Methods of Computational Physics
Sheet 2 - Molecular Dynamics

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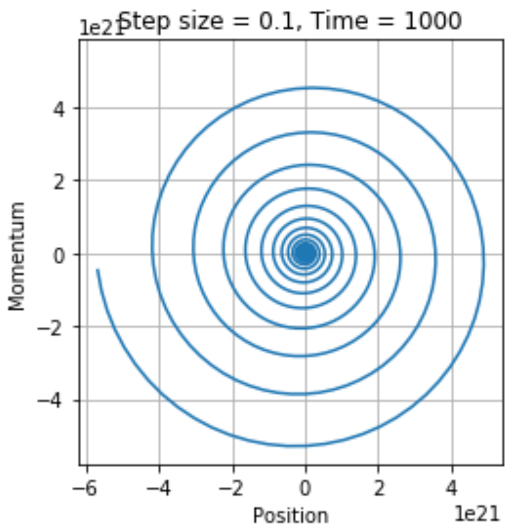
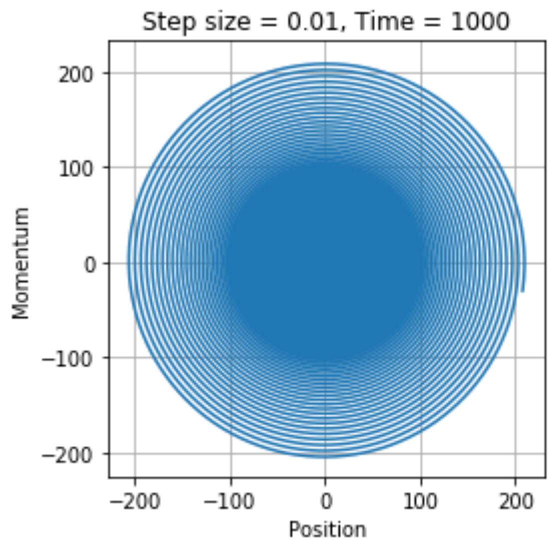
- **Harmonic Oscillator in the microcanonical ensemble**

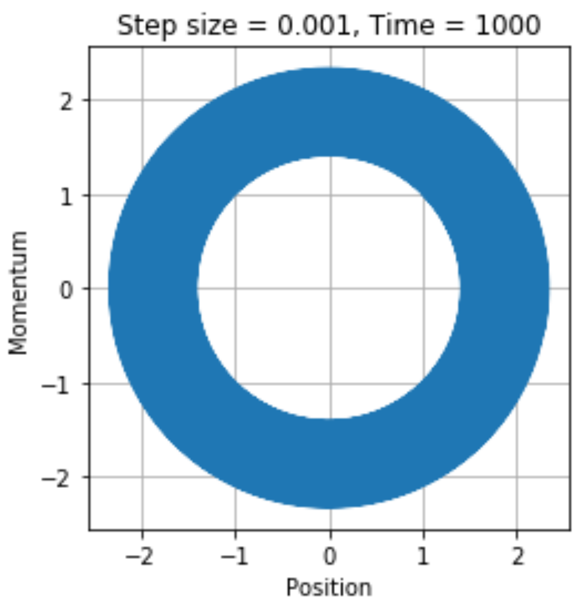
a) $L = \sqrt{\dfrac{E}{m\omega^2}},\ T = \dfrac{1}{\omega},\ E = \dfrac{mL^2}{T^2}$

b) Euler Forward Scheme :

$$q[t+h] = q[t] + h \times p[t]\ ;\ p[t+h] = p[t] - h \times q[t]$$

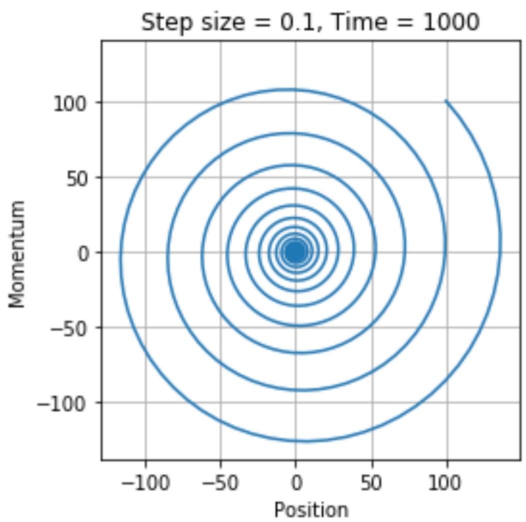


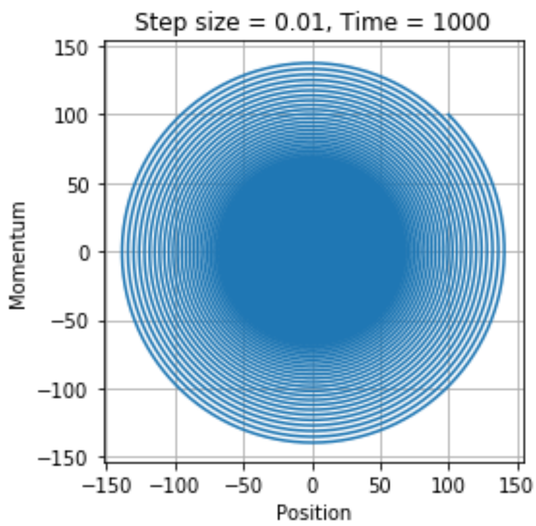


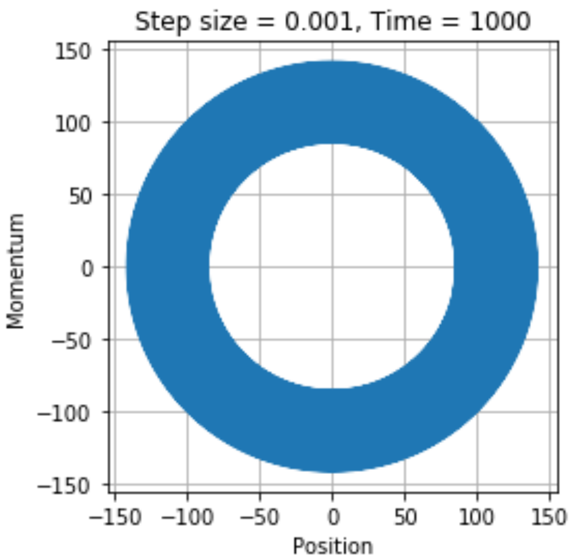


c) **Euler Implicit Scheme :**

$$q[t+h] = \frac{(q[t] + h \times p[t])}{1+h^2} \; ; \; p[t+h] = \frac{(p[t] - h \times q[t])}{1+h^2}$$



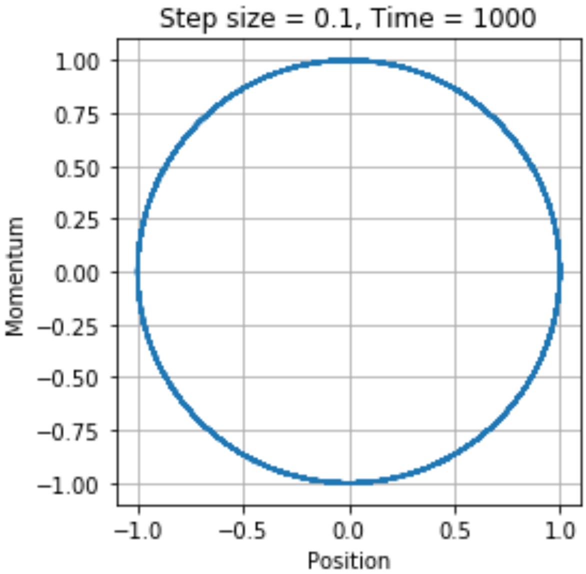


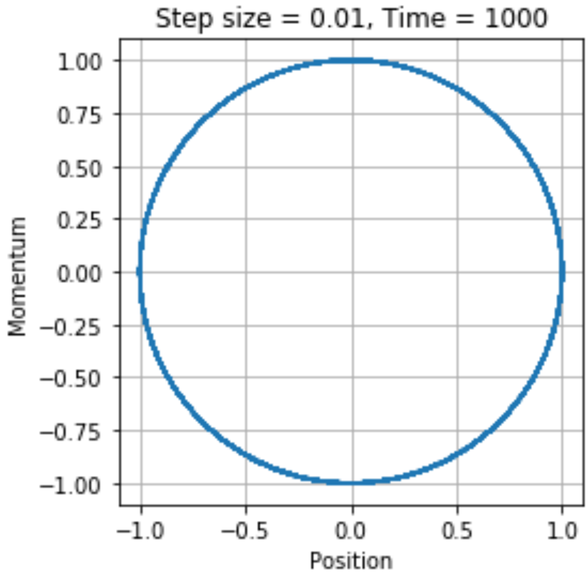


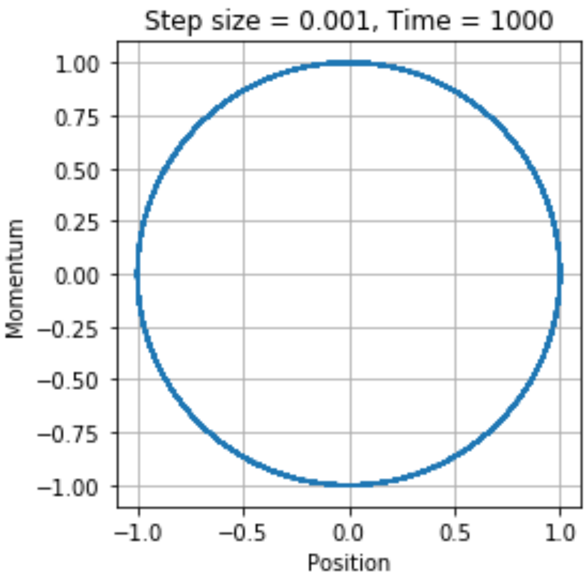
d) **Runga-Kutta algorithm of fourth order (RK4)**

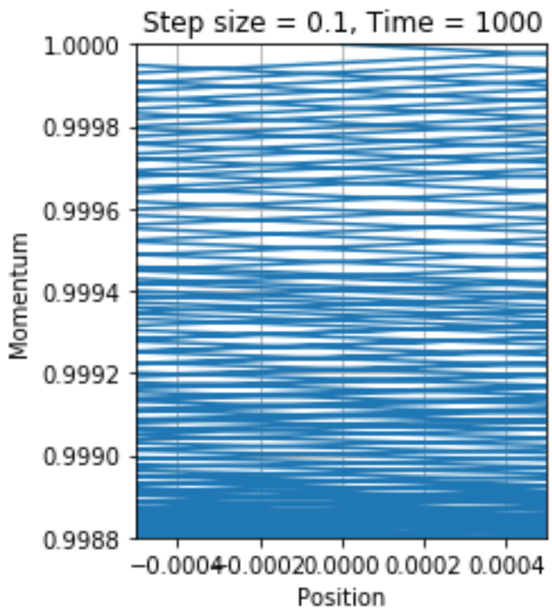
$qk_1 = p[t]$
$pk_1 = -q[t]$
$qk_2 = p[t] - q[t] \times h/2$
$pk_2 = -q[t] - p[t] \times h/2$
$qk_3 = p[t] - q[t] \times (h/2) - p[t] \times h^2/4$
$pk_3 = -q[t] - p[t] \times h/2 + q[t] \times h^2/4$

$$qk_4 = p[t] - q[t] \times (h) - p[t] \times h^2/2 + q[t] \times h^3/4$$
$$pk_4 = -q[t] - p[t] \times h + q[t] \times h^2/2 + p[t] \times h^3/4$$
$$q[t+h] = q[t] + h/6 \times (qk1 + 2 \times qk2 + 2 \times qk3 + qk4)$$
$$p[t+h] = p[t] + h/6 \times (pk1 + 2 \times pk2 + 2 \times pk3 + pk4)$$









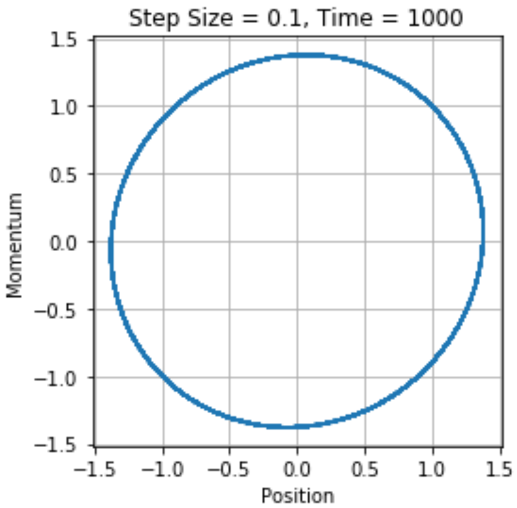
e) **Symplectic Euler**

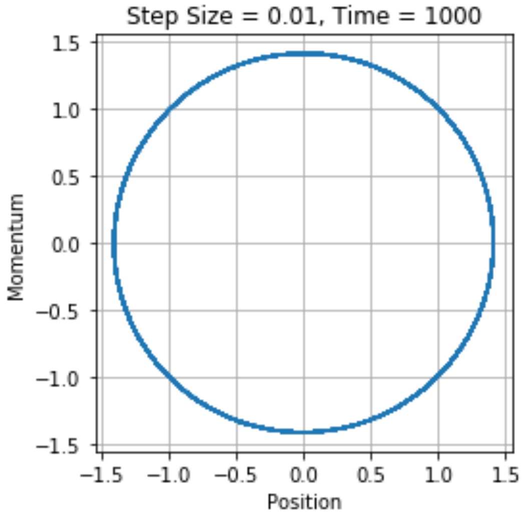
$$T(\Delta t) = e^{\Delta t \frac{\partial H}{\partial p}\frac{\partial}{\partial q}} e^{-\Delta t \frac{\partial H}{\partial q}\frac{\partial}{\partial p}}$$

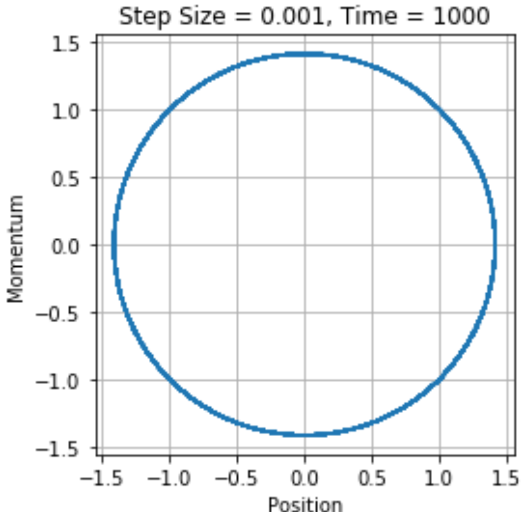
$$Z(t+\Delta t) = T(\Delta t)Z(t) = e^{\Delta t \frac{\partial H}{\partial p}\frac{\partial}{\partial q}} e^{-\Delta t \frac{\partial H}{\partial q}\frac{\partial}{\partial p}} \begin{pmatrix} q(t) \\ p(t) \end{pmatrix}$$

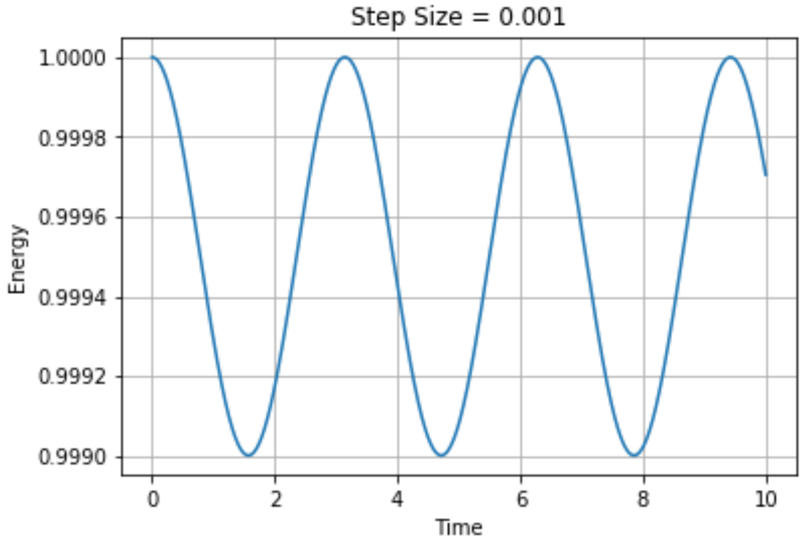
Using $p = \dfrac{\partial H}{\partial p}$; $q = \dfrac{\partial H}{\partial q}$, solving gives -

$$q[t+h] = q[t] \times (1-h^2) + h \times p[t] \ ; \ p[t+h] = p[t] - q[t] \times h$$

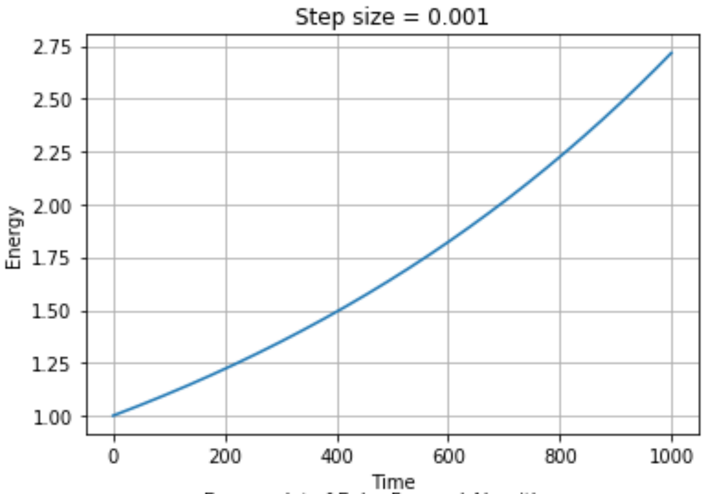




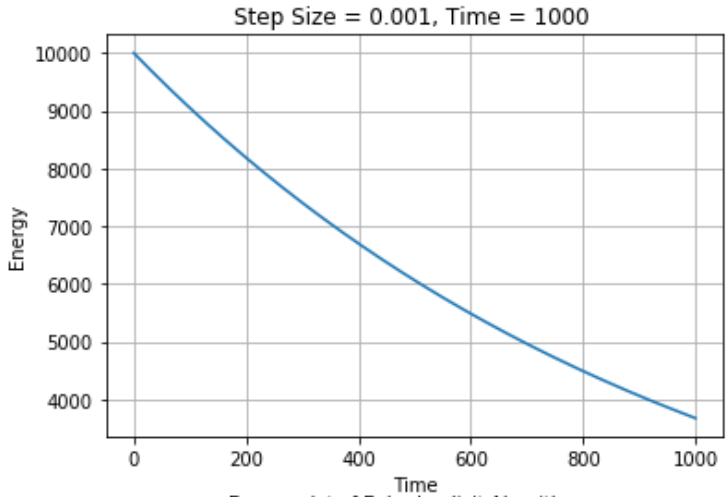




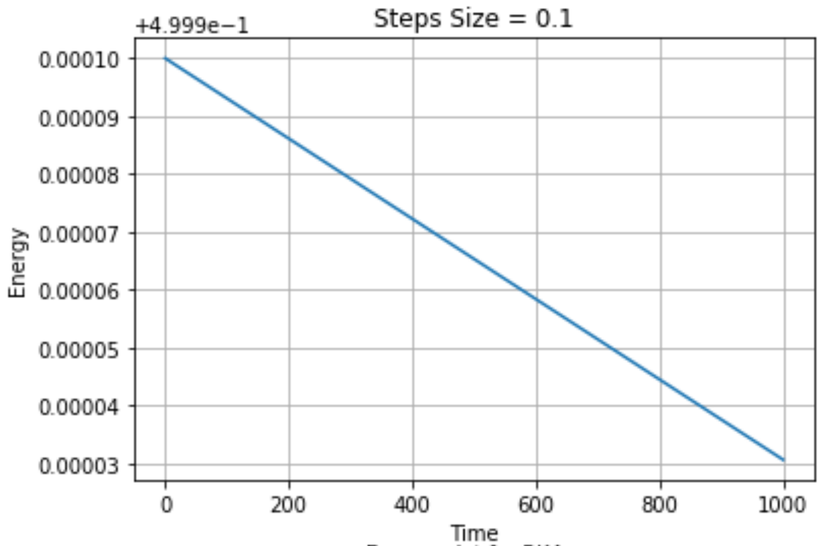
Energy plot of Symplectic Euler



Energy plot of Euler Forward Algorithm



Energy plot of Euler Implicit Algorithm

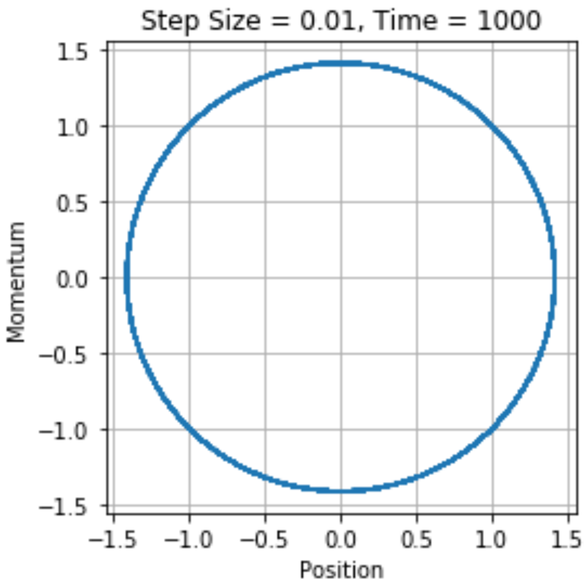


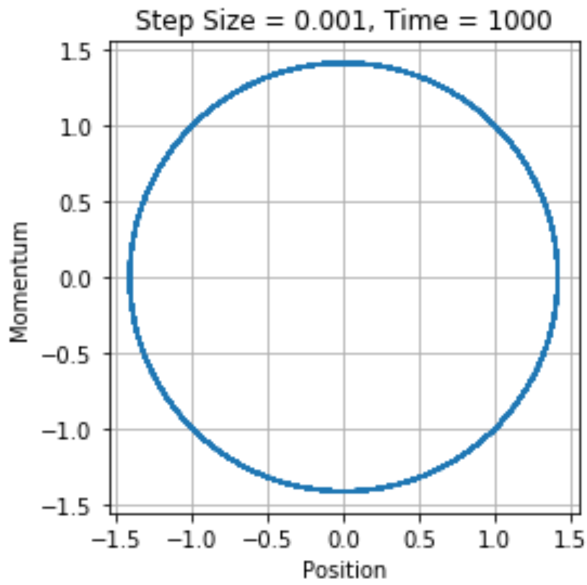
Energy plot for RK4

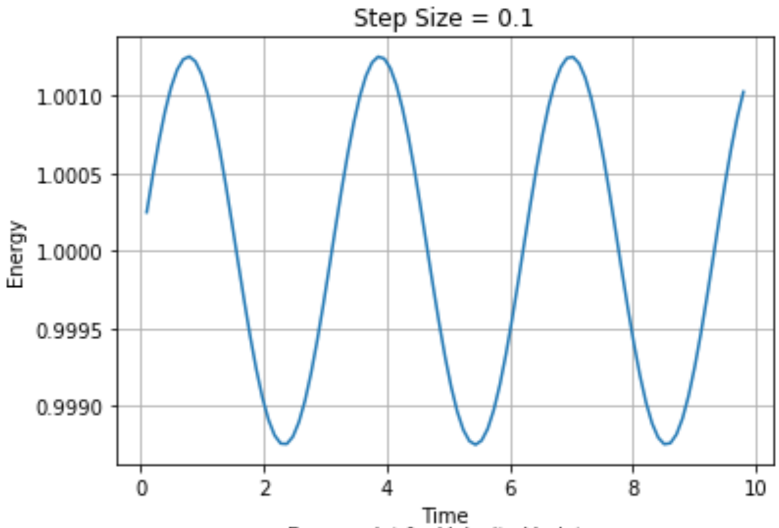
Energy plots suggests that energy is much more bounded and approximately conserved for symplectic Euler.
For Euler Forward, energy explodes exponentially. For Euler Backward, energy drops to 0. RK 4 conserves energy quite well for a range of time, but energy still falls with time.

f) **Velocity-Verlet algorithm :**

$$q[t+1] = q[t] + p[t] \times h - q[t] \times h^2/2$$
$$p[t+1] = p[t] \times (1 - h^2/2) + q[t] \times (h^3/4 - h)$$







Energy plot for Velocity-Verlet

g) **Shadow Hamiltonian $\mathscr{H}_s$ for the velocity-verlet algorithm.**

Using the Baker Campbell Hausdorff Formula and Trotter's Product Formula, we have -

$$i\mathscr{L}_s = i\mathscr{L} - \frac{\Delta t^2}{24}[i\mathscr{L}_p,[i\mathscr{L}_p,i\mathscr{L}_q]] + \frac{\Delta t^2}{12}[i\mathscr{L}_q,[i\mathscr{L}_q,i\mathscr{L}_p],$$

where $i\mathscr{L} = i\mathscr{L}_q + i\mathscr{L}_p$ and $i\mathscr{L}_q = p\frac{\partial}{\partial q}$; $i\mathscr{L}_p = -q\frac{\partial}{\partial p}$, for the described harmonic oscillator.

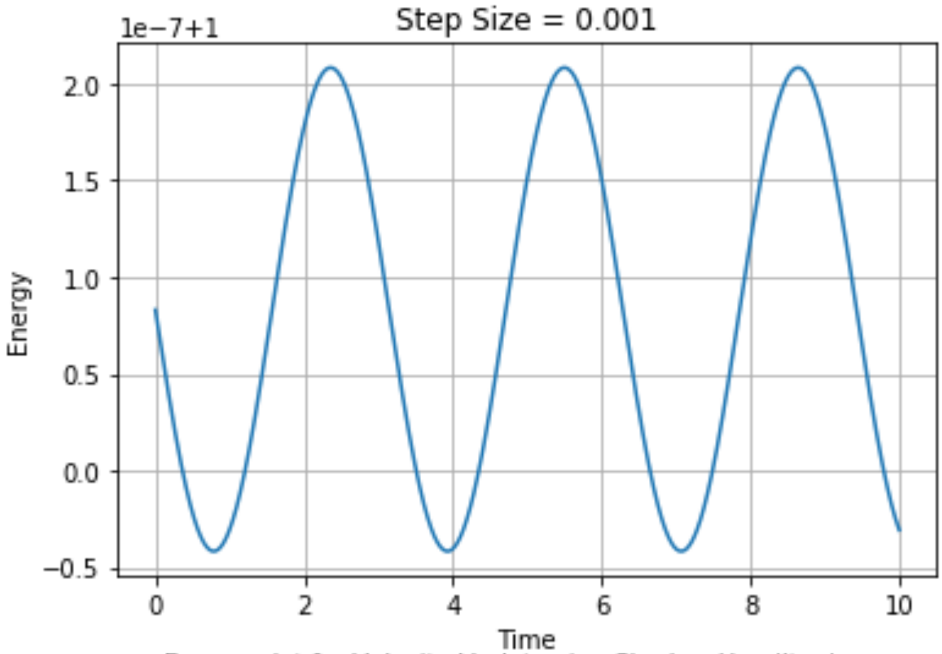
Solving the commutation relations, we get -

$$i\mathscr{L}_s = \frac{\partial H_s}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H_s}{\partial q}\frac{\partial}{\partial p} = (-q + \frac{\Delta t^2}{12}q)\frac{\partial}{\partial p} + (p + \frac{\Delta t^2}{6}p)\frac{\partial}{\partial q}$$

Now comparing coefficients such that -

$\dfrac{\partial H_s}{\partial q} = -q + \dfrac{\Delta t^2}{12}q = q_s$ (say), $\dfrac{\partial H_s}{\partial p} = p + \dfrac{\Delta t^2}{6}p = p_s$ (say)

Now $\mathscr{H}_s = \dfrac{p_s^2 + q_s^2}{2}$, this implies - $\boxed{\mathscr{H}_s = \dfrac{(-q + \frac{\Delta t^2}{12}q)^2 + (p + \frac{\Delta t^2}{6}p)^2}{2}}$



Energy plot for Velocity-Verlet using Shadow Hamiltonian

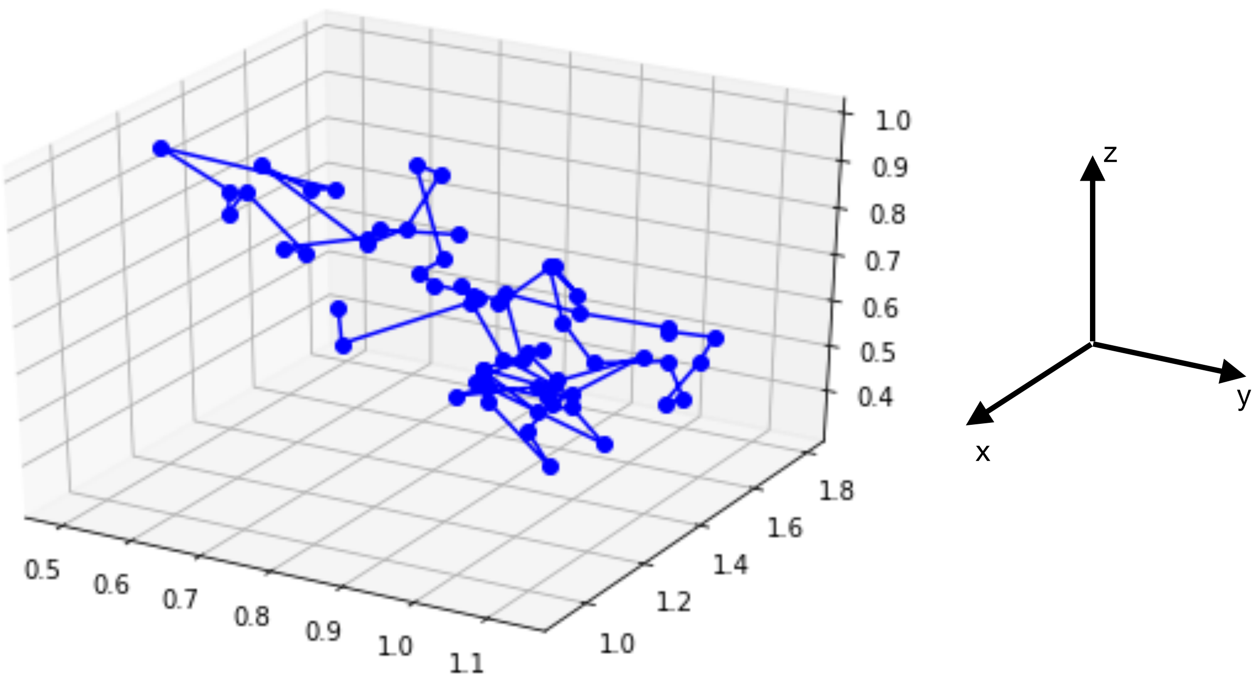
Shadow Hamiltonian strictly conserves energy within the variation order of 10^{-7} for T=10 and step size = 0.001.

- **Rouse Polymer in the microcanonical and canonical ensemble**

a) An equilibrium conformation $\{r_i\}$ from the statistics of a Gaussian polymer (random walk with variance of step length $R_e^2/(N-1)$), and the velocities from the Maxwell-Boltzmann distribution.

$$< (r_i - < r_i >)^2 > = \frac{1}{3(N-1)}$$

$\rho_{i\alpha} = \frac{1}{\sqrt{2m_iKT}} e^{-p_{i\alpha}^2/2m_iKT}$ (Maxwell-Boltzmann distribution) -i^{th}particle and α direction.

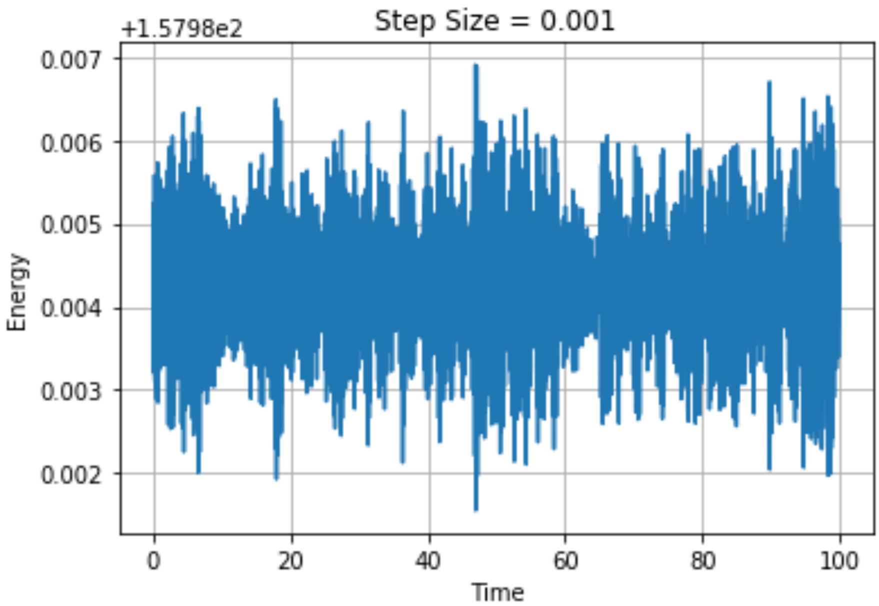


b) Velocity-Verlet for Rouse Polymer

$$q_i[t+h] = q_i[t] + p_i[t] \times h + F_i[t] \times \frac{h^2}{2}$$

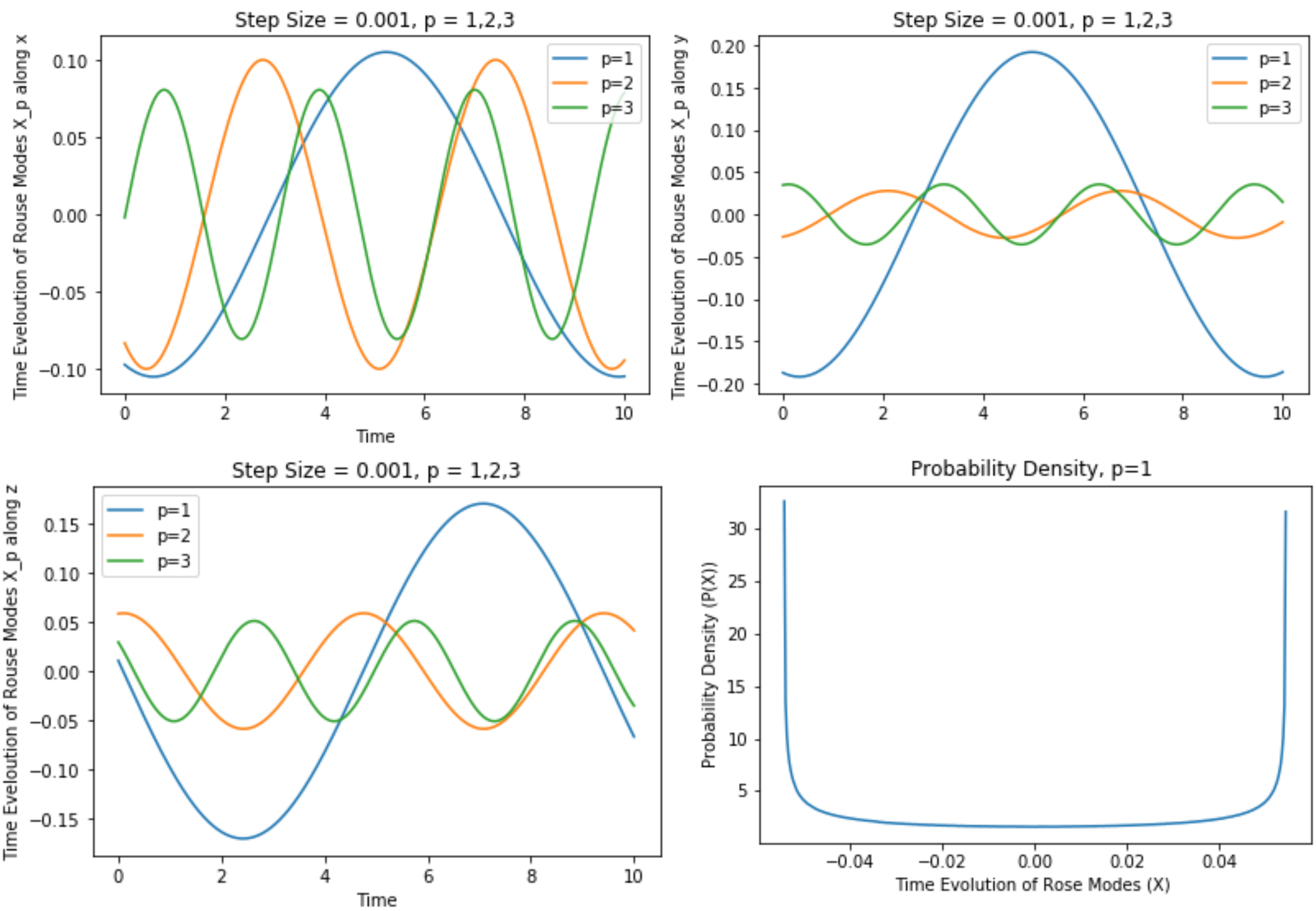
$$F_i[t+h] = -\frac{3}{2}(N-1)\frac{\partial}{\partial q_i}\sum_{i=1}^{N-1} |q_{i+1}[t+h] - q_i[t+h]|^2$$

$p_i[t+h] = p_i[t] + F_i[t] \times \frac{h}{2} + F_i[t+h] \times \frac{h}{2}$, for i^{th} particle.



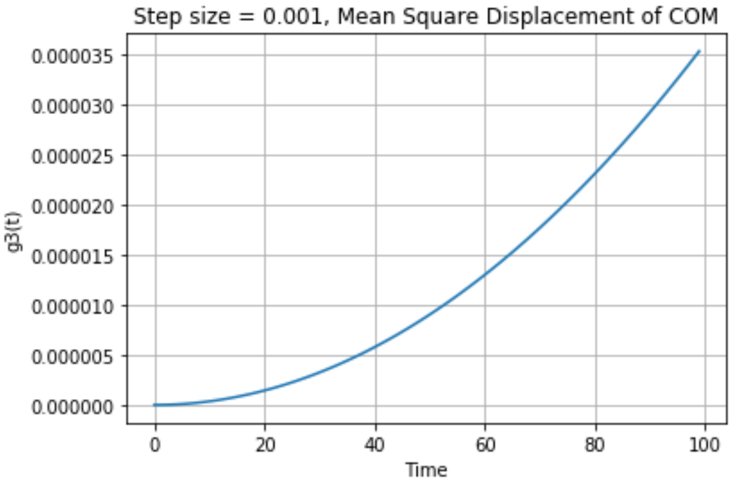
c) Rouse Modes: Calculated along x, y and z.

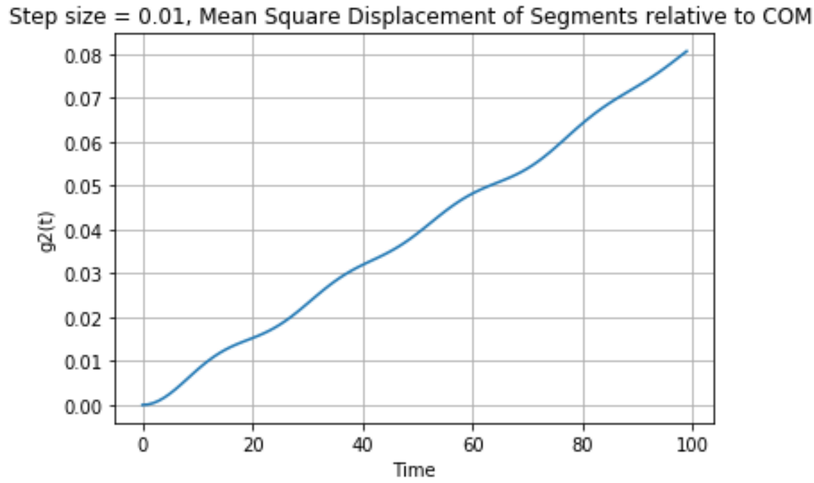
Total Time = 10. No. of Evolution steps = 10/0.001=10000

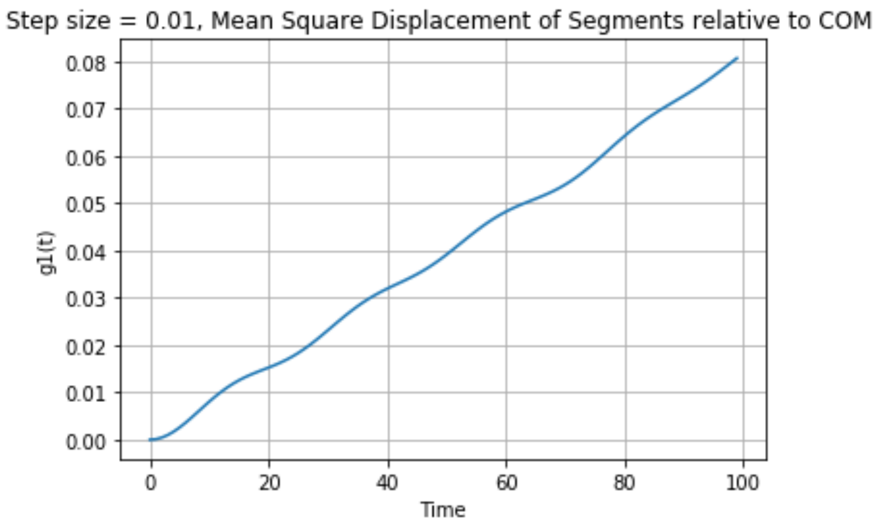


The sinusoidal (periodic) nature of plots suggest ergodicity.

d) Mean Square Displacements of COM, segments and relative between COM and segments: Total Time (T) = 100. No of evolution steps = T/h = 100000.

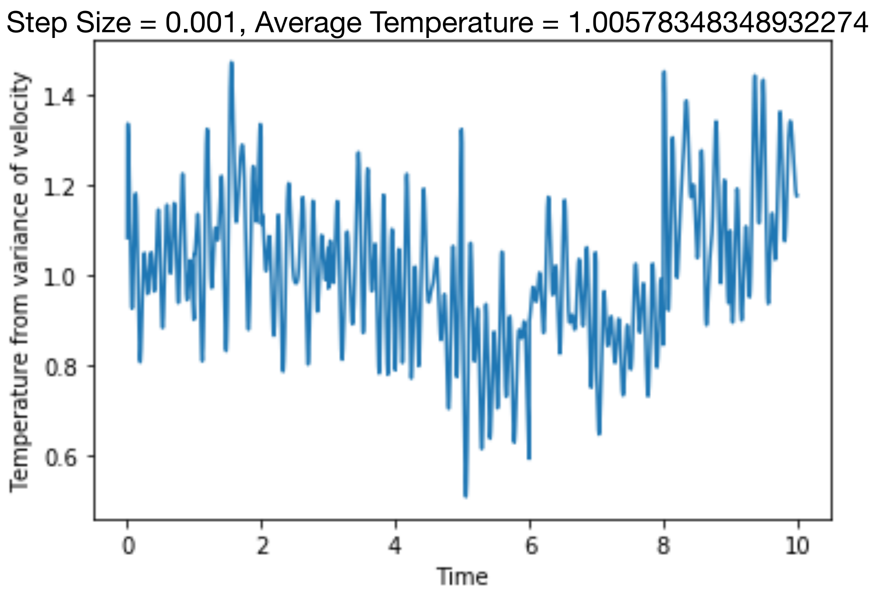


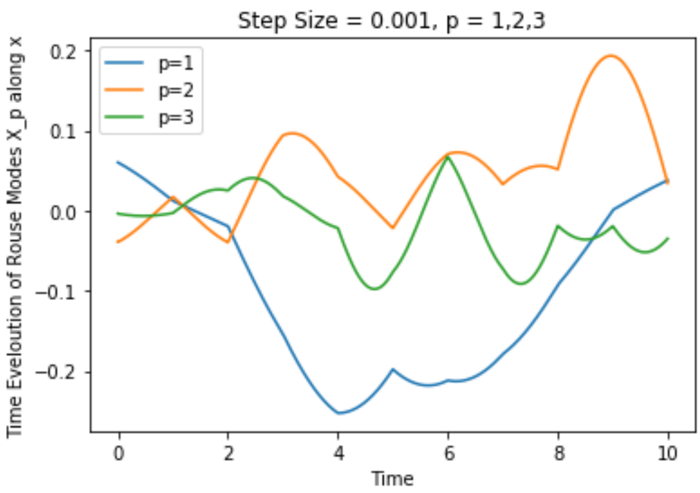


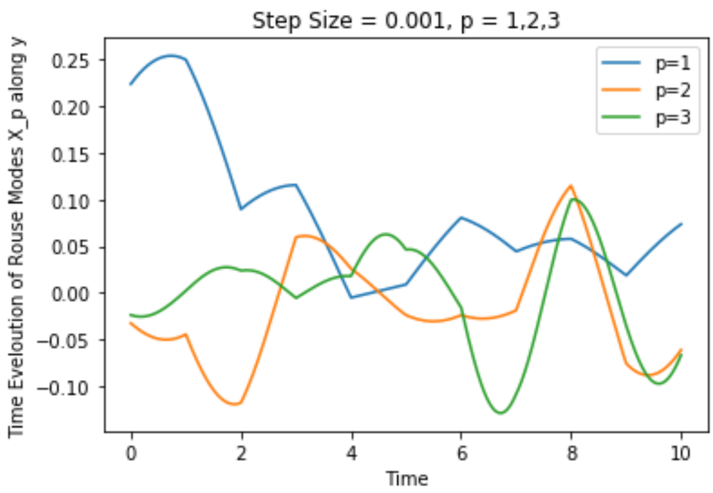


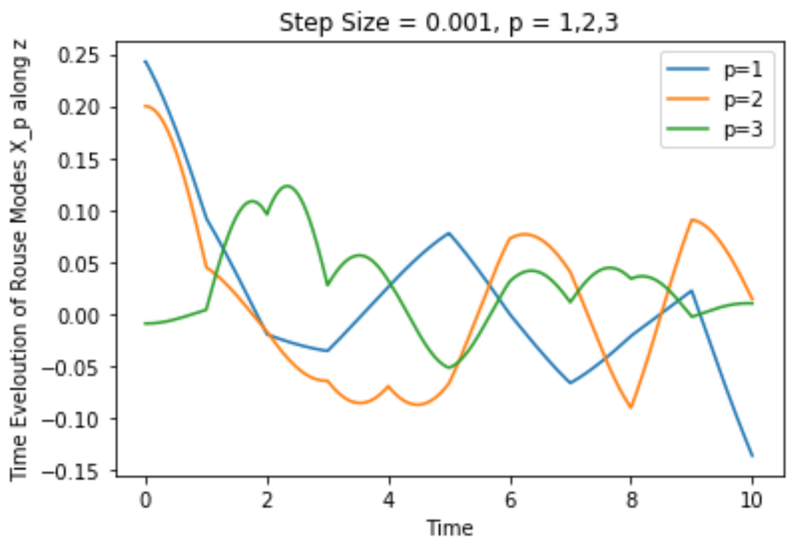
e) Anderson Thermostat: $\Delta t_{AT} = 1000$, after every 1000 steps I dump in new momenta to the system using the $\rho_{i\alpha} = \dfrac{1}{\sqrt{2m_i KT}} e^{-p_{i\alpha}^2/2m_i KT}$ (Maxwell-Boltzmann distribution) -i^{th} particle and α direction. Total time (T) was taken to be 10 for calculating Rouse Modes, and 100 for calculating Mean Square Displacements.

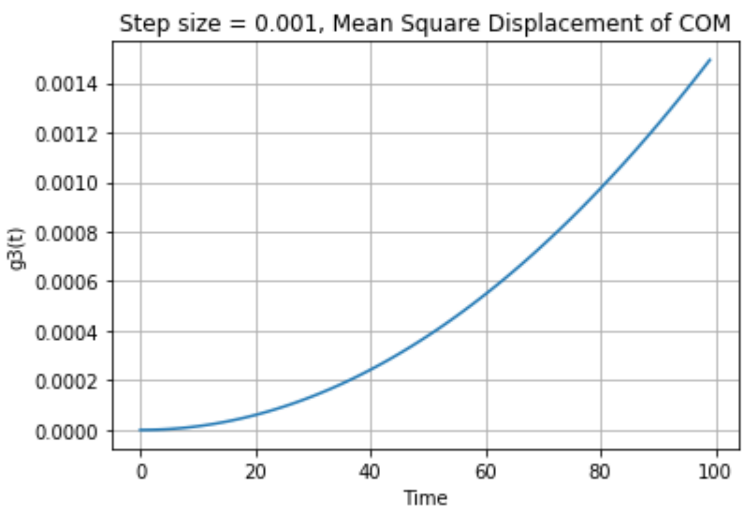
Thermostat keeping temperature almost constant.

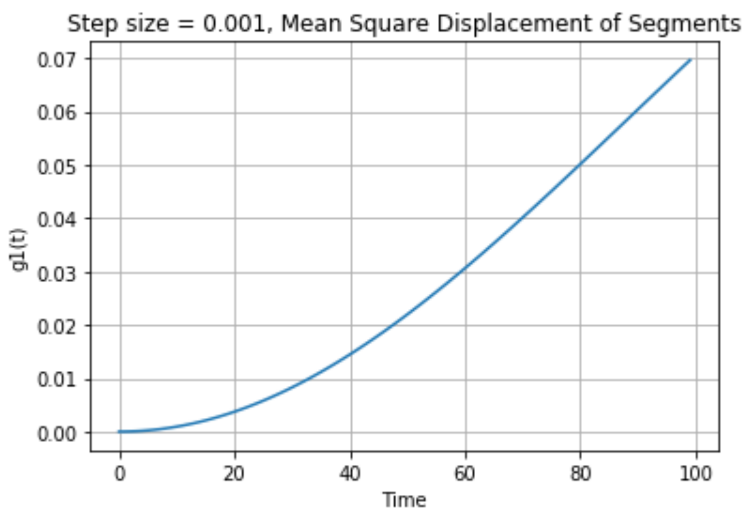


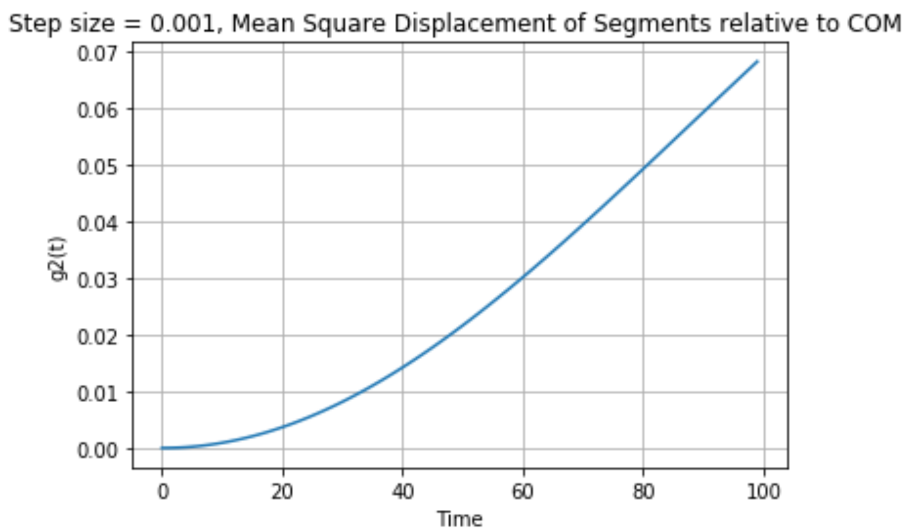

Step Size = 0.001, p = 1,2,3
Time Eveloution of Rouse Modes X_p along x
Time
p=1
p=2
p=3


Step Size = 0.001, p = 1,2,3
Time Eveloution of Rouse Modes X_p along y
Time
p=1
p=2
p=3


Step Size = 0.001, p = 1,2,3
Time Eveloution of Rouse Modes X_p along z
Time
p=1
p=2
p=3


Step size = 0.001, Mean Square Displacement of COM
g3(t)
Time


Step size = 0.001, Mean Square Displacement of Segments
g1(t)
Time


Step size = 0.001, Mean Square Displacement of Segments relative to COM
g2(t)
Time