Tata Institute of Fundamental Research
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Webinar

Exploring Protein Dynamics: Conformational heterogeneity and Collective Variables

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As non-static objects, proteins proliferate a huge pool of conformations attained as a consequence of numerous modes of perpetually incessant stochastic fluctuations occurring simultaneously at various locations in the protein 3D structure. Switching between these numerous states calls for transitions occurring over a variety of length scales (ranging from tens of angstrom to nanometers) and time scales (ranging from nanoseconds to seconds) which have been reported to be associated with relevant phenomena such as allosteric signalling and enzymatic catalysis. Tracking systems exhibiting these complex transformations requires development and programming of lower dimensional Collective Variables (CV) which can guide us in capturing and analyzing various crucial bottleneck transition events separating the different metastable states. Pointing out the shortcomings and the inability of the traditional CVs to capture local functionally relevant conformation changes, we propose to formalise a CV that can filter out subtle non-trivial fluctuations from a stochastic reservoir of random background noise. Identification of non-affine fluctuations in protein offers a distinct advantage for understanding the bio-macromolecular dynamics. We have shown that all the key dynamical phenomena like allostery, ligand-binding and folding can be investigated by tracking down the various regional predominant non-affine modes of fluctuations.

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