

Seminar 2016

Multi-scale models in biophysics: developments and applications



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In this seminar I'll discuss several recent developments of multi-scale computational models for biophysical applications. First, I'll give an overview of an approximate density functional model, DFTB3 and its integration with molecular mechanics (MM) for the analysis of chemical processes in solution and proteins. I'll discuss several recent applications to illustrate the value of such DFTB3/MM approach. In the second part of the talk, I'll touch upon method development for the analysis of protein-membrane interactions, which play an important role in processes such as cellular localization of proteins. I'll illustrate the approach with an application to RecA-membrane interaction, which highlights the interplay of electrostatics, hydrophobic insertion and lipid packing defects in determining the orientation, insertion depth and binding affinity of proteins at membrane surface. If time permits, I'll also briefly discuss the value of coarse-grained models for understanding peptide/membrane interactions.

Friday April 8, 2016

2:30 PM

Laufer Center Lecture Hall 101

Host: Ken Dill

Refreshments following seminar

