سمینار هفتگی ماده چگال نرم

Fluid membrane triangulation with dynamic area redistribution

Abstract

Lipid bilayers are one of nature's solutions to confine and compartmentalize molecules and micro-organisms. The simplest type of membrane, vesicles, is made of two layers of amphiphilic lipid molecules that enclose a fluid. Although vesicles are relatively simple systems, they have a plethora of interesting applications and properties that have been the subject of research during the past 50 years. Due to the high demand for computational resources, coarse-grained models are the number one choice for the study of membranes as small as 100nm up to a couple of tens of microns. Tri-angulated surfaces are the most popular discretization method to study the mechanical behavior of vesicles and fluid membranes since the elastic and bending moduli can be easily defined. The difficulty in simulating fluid membranes lies in correctly calculating the bending energy. A Monte Carlo (MC) based algorithm, called the dynamics triangulation algorithm, was developed around 30 years ago that opened a path for simulating these systems. The algorithm comes with many restrictions that do not allow a pure Molecular Dynamics (MD) implementation.

We have developed a new method to simulate fluid membranes, coined the dynamic area redistribution (DAR), that is fully compatible with MD and can take advantage of all the perks of MD simulation packages such as OpenMM and HooMD.

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