Monte Carlo Problems for Diatomic Molecular Systems

# Problem 1: Estimating Bond Length Distribution

You simulate 10 bond lengths (in Å) for a diatomic molecule (e.g., H₂) from a uniform distribution between 0.5 and 2.0 Å:  
1.0, 1.3, 0.8, 1.6, 1.2, 1.9, 0.7, 1.5, 1.1, 1.4

Tasks:

• Calculate the average bond length

• Calculate the standard deviation using:

σ = sqrt((1/N) \* Σ(xᵢ - x̄)²)

# Problem 2: Estimating Potential Energy from Lennard-Jones

Given 5 interatomic distances (in Å): 0.9, 1.2, 1.5, 2.0, 2.5  
With Lennard-Jones parameters: ε = 0.2 kcal/mol, σ = 1.0 Å

Use the Lennard-Jones potential:

V(r) = 4ε[(σ/r)^12 - (σ/r)^6]

# Problem 3: Metropolis Monte Carlo Acceptance

A trial move increases system energy from 1.5 to 2.0 kcal/mol.  
Given: T = 300 K, k\_B = 0.001987 kcal/mol·K

Calculate probability of acceptance using:

P = exp(-ΔE / (k\_B T))

# Problem 4: Estimating Radial Distribution Function (RDF)

Distances: 1.0, 1.5, 2.0, 2.5, 1.2, 2.2, 1.8, 2.7, 3.0, 2.3  
Bin edges: [1.0–1.5), [1.5–2.0), [2.0–2.5)

# Problem 5: Estimating Configurational Integral

Bond lengths: 0.7, 1.0, 1.3, 1.7, 1.9  
Potential function:

V(r) = Dₑ(1 - e^{-a(r - rₑ)})²

Estimate configurational integral using:

Z ≈ (2.0 - 0.5)/5 \* Σ exp(-V(r)/k\_BT)

# Detailed Solutions

## Problem 1

Average bond length = 1.25 Å

Standard deviation ≈ 0.35 Å

## Problem 2

V(r) values:  
0.9 → 0.908  
1.2 → -0.128  
1.5 → -0.153  
2.0 → -0.087  
2.5 → -0.041  
Average ≈ 0.1 kcal/mol

## Problem 3

ΔE = 0.5 kcal/mol  
k\_B T = 0.5961  
P = exp(-0.839) ≈ 0.432

## Problem 4

Bin [1.0–1.5): 2  
Bin [1.5–2.0): 2  
Bin [2.0–2.5): 3

g(r) = count / (bin width × total samples)

## Problem 5

V(r) values:  
0.7 → 2.57  
1.0 → 0.75  
1.3 → 0.11  
1.7 → 1.32  
1.9 → 2.09

Boltzmann weights:  
0.014, 0.285, 0.832, 0.106, 0.031

Z ≈ 0.254