

Biophysics seminar

Multi-Resolution Simulations of Biological Systems

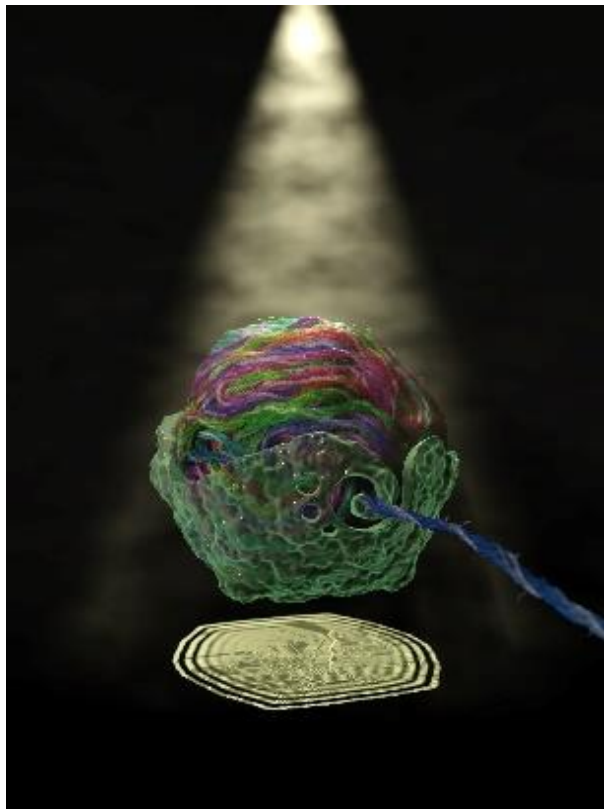
Speaker : **Professor Aleksei Aksimentiev**

Biological Physics University of Illinois at Urbana-Champaign

Date: **April 22, 2024 13:15~**

Venue: **Graduate School of Science Bldg. No.1, 106**
(理学研究科1号館 106号室 BP1)

Notwithstanding dramatic advances in experimental characterization of nanoscale systems, some of the nanoscale processes are simply too fast to register by experimental approaches or involve displacements at scales too fine for direct experimental observation. Microscopic simulations have emerged as a kind of a computational microscope that can characterize processes inaccessible to experimental techniques, revealing not only the sequence of events underlying an experimental measurement but also the forces and energies involved. This lecture will use several systems to illustrate the application of high-end all-atom, coarse-grained, and multi-resolution simulations to obtain information inaccessible to experimental approaches. The topics to be covered will include DNA replication, transport through nuclear pores, and packaging of viral genomes. The lecture will provide a forward-looking perspective on modeling an entire biological cell at all-atom resolution.



References:

- Christopher Maffeo, Han-Yi Chou, and Aleksei Aksimentiev. Single-molecule biophysics experiments *in silico*: Towards a physical model of a replisome. *iScience* 25: 104264 (2022).
- David Winogradoff, Han-Yi Chou, Christopher Maffeo, Aleksei Aksimentiev. Percolation transition prescribes protein size-specific barrier to passive transport through the nuclear pore complex. *Nature Communications* 13:5138 (2022).
- Kush Coshic, Christopher Maffeo, David Winogradoff, Aleksei Aksimentiev. The structure and physical properties of a packaged bacteriophage particle. *Nature* (2024). Doi: 10.1038/s41586-024-07150-4.

Seminar

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