# Polymer Chain Simulation Report

## Abstract

This report outlines the computational simulation performed to analyze the properties of polymer chains in three-dimensional space. The purpose of this study was to estimate the mean squared end-to-end distance as a function of chain length, thereby elucidating the scaling behavior in a stochastic environment. Understanding these properties is pivotal as they have extensive applications in materials science, chemistry, and biological systems modeling. The Polymer chain simulation provides critical insights into the dynamics and structural characteristics of polymers which are essential for developing advanced materials.

## Introduction

The physical behavior of polymer chains is a fundamental aspect of material science and biophysics which drives significant research interest. Polymer chains can exhibit a range of mechanical, chemical, and electrical properties based on their length and configuration in space. This report investigates the statistical properties of polymer chains using a computational approach to simulate their random walk in three-dimensional space. By varying the number of segments in the polymer chains, we examined how the distance from the start to the end of the chain scales with the number of segments. Such understanding helps in predicting the behavior of real-world polymers in various applications.

## Methods

To simulate the wanderings of a polymer chain in 3D space, a Python script was crafted to generate 2000 independent polymer chains for selected segment lengths (10, 50, 100, 200, 400 segments). Each segment is modeled as a vector of unit length, pointing in a random direction uniformly distributed across all possible orientations. This uniform distribution was achieved using spherical coordinates with angles chosen according to correct statistical methods to prevent clustering at the poles. This model represents an idealized free-jointed chain where each segment freely rotates relative to its neighbors without any external constraints. The end-to-end distance, or the displacement of the polymer after N steps, was then computed for each simulation, and the squared displacements were averaged over all simulations to estimate the mean squared end-to-end distance.

## Results

The results from the simulations indicate a clear scaling relationship between the mean squared end-to-end distance of the polymer chains and the number of segments, which suggests a power-law behavior typical of random walk phenomena in physics. The scaling exponent, calculated through linear regression of the logarithm of the mean squared end-to-end distances versus the logarithm of the number of segments, was found to be approximately 1.02. This value is consistent with theoretical predictions for the ideal random coil model of polymer chains in a good solvent. Plots of the polymer configurations for different chain lengths clearly show the increase in spatial extent as the chain length increases. These results validate the model and the computational approach used in this study.

All detailed graphs and polymer chain configurations are provided below for reference:

Fig. 1: Chain3D10.png

Fig. 1: Chain3D50.png

Fig. 1: Chain3D100.png

Fig. 1: Chain3D200.png

Fig. 1: Chain3D400.png

Fig. 2: h2vsN.png