

Multi-scale Modeling of Proteins and Membranes

Ravi Radhakrishnan, PhD

Department of Chemical and Biomolecular Engineering, Department of Bioengineering, Department of Biochemistry and Biophysics, Penn Institute of Computational Science, University of Pennsylvania

Abstract: The talk will describe applications of multiscale modeling in the length scale of Angstroms to microns and timescale of picoseconds to seconds with applications to protein dynamics, biological membrane conformations, and protein-membrane interactions. We will discuss electronic structure, molecular dynamics, particle as well as field-based coarse-grained methodologies and how they can be combined to address functionally relevant questions in structural biology and biophysics. We will demonstrate that beyond fundamental molecular-level insight, such modeling can directly lead to an understanding of signaling. We will also discuss long-time sampling methods and how more modern methods based on data science can be combined with molecular simulations to facilitate analysis and gain mechanism-based insight.

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