Q1. For 3D Ising model (10x10x10 = 1000 spins) at zero field, compute the specific heat (C) as a function of temperature across the critical temperature (T_c) using the following methods:

i. $C = \frac{\partial \langle E \rangle_T}{\partial T}$, where $\langle E \rangle_T$ is the average potential energy computed at each temperature T. The derivative may be computed numerically.

ii. $C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}$ (See this for related derivation/discussion: https://www.sccs.swarthmore.edu/users/02/no/pdfs/fluct.pdf)

Q2. For 3D Ising model (10x10x10 = 1000 spins) at zero field, compute the Binder cumulant as defined below across the critical temperature:

$$U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}$$

where, *m* is the order parameter (magnetisation).

Q3. Write a program to numerically evaluate the following integral using Monte Carlo method (importance sampling). Your program must check for numerical convergence with tolerance 10^{-2}.

$$f = \frac{\int_{-\infty}^{\infty} x^4 \, e^{-x^4} \, dx}{\int_{-\infty}^{\infty} e^{-x^4} \, dx}$$

Q4. The supplied data file "unknown.xyz" has Cartesian coordinates (x,y,z) of the atoms of a molecule. The format of the file is as follows:
Line 1: Number of atoms
Line 2: Dummy text (comment)
Line 3 to end of file: Atom name and x, y, z coordinate of the atoms

The atom names are unknown (X) as of now. Consider the following algorithm to determine that information:
If the distance between two atoms is less than 1.6 (in the same unit as supplied coordinates), then the two atoms are bonded (connected) to each other. This molecule is known to have only carbon (C), nitrogen (N), oxygen (O), and hydrogen (H) atoms. The number of bonds that can be formed by these atoms are 4, 3, 2 and 1 for C, N, O and H, respectively.

Write program(s) to perform the following tasks and report the answers:
(i) Find the total number of bonds (connections) in this molecule.

(ii) Count the number of atoms corresponding to each element in the molecule, and determine the empirical molecular formula, e.g. if there are 4 C and 4 H atoms, the formula would be C_4H_4.
(iii) Write a new file "solution.xyz" such that the first column "X" would be replaced by the correct atom name. You may use software like "Avogadro" to visualise this molecule now.