COMPUTATIONAL BIOPHYSICS **SEMINAR**

Investigating mechanisms of biomolecular self-organization by integrating physics-based simulations and AI

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Molecular self-organization, driven by many-body interactions, plays a critical role in forming ordered structures in both living and inanimate matter. Molecular dynamics simulations and single-molecule experiments offer high-resolution insight into these processes, but limitations exist. Machine learning and artificial intelligence (AI) can help overcome these challenges. In the first part of the talk, I will present an autonomous AI that learns molecular mechanisms from computer simulations. The AI agent predicts rare events by driving parallel simulations and aids in mechanistic interpretation. Applications include nucleation processes, membrane protein assembly in lipid bilayers, and polymer and protein folding. In the second part, I will discuss the integration of physical modeling and AI to extract mechanistic understanding from single-molecule force spectroscopy. Despite offering the possibility to measure fundamental quantities like free energies, these experiments often yield incomplete and indirect measurements. Bayesian inference and simulation-based inference are presented as powerful solutions, with neural network-based density estimation improving the accuracy of molecular free energy estimates.

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