Seminar/Talk

Investigating mechanisms of biomolecular self-organization with computational intelligence

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Host: Andela Saric

Molecular self-organization driven by concerted many-body interactions produces the ordered structures that define both inanimate and living matter. Understanding the physical mechanisms that govern the formation of molecular complexes is key to controlling the assembly of nanomachines and new materials.Physics-based simulations and single-molecule experiments offer the unprecedented possibility to reveal mechanisms of molecular self-organization in high resolution. However, outstanding limitations remain. Computational intelligence is an emergent field that integrates multi-scale simulations, high-performance computing, and machine learning, which promises to overcome fundamental challenges.In the first part of my talk, I will present an integration of machine learning and molecular dynamics simulations to learn complex molecular mechanisms. The framework learns how to optimally sample infrequent and stochastic molecular reorganizations. Using interpretable machine learning, we distill simplified quantitative models that reveal mechanistic insight in a human-understandable form.In the second part of my talk, I will discuss how simulation-based inference, which integrates physics-based simulators and AI, allows us to connect mechanistic models with experimental observations in a principled way. I will introduce cryoSBI, a computational framework that builds on probabilistic deep learning and neural density estimation to make Bayesian inferences of molecular configurations from cryo-electron microscopy data.In conclusion, integrating physics-based models and AI provides a powerful way to extract accurate quantitative information from simulations and biophysical experiments.

Thursday, October 5, 2023 11:00am - 12:00pm

Office Bldg West / Ground floor / Heinzel Seminar Room (I21.EG.101)

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