EFFECTIVENESS OF MACHINE LEARNED COLLECTIVE VARIABLE PROJECTION IN BIO-MOLECULAR ENERGY LANDSCAPES

NEELANJANA SENGUPTA

Pallab Dutta, Hindol Chatterjee and Neelanjana Sengupta*
Indian Institute of Science Education and Research (IISER) Kolkata
Mohanpur 741246, West Bengal, India

Capturing biomolecular behaviour with physical-based simulation is beset with several challenges, primary amongst which are delineation of the most important degrees of freedom (DOF) of many-body system. Simplistic collective variables (CVs), while physically intuitive, may not be orthogonal, and moreover, may not capture the essential bio-physical dynamics. Part amelioration of this problem has been achieved by leveraging the latent space of artificial neural networks (ANNs), though these methods challenge physical interpretability. Our recent efforts towards capturing the essential DOFs in bio-molecular simulations will be presented in this seminar. Our work, incorporating dihedral principal component analysis (dPCA), structural biology based efforts coupled with statistical correlations, as well as latent space elucidation, has been applied to a range of bio-molecules, including an intrinsically disordered protein (IDP), the Abelson Tyrosine Kinase (Abl), and fragments of bacteriorhodopsin (bR) embedded in a biological membrane bilayer. Further integrative efforts on the way will be discussed.

Reference:
1. Hindol Chatterjee, Pallab Dutta, Martin Zacharias and Neelanjana Sengupta*, Journal of Chemical Physics, 162, 104110 (2025)
2. Pallab Dutta, Abhay Kshirsagar, Parth Bibekar and Neelanjana Sengupta*, Biophysical Journal, 122, 2948-2959, (2023)
3. Pallab Dutta and Neelanjana Sengupta*, ChemPhysChem, 1-12, e202200 (2022)
4. Pallab Dutta and Neelanjana Sengupta*, Journal of Chemical Physics, 153, 154104 (2020)