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Coarse-grain Modeling in Biological Membranes

Atomistic simulations of biomolecular systems have been used for decades to complement experiments. However, even with the rapid increase in the available computational power, atomistic simulations are still strictly limited to the nanoscale regime. Contemporary classical atomistic MD simulations typically feature ~10,000 - 1,000,000 atoms, studied over time scales of ~10 - 1,000 ns. These limitations prohibit studies of many important processes involving biological macromolecules. Examples of such processes include phase behaviour in lipid bilayers, vesicle fusion, and dynamics of proteins and their aggregates. Moreover, a direct comparison of atomistic simulations to experiments is often hampered due to the inherent limitations in resolution of the experimental methods used.
A powerful solution to the time and length scale problem in molecular simulation is to coarse-grain (CG) the atomistic system studied to one with a lower spatial resolution. Consequently, interactions between single atoms are replaced by effective interactions between the CG units. This process dramatically decreases the degrees of freedom of the model, resulting in a speed-up of the simulations by several orders of magnitude. Not surprisingly, the application of such methods to study entirely new problems of biological importance has been rapidly gaining increased attention in the biomolecular simulation community.
There is no unique way to formulate the CG units, nor the interactions between them. Since in the coarse-graining procedure some chemical detail of the underlying atomistic system is lost, for meaningful application of CG models it is crucial to understand how the CG methods used have been constructed and what is their range of applicability.
Our aim is to study these stuff using coarse-grain approach:

- Simulation of lipids self-assembly in membrane
- Drug design, binding, delivery, transport and metabolism
- Membrane transport phenomena; How flip- flops between the leaflets affect shape of the membrane?
- Phase transitions in lipid bilayer systems
- Computational Protein Design

Summary

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