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ICTS Biophysics Seminar

Title : Molecular simulations of nucleic acid packaging: Physical Virology and beyond

Speaker : Kush Coshic (Max Planck Institute of Biophysics, Germany)

Date : Thursday, 01 May 2025

Time : 3:00 PM (IST)

Abstract : Packaging of nucleic acids is essential for all life, occurring across diverse scales and complexities. Virus particles, with their dense packaging, allow us to study fundamental packaging principles. I will begin by introducing a multi-resolution (MR) approach to determine the complete structure of bacteriophage HK97, including its 39,732 base pair genome [1]. Mimicking the action of a packaging motor, we simulated genome loading and refined the packaged capsid structure at increasing resolutions, generating a 26 million atom model of the entire virion, including internal water and ions. Surprisingly, our simulations reveal a loop extrusion mechanism for DNA packaging, resulting in diverse genome configurations and unique viral particle attributes. Microsecond-long all-atom simulations explored the packaged genome's impact on capsid structure, internal pressure, electrostatics, and the diffusion of water, ions, and DNA. This adaptable methodology can be applied to other dsDNA viruses, like herpes. I will then broaden the scope to discuss my ongoing work on modeling RNA packaging — both in the context of viruses such as Dengue, and in understanding the role of ribonucleoproteins (RNPs) and other packaging factors involved in RNA packaging inside living cells. Time permitting, I will very briefly talk about some of my relevant publications and ongoing projects.

1] Coshic K., et al. Nature 627, 905–914 (2024)

Venue : Feynman Lecture Hall

Zoom Link: <https://icts-res-in.zoom.us/j/94744713813?pwd=24123KFWsjtJdcYDWfuy6Z6ZgRbJOB.1>

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