Numerical Solution of ODE Assignment-I

V.Aravindan, 2017B4A70849P

3/10/2020

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1 Question 10

The hamiltonian plots for different N values along with their observations are described the the follwing subsections.

I discuss the deviation of the Hamiltonian function from its initial condition for N=1000 and N=2000 using the Embedded Runge-Kutta (RKDP45) Method. Furthermore, I also discuss the covergence of the RKDP45 and Classical RK4 methods.

All figures are present in this document and are referenced at appropriate positions.

The Hamiltonian is the total energy of the system and shall be referenced as such.

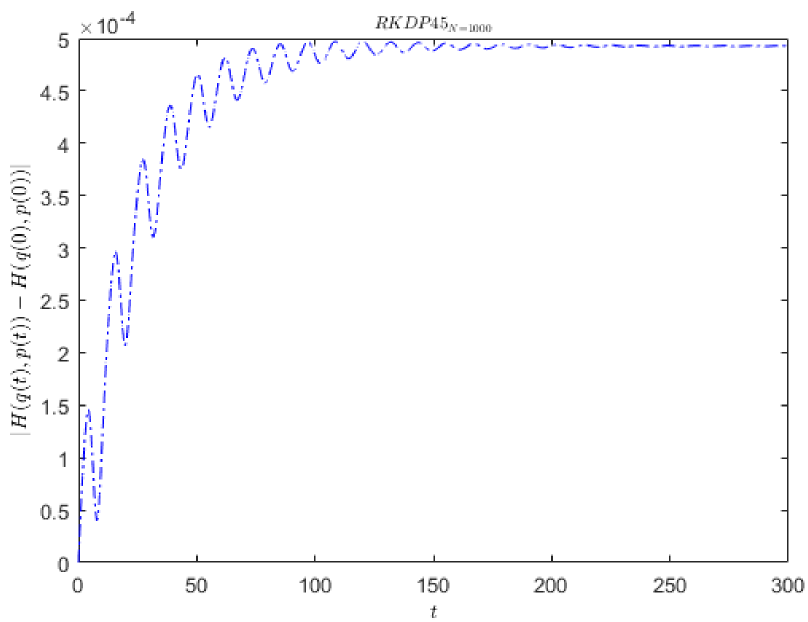
Sometimes to get a better understanding, I also plot a magnified look of the plot by reducing the number of time points to lower values.

1.1 N=1000

The absolute value of the error of the hamiltonian from its initial value is plotted. The energy of the system can be seen to deviate quite sharply initally and then becomes constanst implying a steady state condition after a certain amount of time. This is clearly visible in the magnified plot 1.

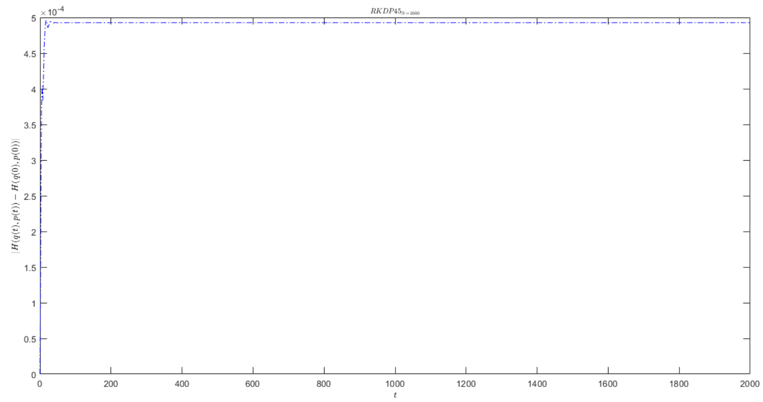
There are differences in the point at which the energy stabilises. This can be seen once the case for N=2000 has been analysed. For N=1000, it was the value 200 from which the energy barely deviated.

Figure 1: Hamiltonian Error plots of Embedded Runge Kutta-45 Magnified(N=1000)



To see the plot across the entire timespan of 2000 points, I plot it in 2. There is initially a steep increase in the error and then it remains constant for the rest of the time.

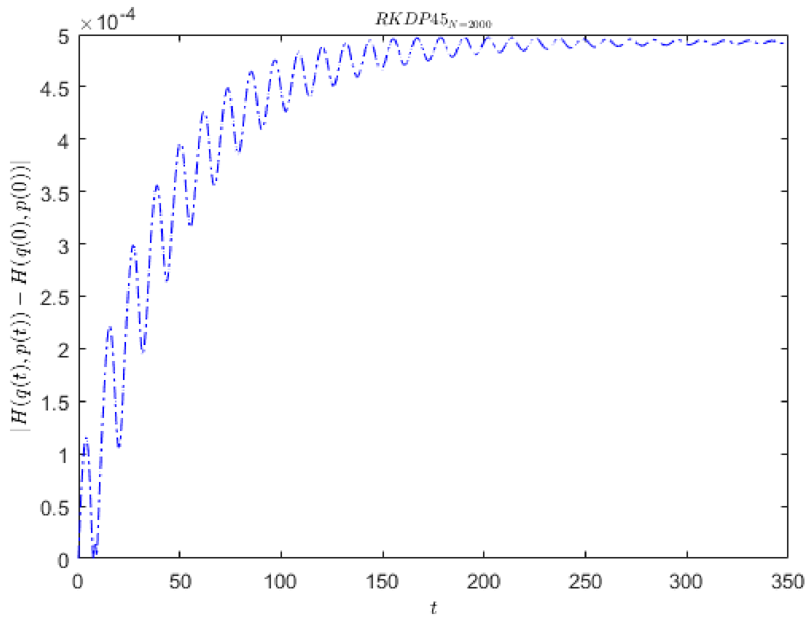
Figure 2: Hamiltonian Error plots of Embedded Runge Kutta-45 (N=1000)



1.2 N=2000

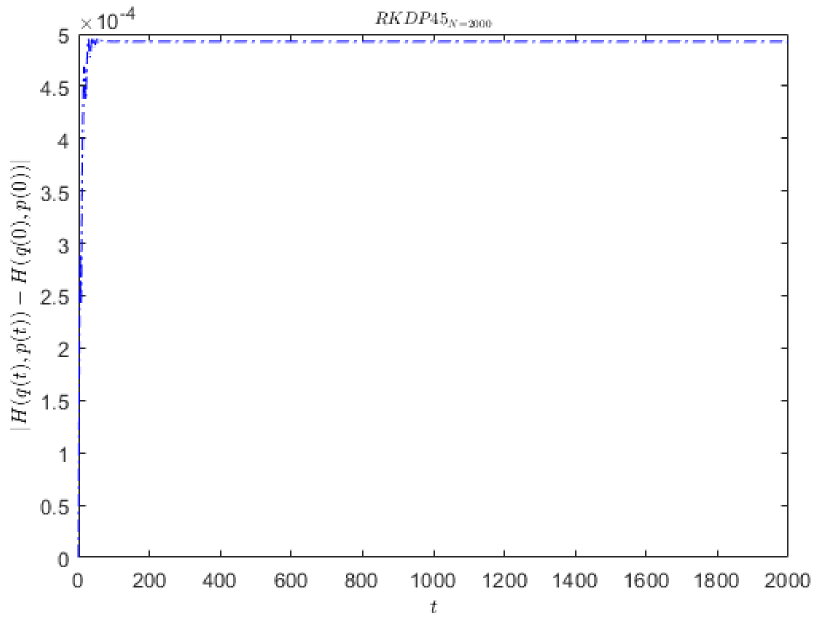
By increasing the number of discretization points, I observe that the energy stabilises at a much later time point than for lower discretization steps. The damped oscillations also seem to show higher frequencies.

Figure 3: Hamiltonian Error plots of Embedded Runge Kutta-45 Magnified(N=2000)



For T=2000 as the end time, the process behaviour is observed in the long run. The plot obtained shows the same level of information obtained for N=1000. With careful the stabilizing point can be seen at a later time point than for the case when N=1000.

Figure 4: Hamiltonian Error plots of Embedded Runge Kutta-45 (N=2000)



1.3 Convergence

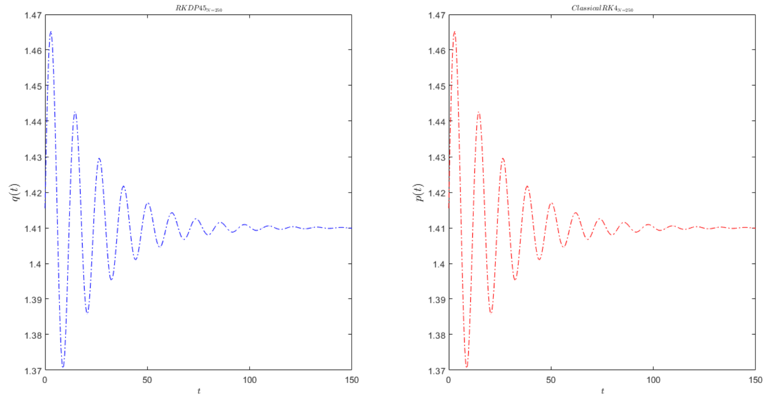
The plots of the molecular position $Q(t)$ are observed for convergence. The energy deviation of the system is also plotted , just to draw up inferences between the energy as well as the position at a given point in time.

The figures are first plotted and then a summary of the conclusions is provided at the end.

1.3.1 N=250

The first plot is that of the molecule position[5], followed by a plot of the energy deviation when 250 discretization points are taken.[6]

Figure 5: $Q(t)$ for N=250



1.3.2 N=500

The first plot is that of the molecule position[7], followed by a plot of the energy deviation when 500 discretization points are taken.[8]

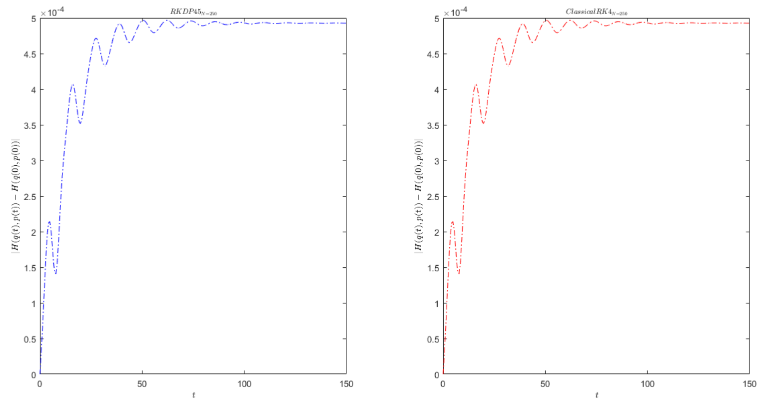
1.3.3 N=1000

The first plot is that of the molecule position[9], followed by a plot of the energy deviation when 1000 discretization points are taken.[10].

1.3.4 N=2000

The first plot is that of the molecule position[11], followed by a plot of the energy deviation when 2000 discretization points are taken.[12].

Figure 6: Hamiltonian difference for N=250



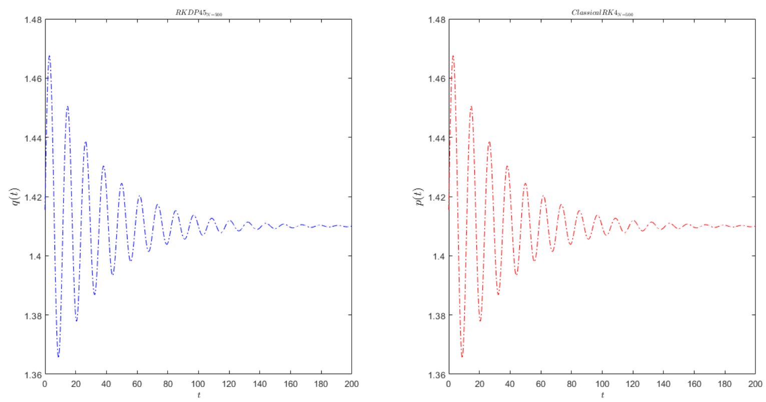
1.3.5 N=4000

The first plot is that of the molecule position[13], followed by a plot of the energy deviation when 2000 discretization points are taken.[14].

1.3.6 Observations

- Proper convergence of solution $q(t)$ was observed only when N=1000,2000,4000 for the last time taken to be 2000. For N=250,500 the solution diverged to infinity. This can be attributed to the lack of stability in the system.
- However, when lower end times were taken all like T=300, all values of N showed convergence behaviour to a steady state position. Both RKDP45 and CRK4 showed the exact same behaviour for all values of N. And when N increases the time taken for the molecule to stabilise also increases, like stabilising

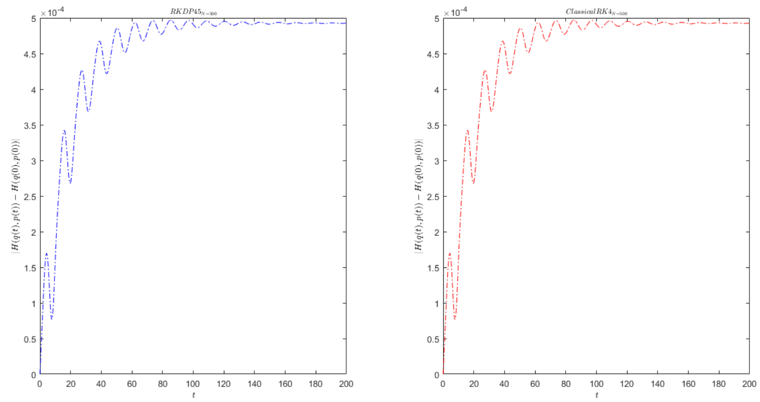
Figure 7: $Q(t)$ for N=500



within 100 units of time when 250 discretization points were considered and on the other end persistence till 500 time units when 4000 discretization points were considered. The amplitude of the particle also shows a slower damping as the discretization points increase in both methods.

- The corresponding plots of the hamiltonian deviations also confirm our observation as the energy stabilises so does the molecule's position.

Figure 8: Hamiltonian difference for N=500



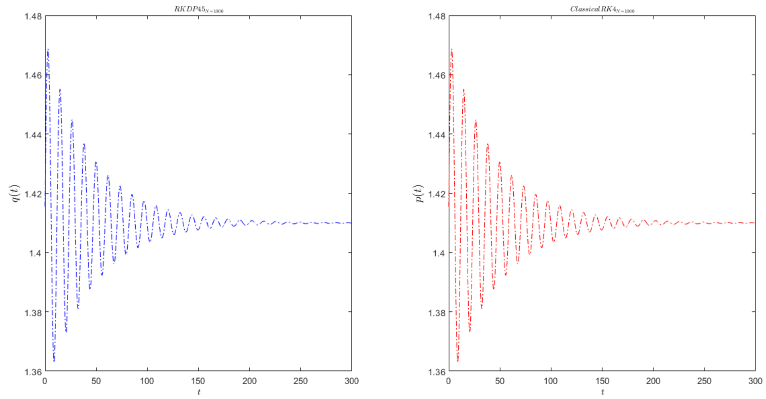
2 Question 11

1000 points with the given step sizes of 2, 2.3684, 2.3685 are considered as per the question. However, h=2.2 is also analyzed because its plot seems to show interesting trends.

2.0.1 Observations

- When forward euler was used. It can be observed that the error increases. The error first shoots up abruptly and then then remains constant for the rest of the time.15
- Symplectic Euler shows no visible trends in the Hamiltonian discrepancy, the data is quite noisy on first glance. However, the maximum error can be shown to increase from $8 * 10^{-4}$ to 10^{-3} when the step sizes increase. A peculiar trend in observed when h=2.2 is taken.16

Figure 9: $Q(t)$ for N=1000



- Similar to Symplectic Euler, the leapfrog method also shows that the maximum error increases when h increases with a similiar peculiar trends for values within 2.1 to 2.3.

Figure 10: Hamiltonian difference for N=1000

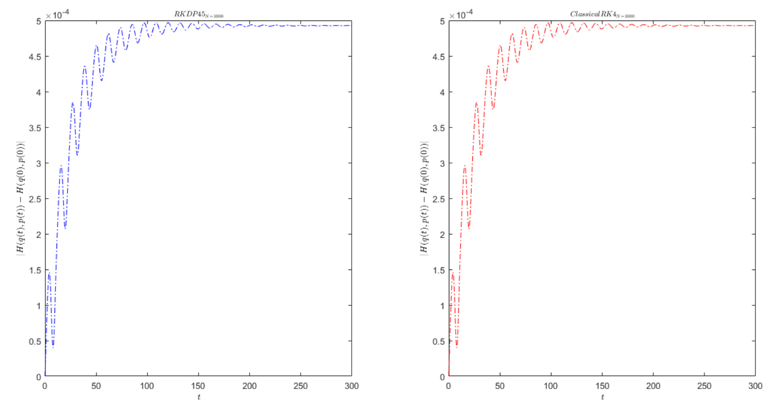


Figure 11: $Q(t)$ for N=2000

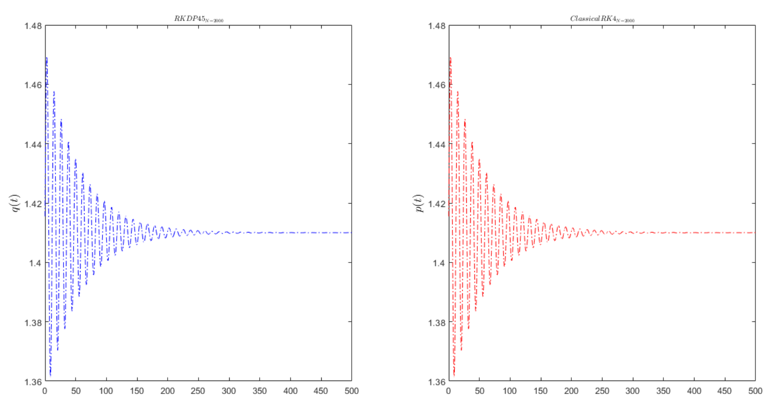


Figure 12: Hamiltonian difference for N=2000

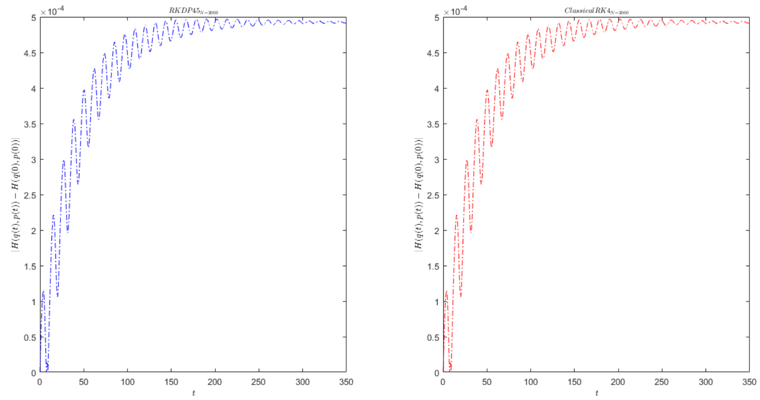


Figure 13: $Q(t)$ for N=4000

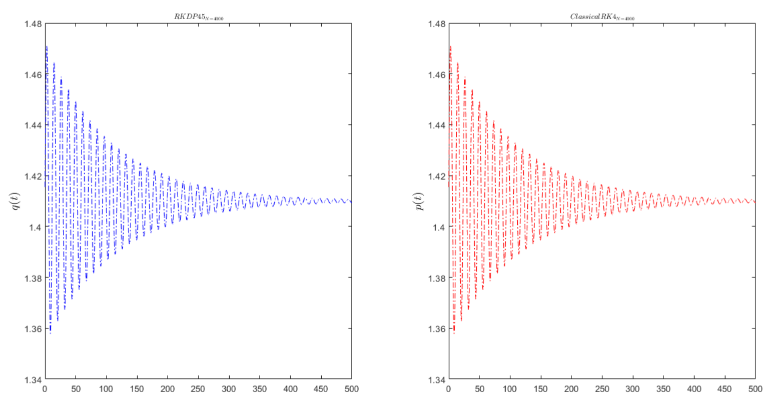


Figure 14: Hamiltonian difference for N=4000

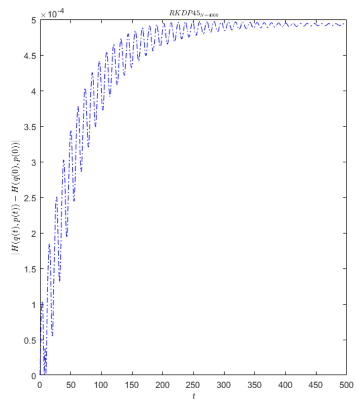


Figure 15: Forward Euler Discrepancy

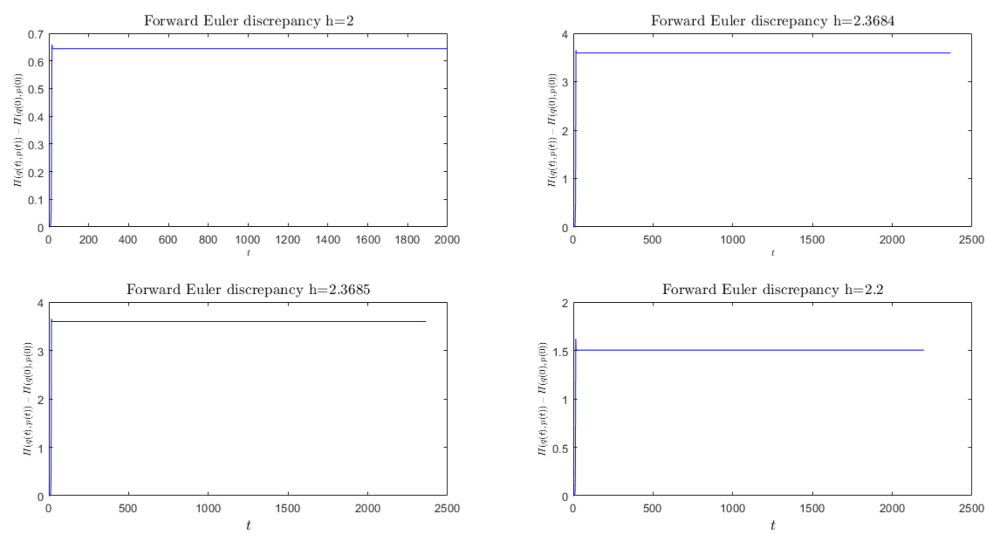


Figure 16: Symplectic Euler Discrepancy

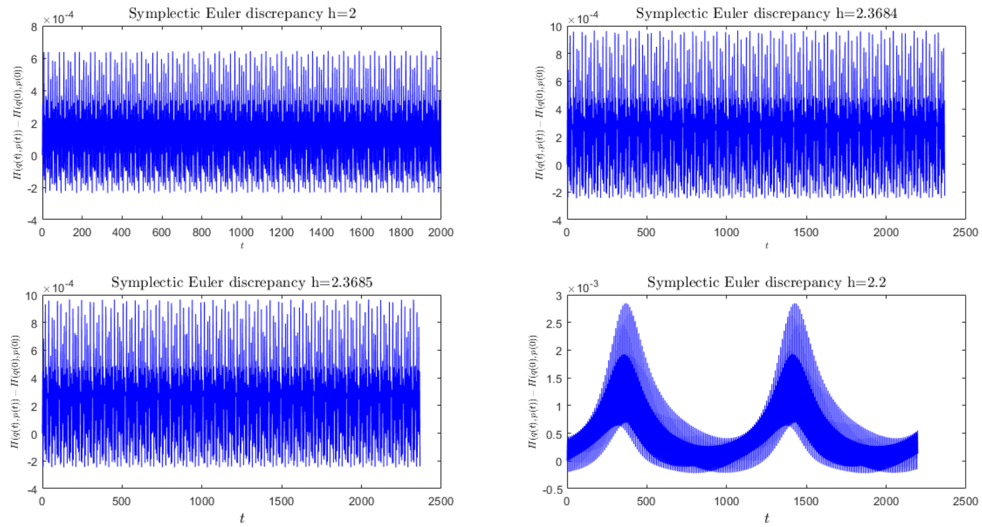


Figure 17: Leapfrog Discrepancy