Incorporation of Solvent Fluctuations into Variational Implicit-Solvent Model

Abstract:
Solvent fluctuations play a fundamental role in many water-mediated molecular interactions. The significance of an efficient implicit-solvent model that can capture solvent fluctuations cannot be overemphasized. In this talk, solvent fluctuations are incorporated into a variational implicit-solvent model in two different approaches. In the first approach, solute-solvent interface fluctuations are taken into account by using a stochastic level set method with noises in the normal velocity. Numerical simulations show that the method can capture dewetting transitions of hydrophobic confinements and can estimate the activation energy barrier of such transitions. The other approach employs a binary level-set representation of the solute and solvent regions. The solvent fluctuation is incorporated through Ising-type Monte Carlo flips of the binary level-set values. Coupled with solute fluctuations, this approach is able to study the folding and unfolding processes of a hydrophobic polymer. Some preliminary results are presented.