Assignment 4:

This program solves driven morse oscillator model. The hamiltonian is H(x, p) = p**2/2 + (1 - exp(-x))**2 - a*x*sin(wt), where a = 0.04, w = 0.25.
I used two two-dimensional array y and dydt to represent x, p, and the derivatives of them.

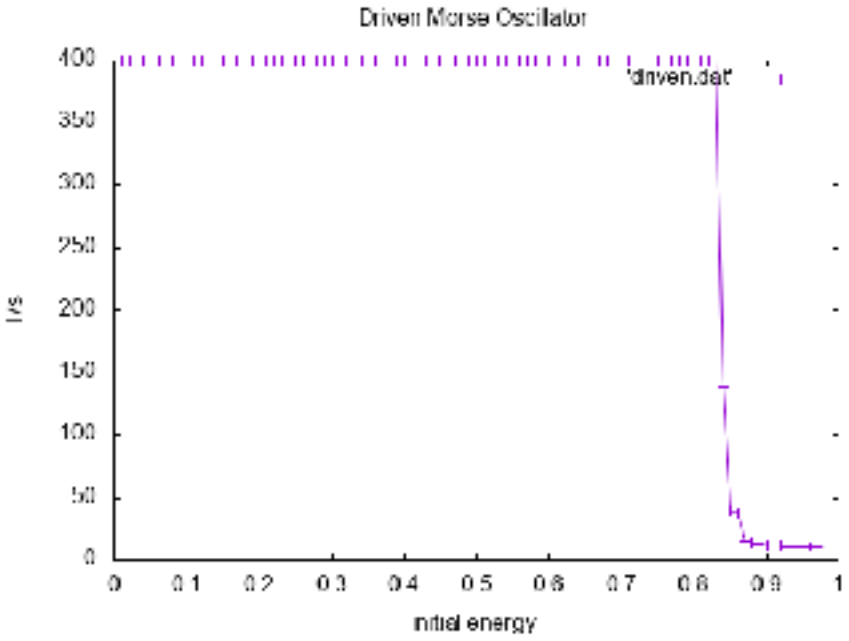
y[0] == x
y[1] == p
dy[0]/dt = p
dy[1]/dt = (-2)*(exp(-x)-exp(-2*x))+0.04_dp*sin(0.25_dp*t)

Firstly, I Started 99 trajectories at equally spaced energies between E = 0.01 and E = 0.99 with x(t=0) = 0 and momentum chosen as initial_p = sqrt(2*initial_E) . I computed the time evolution for each of these trajectories with the time step h = 0.1s until arriving maximum time of t = 400. When E > 1 the program will be automatically stopped, since the molecule is ionized. At last, I use Gnuplot to output a graph named driven.png from the data file driven.dat, which shows us how the time for ionizing changes with the initial energy.

The program driven_Morse.f90 has three major part: main program driven_Morse and two subroutines derivatives and runge_kutta_4.
The subroutine derivatives takes time and the value of x and p as input, outputting the corresponding derivatives for x and p.
The subroutine runge_kutta_4 implement the 4th order of runge_kutta algorithm. It inputs x and p, and their derivatives. What it outputs is the final value for x and p. The subroutine runge_kutta_4 calls subroutine derivatives three times.

The Runge-Kutta algorithm are more symmetric than Euler's method, and it use a trial step at the midpoint of an interval to cancel out lower-order error terms. The second-order formula Requires two function evaluations per step, which makes it better to Euler's method, because Euler's method would only reduce the error by a factor of two. The 4th Runge-Kutta algorithm uses Simpson's formula for integral, thus has error order O(h^5).

As we can see from the graph, when the initial energy is near 0.85, the time for ionization decrease dramatically, which match the prediction from the paper.


Driven Morse Oscillator
'driven.dat'
I*s
initial energy
400
350
300
250
200
150
100
50
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1