Seminar

Learning Optimal Collective Variables for Biophysical Processes via Dimension Reduction

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Computer simulation has now become a very powerful technique for modelling biologically relevant processes with molecular details on both spatial and temporal resolution. Over the past several decades, with the advent of GPU-based hardware coupled with invented fast modern algorithms, MD simulations are currently sampling bio-molecules at multi-microsecond time scales on a routine basis. Consequently analysis of all such data will be very tedious due to the presence of high inherent complexities. Generally these large bio-molecules are associated with huge number of internal dimensions involved. Hence in order to comprehend and interpret these large amount of high dimensional data, we need to have some dimension reduction algorithms to extract the significant and meaningful information in order to infer nice human interpretation in an affordable amount of time. In my entire work we have performed a series of studies on the learning of some mathematical variables also called as Collective Variables to track down such biophysical phenomena. Our analysis revealed that learning the optimal collective variables from dimension reduction is very crucial in order to understand and explain all these bio-physical processes.

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04:00 PM (Tea / Coffee 03.45 PM)

Auditorium, TIFR-H