Dynamics of Biomolecular Processes: From Atomistic Representations to Coarse-Grained Models

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Challenges in protein structure prediction

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Proteins are the central machines of cells, and they perform their actions by interacting with each other as well as with other molecules. Large complexes involving tens or even hundreds of proteins make up the central hubs in biological interaction networks. In human cells repeated domains are frequent among these hubs. Today, large-scale efforts in genomics, proteomics, lipidomics and metabolomics are producing complete lists of the molecules in entire cell as well as in different sub-cellular compartments. Further, interactions between molecules can be studied at different levels of detail. In small-scale studies it is possible to obtain detailed information about the interaction of a few molecules, while in large-scale studies less detailed information for a larger set of molecules can be obtained. Only for a small number of the large complexes atomistic details have been possible to obtain and in particular molecular complexes embedded in the membrane have been difficult to study experimentally.

A major aim within the field is to reveal detailed structural information about large biological complexes. To obtain this goal a mix of experimental and computational methods needs to be applied. A major source of information is coming from the rapid increase in genomic sequence data. Here, I will discuss how to combine computational and experimental studies to obtain increased understanding of the formation of large molecular complexes particularly in the membrane.

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