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S E M I N A I R E

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« Less (detail) is more (information): leveraging multi-scale modelling to understand complex biomolecules »

One of the outstanding challenges of computer-aided investigation of biological macromolecules, such as proteins and protein complexes, is represented by the intrinsic multi-scale nature of several processes and phenomena; these range from large conformational changes induced by ligand binding to the epigenetic regulation of gene expression and beyond. A unique framework for the in silico study of such phenomena is impossible and inappropriate, as different properties take place at distinct characteristic length- and time-scales; consequently, models and representations at various resolutions have been developed, which address each property specifically. A critical issue, however, is how to integrate these models to account for the interplay of processes occurring at different scales.
In this talk I will present methods and techniques that have been recently developed and applied to fill this gap. Particular attention will be posed on those strategies aimed at identifying functionally relevant sites or regions of proteins, based on the amount of information that a reduced representation can preserve from the underlying high-resolution model. Subsequently, I will discuss the general properties of these reduced representations and the issue of integrating models at different levels of detail in the same setup. Finally, I will hint at multi-disciplinary applications that these methods would allow in fields even very far from molecular biophysics, e.g. neuroscience and quantitative finance.

Lundi 10 octobre 2022 à 14h00

Salle de conférence