Simulation Experiment Report

# **Abstract**

This report outlines the simulation results of generating 2000 random polymer chains with varying segment lengths and evaluating their structural properties in 3-D space.

# **Introduction**

The purpose of this analysis is to explore the behavior of polymer chains by simulating their random walks in a three-dimensional space. The focus is on determining the scaling relationship of mean squared end-to-end distance with respect to the number of segments in a polymer chain.

# **Methods**

We employed a Python script to generate chains wherein each segment's orientation was assigned randomly in 3D space with uniform distribution. Specifically, segment angles were chosen to ensure a statistically uniform distribution over the sphere. The end-to-end distance vector was computed for each polymer chain, and the mean squared distance was calculated by averaging over 2000 samples.

# **Results**

The mean squared end-to-end distance h2(N) was plotted against the number of segments N, demonstrating a clear scaling relationship. The scaling exponent v, estimated through linear regression of the log-transformed values, was found to be approximately 1.022. Simulated chain conformations are shown in Fig. 1 to Fig. 5, corresponding to different segment counts.  
Fig. 1: 3D view of 50 random polymer chain conformations with 10 segments.  
  
Fig. 2: 3D view of 50 random polymer chain conformations with 50 segments.  
  
Fig. 3: 3D view of 50 random polymer chain conformations with 100 segments.  
  
Fig. 4: 3D view of 50 random polymer chain conformations with 200 segments.  
  
Fig. 5: 3D view of 50 random polymer chain conformations with 400 segments.









