Pranav Parakh PHYS 212 Project Proposal

Topic: Self-Avoiding Random Walks with Application to Polymers

In this project, we aim to implement the Pivot Monte-Carlo algorithm to generate self-avoiding random walks (SAWs), with the aim of simulating their behaviour in 2 and 3 dimensions. Self-avoiding random walks are thought to obey power laws for the mean-squared end-to-end distance and the mean-squared radius of gyration. By using Pivot Monte-Carlo to sample from the vast space of self-avoiding random walks, we aim to compute these critical exponents to a high degree of accuracy.

Outline:

1. Background and introduction
    a. Discussion of SAWs, the connective constant, end-to-end distance, and radius of gyration
    b. Applicability to polymers and simulation of polymer dynamics
2. Pivot Monte-Carlo algorithm
    a. Theory, implementation, and relevant parameters of Pivot Monte-Carlo. Explanation of parameters that scale with power laws and what critical exponents we will be computing.
    b. Explanation of acceptance probability and how that also scales as a power law in multiple dimensions
3. Discussion of results
    a. Show simulations in 2 and 3 dimensions of SAW and compute the relevant critical exponents
    b. Explanation of convergence speed and dependence on lattice size
    c. Exploration of computational complexity of the SAW problem
4. Bonus (if I have time and space):
    a. Fractal dimension of SAWs
    b. Proof of ergodicity
    c. Other algorithms (e.g. repetition algorithm, kink-jump algorithm)
    d. Exact enumeration of SAWs using the transfer matrix methods
5. Appendix:
    a. Implementation in Python and plotting software

References:

https://link.springer.com/article/10.1007/BF01022990 - most cited paper in this field, implements the pivot algorithm developed by Lal and rigorously computes critical exponents. Good discussion of theory and computational complexity of the system.

https://www.hiskp.uni-bonn.de/uploads/media/polymers.pdf - more discussion about relevance to polymers, exploration of various algorithms, both static and dynamic.

https://arxiv.org/pdf/1309.6709 - transfer matrix method for exactly enumerating the number of SAWs on a lattice.

https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.104.055702 - the current best implementation to enumerate SAWs, faster in time and memory complexity than Madras & Sokal, but significantly more complicated algorithm implementation.

https://en.wikipedia.org/wiki/Self-avoiding_walk#cite_note-1 – Wikipedia page, good overview of the field.