

BB 626: Modeling biological systems and processes

Date : 27 Jan 2025

This is NOT to grade

1. Consider two particles connected by spring with spring constant k in 1D. The energy of the system is given

$$E = \frac{k}{2}(x - x_0)^2$$

Simulate this system using Monte Carlo simulation and calculate the following quantities. Take $k = 1$ and $x_0 = 2$.

- (a) Calculate the total energy of the system as a function of Monte-Carlo steps
- (b) Calculate the mean value of the x , standard deviation of x in steady state
- (c) Calculate the probability distribution of x , $P(x)$
- (d) Repeat the above for $k = 10$ and also other values. Calculate the variance corresponding to each k value and note their relation with k

Optional questions:

1. Repeat the simulation by taking two particles in 3D.
2. Repeat the simulation by considering multiple particles connected linearly as a polymer chain