Lab project / internship M1 PPN (1,5 months : 13/05-21/06)

2023-2024

Title of the project: Topological properties of a class of Self-Avoiding Random Walks and protein folding and design

Supervisor(s): Patrick SENET

Laboratory / Department / Team : ICB/PhaP

Collaborations:

Summary:
This internship combines graph theory, statistical physics, machine learning and molecular biophysics to propose a new road to design protein and understand misfolding of proteins. We have defined a class of three-dimensional self-avoiding random walks (SAW) at constant curvature which is generated by a homemade algorithm. We showed that curvature is analogous to an inverse temperature in what is equivalent to a protein folding phenomena. The probability density of the topological properties of the SAW generated follows a non-Gaussian statistic with a long tail in which we detect structures which can serve as scaffold for new stable proteins. These rare structures are difficult to generate for a path of more than 20 steps of the SAW. The internship will consist to 1) test and write a Monte Carlo algorithm to generate the rare structures for longer paths, 2) to establish a database of the curvature of human proteins using molecular dynamics and Alphafold2 (a deep learning program), 3) to test machine learning programs to generate an amino-acid sequence constrained to a given scaffold.

Type of project (theory / experiment): theory, computational

Required skills: Python, mathematics, physics.