Lab project / internship M1 PPN-QuanTEEM (1,5 months : 15/05-30/06)

2022-2023

Title of the project: Modelization of the growth of self-avoiding walks

Supervisor(s): Christophe Laforge & Patrick Senet

Laboratory / Department / Team : ICB/Nanosciences/PhaP

Collaborations: -

Summary:

A self-avoiding walk is a path on a graph that does not visit the same site twice. Despite this apparent simple definition, self-avoiding walks (SAW) are still today the focus of numerous research efforts. Indeed, every step forward in the understanding of SAW potentially lead to a better understanding of polymers for which they are an idealistic model. Applications of SAW in our team are protein folding and intrinsically disordered proteins.

During the internship, you will implement an algorithm simulating the growth of interacting self-avoiding walks. You will first reproduce and verify recent scientific results concerning a phenomenon named trapping in which the growth of the walks is prevented by the steric constraint (1). You will also verify some statements that are made in the paper but for which no data or evidence are presented. Reproducing scientific results is an important step in the construction of scientific knowledge.

Based on your progress, you could move on to an original investigation. Indeed, the model can be easily modified to the fabled lattice protein model: the 2D-HP which mimics the hydrophobic/polar amino-acid interactions. The study of trapping for the 2D-HP model, certainly not a trivial question, is waiting for a curious mind to be explored.

Finally, you will be exposed to modern numerical methods as the so-called deep learning technique currently explored in the team.

(1) *Trapping in self-avoiding walks with nearest-neighbor attraction*, W. Hooper & A.R. Klotz, Phys. Rev. E 102, 032132 (2020)

Type of project (theory / experiment): theory

Required skills: Python programming skills