1. (10 marks)
(a) Explain how a uniform random number generator works and describe the underlying probability distribution from which such numbers are drawn.
(b) Specify the random number generator used in your code and write the syntax for generating a uniform random number.
(c) Describe how you would modify the code to generate random numbers in the range −100 to +100.

2. (12 marks)
Using the one-dimensional random walk model:
(a) Derive the diffusion equation starting from the discrete random walk.
(b) Clearly define the diffusion constant.
(c) Write down the discrete approximations for the first and second spatial derivatives that appear in the derivation.

3. (10 marks)
You are given a time series of a random variable sampled from a uniform distribution.
Write a pseudo-code to compute:
(a) the mean displacement,
(b) the mean-square displacement, and
(c) the histogram of the variable.

4. (16 marks)
Consider a system of 108 water molecules confined in a cubic box of volume V.
(a) Write the classical Hamiltonian for this system. (6 marks)
(b) Write the quantum Hamiltonian for the same system. (6 marks)
(c) What is the Born–Oppenheimer approximation, and how is it used to obtain the electronic potential energy surface? (4 marks)

5. (12 marks)
Explain the gradient descent method for minimizing the potential energy surface of a system of N interacting particles governed by an arbitrary potential energy function. Include the update rule and the physical interpretation of force-based minimization.