Exercise sheet 4

Polymers

Theoretical Biophysics
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Exercise 4.1 Radius of gyration label

Calculate the radius of gyration of a freely jointed chain and compare it to the average squared end-to-end distance. The radius of gyration is defined as

\[
R_g^2 = \frac{1}{N} \left( \sum_{i=1}^{N} (\vec{R}_i - \vec{R}_{CM})^2 \right)
\]

where \( \vec{R}_{CM} = \frac{1}{N} \sum_{i=1}^{N} \vec{R}_i \) is the center of mass of the polymer and \( \vec{R}_i = d \sum_{j=1}^{i-1} \vec{e}_j \) is the position of the \( i \)th monomer. The center of mass and the radius of gyration are the analogs of mean and variance of a mass distribution.

Exercise 4.2 Self-avoiding random walks

The majority of polymer models discussed in class ignore the fact that a polymer can’t intersect with itself. Accounting for such constraints is challenging mathematically and the ignoring them will often give accurate answers, at least in three dimensions.

- Discuss the different between regular and self-avoiding walks in one dimension (this is really simple, don’t try to come up with anything complicated)
- Simulate random walks in three and four dimensional integer grids with and without self-avoidance (up to \( n = 1000 \) steps). Repeat until you have sufficient statistics. Occasionally your walker will get trapped in a place where all possible steps are already taken.
- Graph the dependence of the average squared end-to-end distance as a function of the number of steps.
- Compare the distribution of end-to-end distances.