Tata Institute of Fundamental Research
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Seminar

Enhanced sampling simulation methods for biophysical problems

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Biophysical theory, modeling, and simulation techniques rooted in statistical mechanics are playing an increasingly important role in elucidating mechanistic details of various cellular processes. Given the large number of degrees-of-freedom in biomolecules, conventional simulation methods remain limited in providing information on conformational statistics – particularly on transiently-populated and metastable states. The knowledge of such states is crucial for rationally designing novel materials and therapeutics. Therefore, many promising simulation approaches that exploit dimensionality-reduction as a tool to explore the vast conformational space of biomolecules in large-yet-finite collective variable (CV) spaces have been proposed. As opposed to coarse-graining methods, CV-based techniques afford enhanced conformational sampling while retaining fully-solvated and atomically-resolved representations of biomolecules. In this talk, I will discuss the algorithmic underpinnings of these methods and their ability in resolving multi-dimensional free-energy surfaces on-the-fly or a posteriori. I will further highlight applications of these methods in the context of several biophysical problems involving a range of conformational motions in multidomain proteins as well as in nucleic acids (specifically, RNA). I will also highlight how conformational heterogeneity can be exploited in the design of novel peptide/small-molecule based therapeutics.

Tuesday, Dec 11th 2018

4:00 PM (Tea/Coffee at 3:30 PM)

Auditorium, TIFR-H