

## Erasmus Mundus Master QuanTEEM Research Project

TITLE	Topological properties of a class of Self-Avoiding Random Walks and protein folding and design.
SUPERVISORS	Patrick Senet
INSTITUTION	Université de Bourgogne
LAB / DEPARTMENT / TEAM	ICB/PhaP
COLLABORATIONS	
TYPE OF PROJECT (theory / experiment)	Theory, computational

### 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.

### Additional Information

Required skills: Python, mathematics, physics.

Duration: from 13/05/2024 to 21/06/2024.