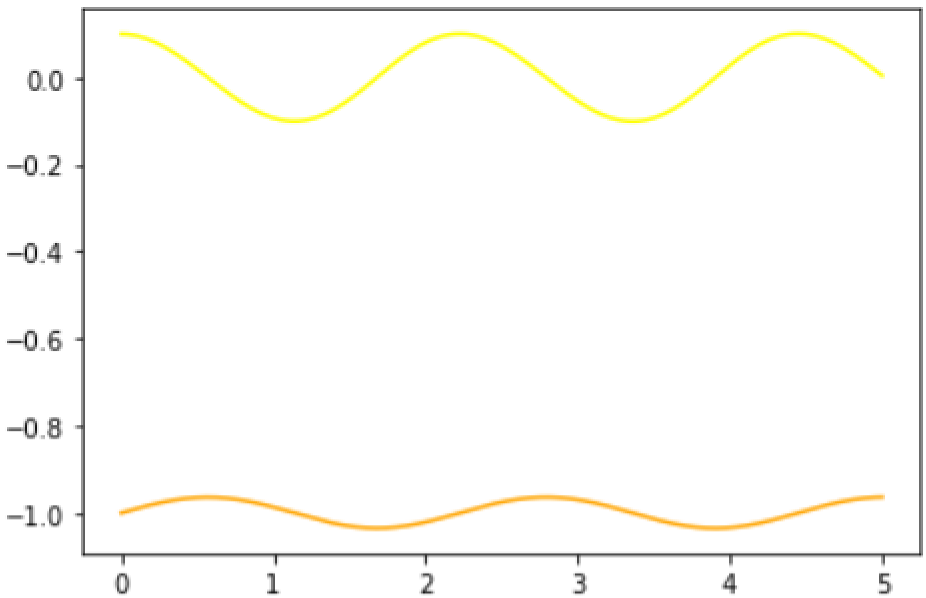
For X = (-1, 0.1)

p vs x

x vs time

p vs time



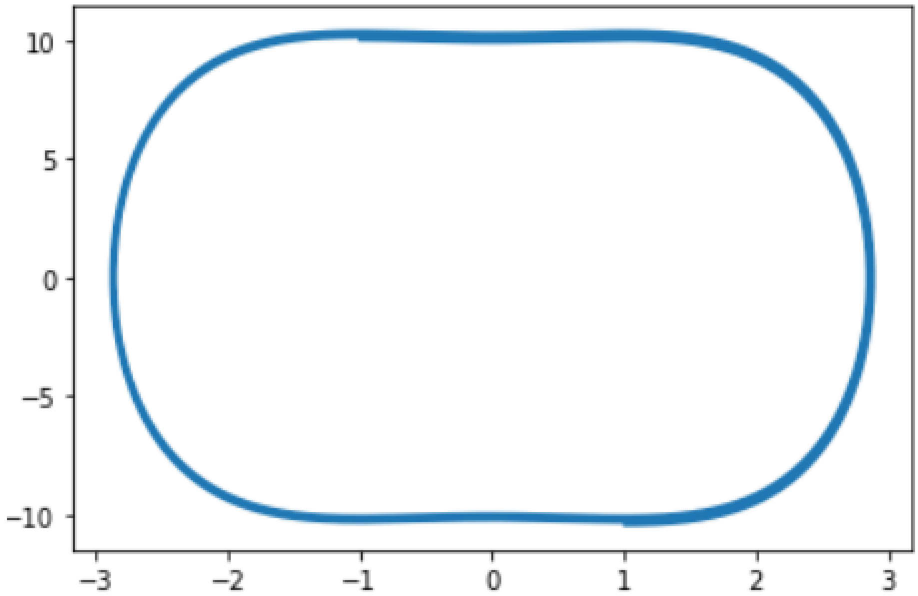


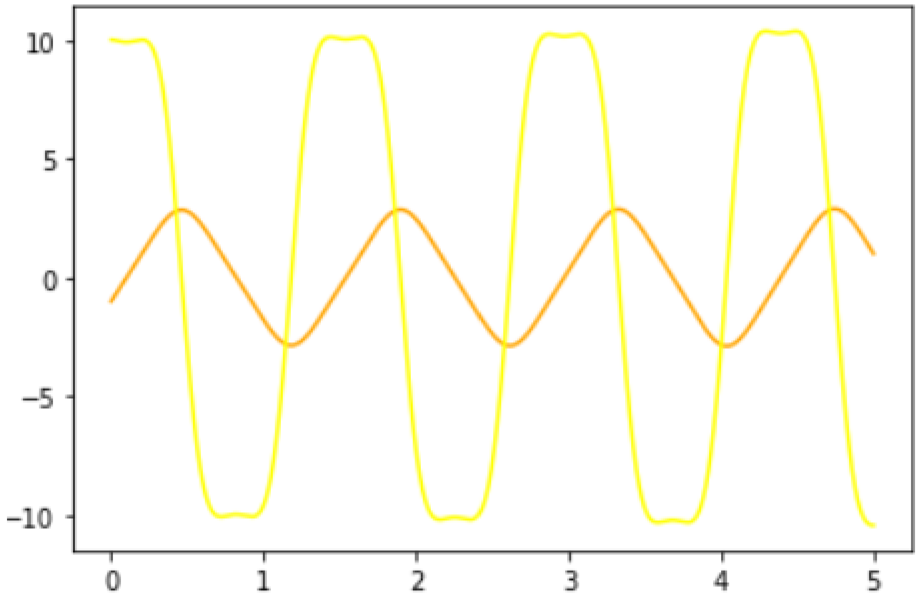
For X = (1, 10)

p vs x

x vs time

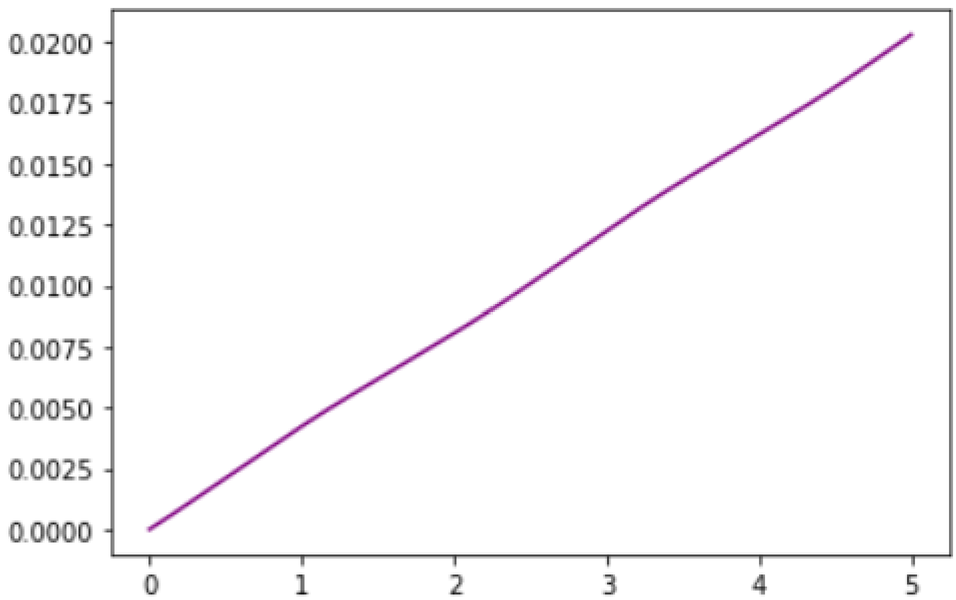
p vs time



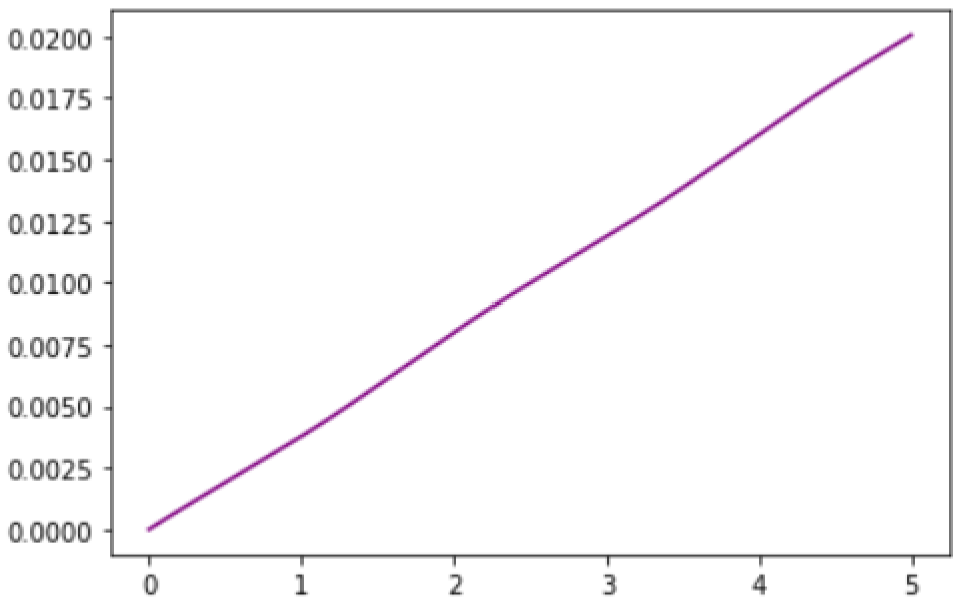


Part - (ii)

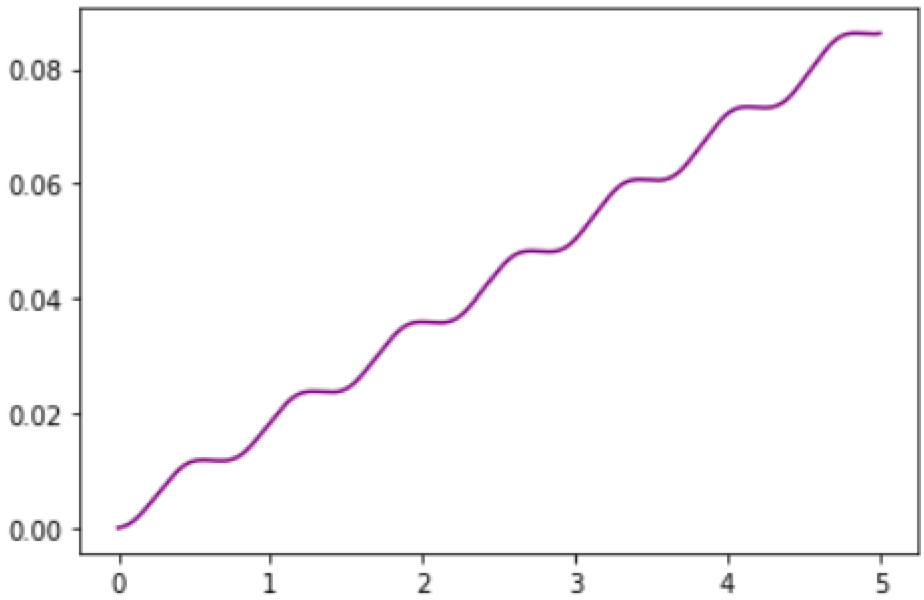
For X = (1, 0.1)



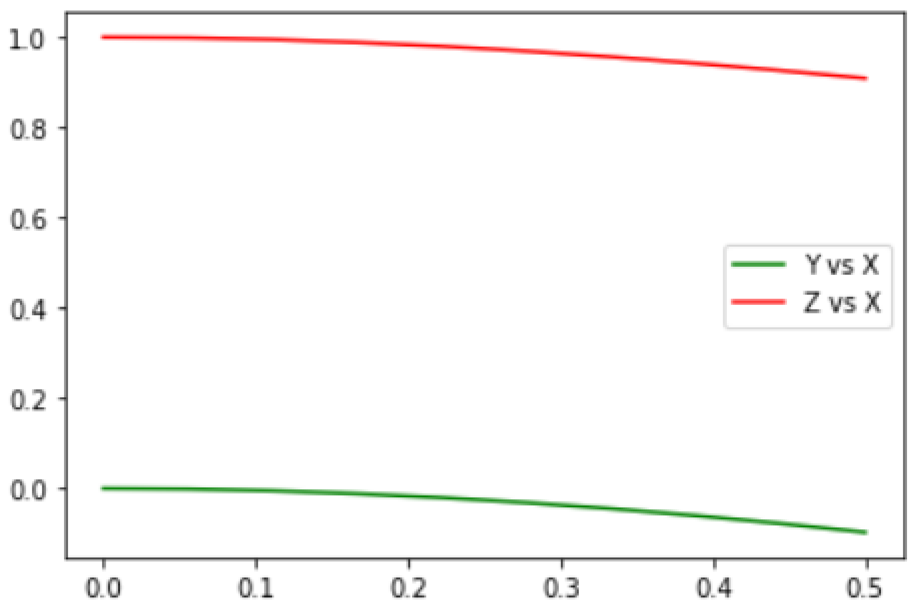
For X = (-1, 0.1)



For X = (1, 10)



For problem-4:

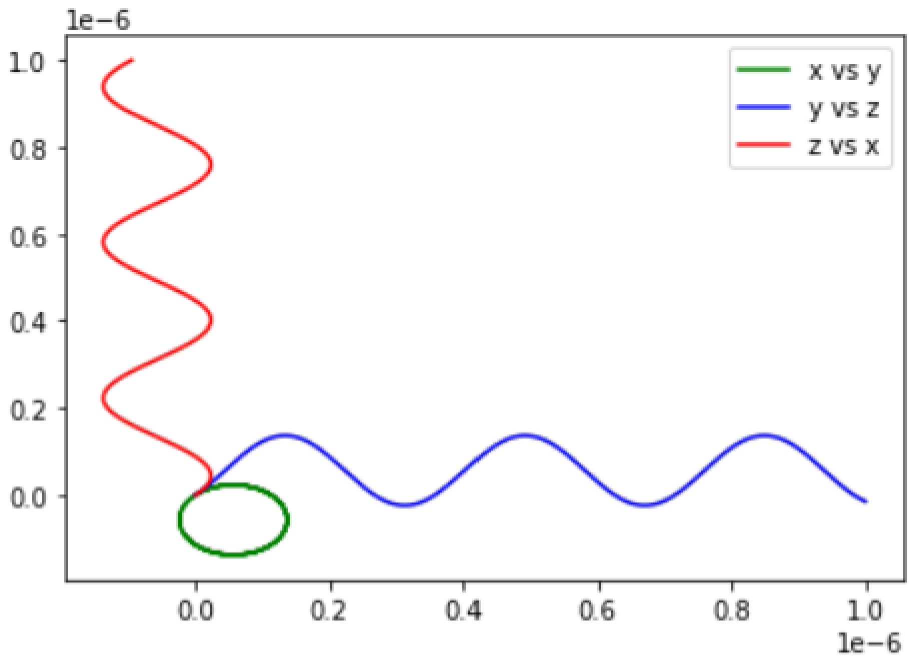


For problem-5:

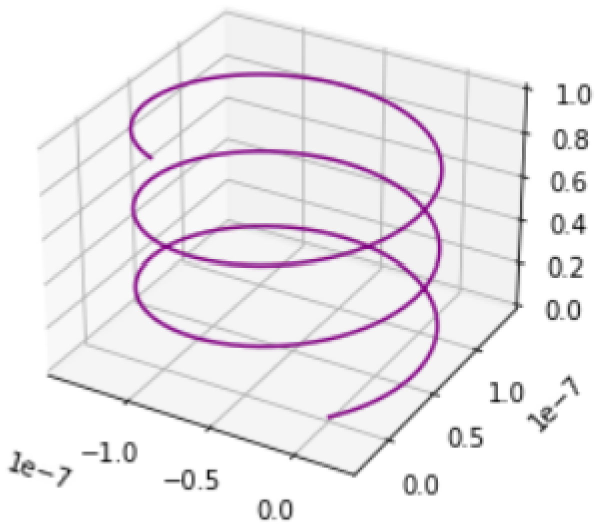
Graphs-

a) For case-1: B is 10^{-4} T along z-axis

In 2D-



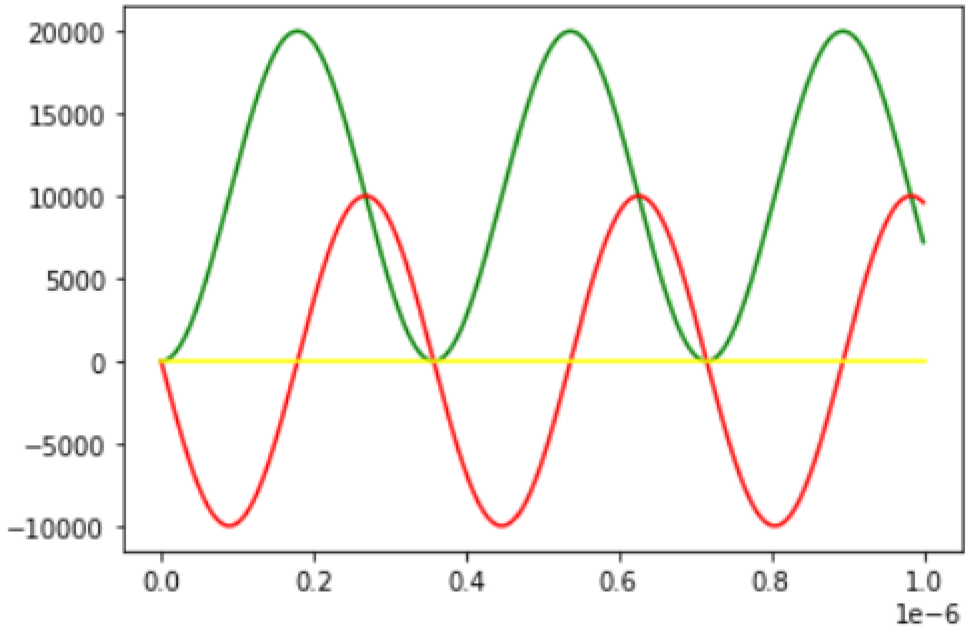
In 3D-



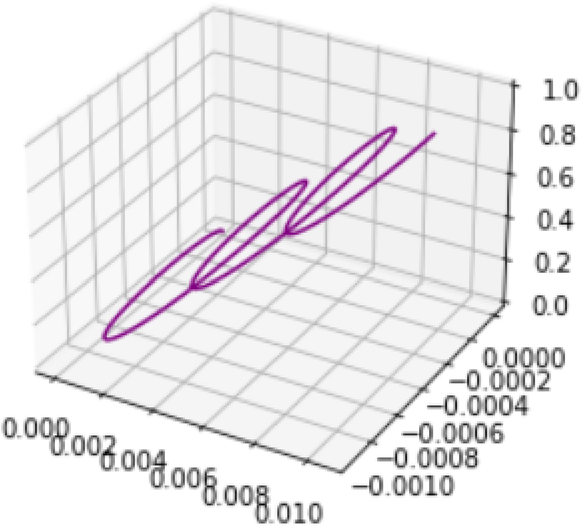
b) For case-1: B is 10^{-4} T along z-axis and E is 1 V/m along y-axis

In 2D-

Green is for x vs y
Blue is for y vs z
Red is for z vs x


20000
15000
10000
5000
0
−5000
−10000
0.0
0.2
0.4
0.6
0.8
1.0
1e−6

In 3D-


1.0
0.8
0.6
0.4
0.2
0.0
0.0000
−0.0002
−0.0004
−0.0006
−0.0008
−0.0010
0.000
0.002
0.004
0.006
0.008
0.010