

The comes and goes of lipid membranes under the lens of computer simulations

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When phospholipids dissolve in water they self-assemble into a variety of structures of which bilayers have the greatest biological relevance. Bio-membranes are the most complex examples of lipid bilayers as they have evolved to accommodate the needs of specialized cells, organelles, and other sub-cellular structures. However, even the simplest lipid bilayer offers a repertoire of behaviours that is amenable of exploration with different levels of resolution in space and time. For example, while certain properties of the membranes are well described considering the membrane as an elastic sheet, others demand a more detailed description that takes into account the atomic nature of the lipids and the forces that keep the bilayer together. Between these two extreme representations of the membrane, one fairly schematic the other very elaborate, there is a range of “coarse-grain” models that can be interrogated with the aid of computer simulations.

The aim of this talk is to provide an overview of how observable membrane properties emerge from the molecular level interactions and the collective action of the lipid molecules. I will first present a brief and simple summary of the current methods, techniques, and models available to simulate lipid bilayers across different length- and time-scales. Secondly, I will discuss what simulations teach us about the transport of nanoparticles, cell-penetrating peptides, and nano-bubbles across lipid bilayers. I will also address the problem of how and where transmembrane pores form in phase-segregated membranes. Finally, I will present some preliminary results concerning multicomponent membranes with realistic composition, and discuss the correlation between membrane curvature and local lipid packing and composition. In all cases, I will emphasize the connection between computational work and experimental observations, advocating the idea that computer simulations are tools that allow us to think, predict, and test hypothesis about the behaviour of real membranes, but within the realms of specific models.