Laboratoire de Biochimie Théorique
Institut de **B**iologie **P**hysico-**C**himique
13, rue Pierre et Marie Curie
75005 PARIS

S E M I N A I RE

Michael Feig, Department of Biochemistry & Molecular Biology,
Michigan State University, USA

" Dynamics and interactions of biomolecules in cellular environments: From traditional simulations to direct sampling via machine learning "

In biological environments biomolecules are present at high concentrations making frequent interactions unavoidable. The resulting crowding leads to altered dynamics but also enables phase separation processes that will be analyzed from a simulation perspective. Recent results with atomistic and coarse-grained models will be presented. A focus will be on the recently developed COCOMO model for modeling intrinsically disordered peptides at a residue level with applications to model liquid-liquid phase separation of peptide and and peptide-nucleic acid systems. The interpretation and prediction of experimental data via such simulations will be discussed in detail. Extensive simulations of IDPs with COCOMO were also the starting point for developing generative machine learning models that can rapidly generate conformational ensembles according without the need for simulations. Such methods are further complemented by new tools based on machine-learning for rapidly converting CG models to accurate atomistic models that have implications for implicit multi-scale sampling and coarse-graining strategies. As a practical example, the rapid refinement of structural models against cryoEM density maps will be demonstrated.

Jeudi 25 avril 2024

14h30

Salle des conférences