Machine Learning Approach To Connect Time-Series Data Of Single-Molecule Experiments With Molecular Dynamics Simulations On Protein Folding Dynamics

02/14/18 4:15PM

MIT Building 4, Room 163

Yuji Sugita

How proteins fold into native structures in physiological conditions is one of the most fundamental questions in molecular biology and biophysics. Until now, a huge number of theoretical, computational, and experimental studies have been carried out to answer this question. In the lecture, I first introduce standard computational approaches, such as coarse-grained simulations based on the Go-model and enhanced conformational sampling algorithms like replica-exchange molecular dynamics (REMD) methods. Then, I explain our machine learning approach connecting time-series data of single-molecule experiments with molecular dynamics simulations. This method is free from the force-field bias and can provide the conformational ensembles of proteins that match with the single-molecule experimental data. I also compare the usage of single-molecule time-series data to the ensemble-average data in the machine learning approach.