سمینار هفتگی ماده چگال نرم

Soft meshes for soft matter: A Molecular Dynamics approach to simulating continuum models of fluid bilayer vesicles

Abstract

The spontaneous curvature model or Helfrich's curvature model is widely used to describe the shape changes and behavior of fluid membranes. The discretization of Helfrich's continuum model on triangulated meshes requires a mesh with a uniform distribution of vertices. The dynamic triangulation algorithm is the state-of-the-art method to simulate mesh shape changes while maintaining a uniform vertex distribution. The dynamic triangulation method is used in Monte Carlo simulations but is incompatible with Molecular Dynamics. Here we introduce a Molecular Dynamics simulation method called dynamic area redistribution that can simulate the fluid behavior of biomembranes using two-dimensional meshes with fixed connectivity. The application of an MD-compatible method for fluid membranes is discussed, and a simple red blood cell composite model is proposed.

Ali Farnudi

Sharif University of Technology

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