Université de Reims Champagne-Ardenne
Unité Matrice Extracellulaire et Dynamique Cellulaire
CNRS UMR 7369

Thesis offer – 2024-2027

MERISM Thesis: Membranes and Matrix Receptors; Interactions by Multi-Scale Simulations

Subject: The dynamic modeling of molecular systems at the mesoscopic scale represents a challenge at the level of matricellular interfaces. Indeed, at this scale, there are no direct observation tools and simulations allow us to better understand the molecular players in these interfaces and their impacts in various pathologies, particularly associated with aging. With this in mind, the MEDyC unit has developed the DURABIN tool based on the dynamics of rigid bodies. However, the membrane representation of the DURABIN tool is succinct and the MERISME thesis project aims to parameterize/improve DURABIN for the study of the dynamics of membrane proteins via the development of a multi-scale approach (all atom AT, large grains CG and rigid bodies CR). A more faithful representation of the membrane is important because it has been shown that its composition and organization plays an important functional role and that large membrane proteins such as integrins, CD44 or CD36, metalloproteinases or the EBP from the Elastin Receptor Complex have an affinity for plasma membrane domains. Modeling techniques will provide a better understanding of the mechanisms of activation and recruitment of matrix receptors to the membrane.

This project involves bioinformatics methods with the construction of models (protein and membrane) and their numerical simulations (molecular and Brownian dynamics) at different resolutions (AT, CG, CR); and IT developments with the use of Unity and Blender to add new features to DURABIN. This project also calls on knowledge in biochemistry and biophysics. Molecular dynamics calculations will mainly be carried out on the regional Romeo server.

Application: The candidate, bioinformatician or computer scientist, must have good knowledge of C++, bash and python programming under Linux. He will join a team of biologists, bioinformaticians and biophysicists of around ten people. The recruited candidate will have skills in computer science, bioinformatics and structural biology. The thesis should ideally begin on September 1 or October 1, 2024.

The candidate must provide a cover letter and a curriculum vitae as well as a letter of recommendation to stephanie.baud@univ-reims.fr

Keywords: scientific computing, molecular modeling, molecular dynamics, multi-scale representations

Team – location: Molecular Modeling and Multi-scale Imaging (MIME) Team
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