

Title: Molecular simulations of cellular membranes: coming of age?

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Abstract:

Cellular membranes play a huge role in a myriad of key cellular processes as diverse and fascinating as vesicle trafficking, receptor functioning or synaptic transmission. Yet, due to intrinsic limitations of biophysical and biochemical methods when dealing with a membrane- mimetic environment, a high-resolution knowledge of the basic physicochemical principles that govern these processes is still limited. In this context, *in silico* modeling is a well-established alternative strategy, since computational-based studies offer the possibility to investigate the behavior of matter directly at the atomistic level under highly controlled conditions.

Recent developments in multi-scale molecular simulations and in HPC infrastructures have helped us providing precise mechanistic insights into key cellular processes involving membranes, including vesicular trafficking (Vanni et al., Nat Comm, 2014; Magdeleine et al, eLife 2016), endocytosis (Pinot et al., Science 2014) and lipid droplet biogenesis (M'Barek et al., Dev Cell 201; Zoni et al, in preparation).

I will highlight how these recent developments have allowed to establish meaningful direct correlations between experimental observations and computational results and I will discuss how important remaining key challenges in membrane simulations can be addressed thanks to continuous improvements in HPC infrastructures.