Investigating Elastic- And Entropic-driven Rupture Mechanisms Of Biomembranes

Salvatore Buonocore[1], Francesco De Angelis[1], Rosario Capozza[2]

[1]Istituto Italiano di Tecnologia
[2]University of Edinburgh

Abstract

Biomemebranes are characterized by several elastic parameters that appropriately describe the energetics of their deformation under thermal fluctuations [1]. When their structure is quasi-two-dimensional (namely lipid bilayer 4-5 nm thick), several recent studies [1,2] showed that their disruption, at finite temperature, can be driven either by elastic or entropic forces depending on its size. However, what happens for thicker structures? Using the computational platform COMSOL Multiphysics that allows the coupling between finite element simulations and Brownian motion models, we show that the entropic contribution to the fluctuations and rupture of biomembranes at finite temperature can be the dominant mechanism not only for structures few nanometers thick but also for thicker structures (of the order of 1 um). The results of this work can help shedding light on the dynamic and failure behavior of biomembranes that are key in tissue engineering and drug delivery. The most remarkable advantage of the proposed approach is the possibility of analyzing dynamical processes of bio-structures spanning dimensional and temporal intervals ranging from nanometers to micrometers and from nanoseconds to microseconds, in a computationally very stable and efficient manner. In these spatial and temporal ranges, the Molecular Dynamics approach is not a viable route

Reference

[1] David Boal, David H. Boal, Mechanics of the Cell. Cambridge University Press, 2012.
[2] Rosario Capozza, Luca Giomi, Carlo A. Gonano, and Francesco De Angelis, How to puncture a biomembrane: elastic versus entropic rupture, arXiv preprint: 1911.05557 (2019).

Figures used in the abstract

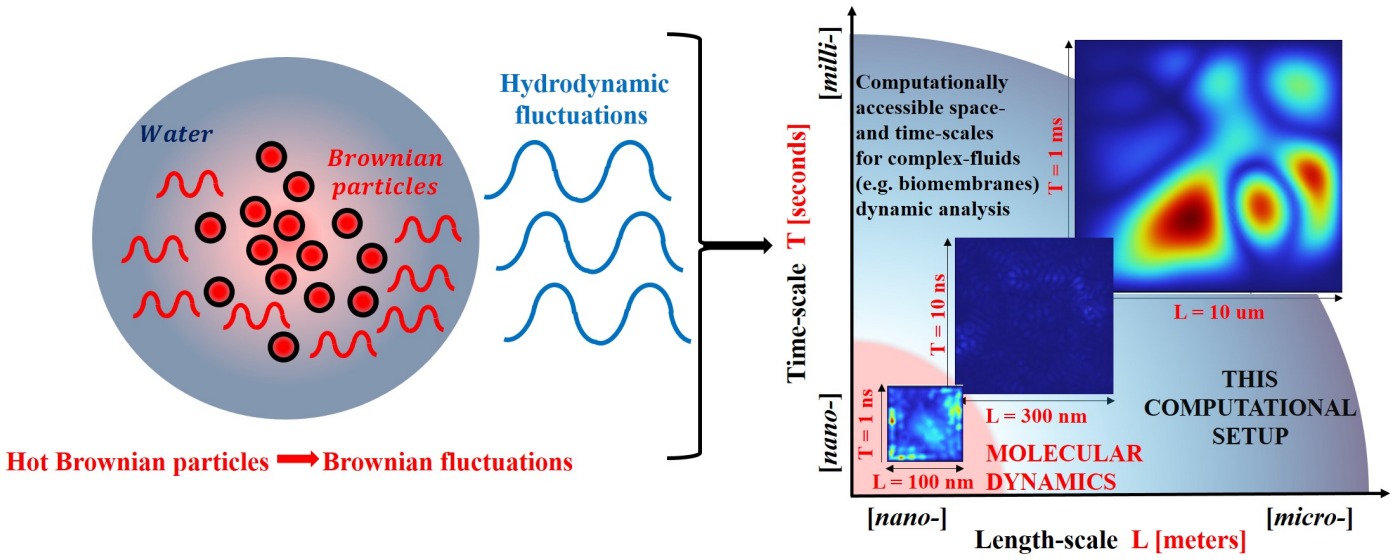

Figure 1 : From left to right: The concept of fluctuations of BIO-membranes (belonging to the class of COMPLEX FLUIDS) modeled by using hot Brownian particles. The resulting Brownian motion causes (drag-induced) hydrodynamic fluctuations that act on the membrane thu