Contribution ID: **50** Type: **Contribucion Oral**

Transfer entropy and graph theory in the analysis of MD trajectories of Lipid Bilayers

Thursday 14 December 2023 11:40 (20 minutes)

Transfer entropy and graph theory in he analysis of MD trajectories of Lipid Bilayers Cellular processes rely on signaling to initiate various activities, often involving the transmission of information to trigger these events. While conventional biochemical signaling pathways typically involve specific molecule arrival, allosterism introduces conformational changes in one site that affect another at a topographically distinct site. The application of transfer entropy (TE) has recently enhanced our understanding of these phenomena. In the case of biological membranes, the lipid raft hypothesis postulates that lipid-lipid interactions can laterally organize them into domains of distinct structures, lipid/protein compositions, and functions; nonetheless, the difficulties of experimentally observing nano-scale dynamic structures have prevented a full characterization. Furthermore, the time required for the spontaneous formation of a raft from an arbitrary initial configuration is still beyond the current capacity of molecular dynamics (MD) simulations. Moreover, the standard tools to analyse MD trajectories are aimed at describing the properties of the whole simulated system. In this work, TE is shown to provide a quantitative tool to evaluate the influence that instantaneous fluctuations of lipid tails have on each other, thus to assess emergent collective behaviors. TE analyses were conducted on all lipid pairs within three distinct MD trajectories of bilayers, each characterized by a specific composition: one with a 55:45 POPC:PSM mixture, a second with a 45:35:20 POPC:PSM:Cholesterol mixture, and a third with a 35:30:35 composition. Leveraging TE results, a directed graph is constructed to facilitate the evaluation of emergent system properties. From the comparison of the results, it is inferred that lipid behavior becomes more intertwined at higher cholesterol concentrations. This methodology can be extended to various different lipid mixtures to study how motion fluctuations can convey structural and dynamic information from one region of a bilayer to another.

Resumen de la contribución

Author: MORENO PÉREZ, Nahuel Armando (ICF, UNAM)

Presenter: MORENO PÉREZ, Nahuel Armando (ICF, UNAM)

Session Classification: Contribuciones Orales