

Student Exit Seminar

Multiscale Simulation of Biophysics, with Emphasis on Rare-Event Sampling



The behavior of a biophysical systems often is quite different when investigated on different length scales and a complete description of such a system typically requires different approaches for these different length scales. At atomic and mesoscopic scales, a considerable number of degrees of freedom are involved. The associated free energy profiles are relatively rugged with energy barriers or kinetic bottlenecks preventing efficient sampling when doing numerical simulations. To alleviate this problem, a variety of sampling strategies have been developed

In this seminar, I will start with a general background of the multi-scale modeling of biophysical systems and review the different sampling strategies that are being used when doing simulations. Next, I will talk about two of my projects. The first one involves reaction-diffusion problems in a confined environment in the presence of attractive interactions. The second one is the diffusion-driven phase separation problem inside a cross-linked network of semi-flexible polymers. I will use these two projects to illustrate how one can apply multi-scale descriptions and sampling techniques to Non-equilibrium Biophysical systems.



Monday, August 23, 2021
3:00 p.m.
Via Zoom