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BioSim Talk #16

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March 26th 2025 (Wednesday), 16:30-18:00

Institute for Protein Science, Osaka U. (Suita Campus)
2nd floor conference room (large)

Unveiling the biological rare events using Parallel Cascade Selection Molecular Dynamics Simulation

Understanding biological processes requires a detailed, atomistic-level comprehension of biomolecular interactions, often achieved through molecular simulations. However, the timescales of these processes typically exceed the computational capabilities of classical molecular dynamics simulations. To address this challenge, we introduce a series of methods known as Parallel Cascade Selection Molecular Dynamics (PaCS-MD) [1], which enhances efficiency in simulating rare biological events while being compatible with distributed computing. By integrating PaCS-MD with Markov State Modeling, we can investigate dissociation (dPaCS-MD [2, 3]) and association (a/dPaCS-MD [4]) events in Protein/Ligand, Protein/Peptide, and Protein/Protein complexes [5-7]. In this seminar, I will discuss the underlying theory of PaCS-MD/MSM and their applications.

Link for online participation via Zoom:
Meeting ID: 810 2315 5765
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