Department of Physics
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Problem set 1: Computational Molecular Physics

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1. Distributions (Computational, 15 points)
Write a small programme (choosing your favourite programming language) to draw $N = 10, 100, 1000, 1000$ samples x from the following distributions.

(i) the uniform distribution $\rho(x) = \frac{1}{b-a}$ for $x \leq x \leq b$.
(ii) the Gaussian distribution $\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[\frac{-x^2}{2\sigma^2}]$.
(iii) the Boltzmann distribution $\rho(x) = \frac{\exp[-\frac{x}{k_B T}]}{Z}$ (for simplicity you can use Z=1)

(a) Plot the histrogram of drawn samples for each N and each distribution.

(b) Calculate the mean and variance from your samples. How do they compare to the expected (theoretical) values of mean and variance?

(c) Choose now your sample y to be the sum of $k = 100, 1000, 10000$ samples from the same distribution. $y = \sum_k x_k$. Draw $N = 10, 100, 1000, 1000$ samples y and plot their distribution as a histogram of the samples. What do you observe?

2. Phase space (15 points)
(a) What is a microstate?

(b) Draw the trajectory in phase space of a classical particle of unit mass that
(i) freely moves with constant velocity and is reflected at $x = \pm a$.
(ii) moves in a quadratic potential $U(x) = kx^2$.

(c) What can you say about the number of microstates of the particle in case (i) and (ii)?

3. Monte-Carlo Sampling (Computational, 20 points)
Choose your favorite programming language and implement a Monte Carlo (MC) algorithm to approximate the following integral:

$$\int_0^\pi \frac{1}{x^2 + cos^2(x)} dx$$

(a) Using the uniform distribution function, explore what happens with N=100, 1000, 10000 generating points and plot the results of each case
(b) Using the function $P(x) = \exp[-x]$, explore what happens with N=100, 1000, 10000 generating points and plot the results of each case

For every MC calculation compute also the corresponding variance.