ZAJEDNIČKI SEMINAR

četvrtak, 20.04.2023., 11:00 sati

Fizički odsjek, PMF, Bijenička cesta 32, predavaonica F - 201

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Biophysical Modeling of Cytoskeletal Motor and Crosslinker Cooperativity

Interactions of cytoskeletal filaments, motor proteins, and crosslinking proteins drive important cellular processes such as cell division and cell movement. Cytoskeletal networks also exhibit automated self organization in vitro, leading to non-equilibrium self-assembly in reconstituted systems. An emerging problem in cytoskeletal modeling and simulation is spatiotemporal alteration of the dynamics of filaments, motors, and associated proteins. This can occur due to motor crowding, obstacles along the filament, motor interactions and direction switching, and changes, defects, or heterogeneity in the filament binding lattice. How such spatiotemporally varying cytoskeletal filaments and motor interactions affect their collective properties is not fully understood. The Cytoskeleton Lattice-based Kinetic Simulator (CyLaKS) was developed to investigate such problems. The simulation model builds on previous work by incorporating motor mechanochemistry into a simulation with many interacting motors and/or associated proteins on a discretized binding lattice. CyLaKS also includes detailed balance in binding kinetics, movement, and lattice heterogeneity. The simulation framework is flexible and extensible for future modeling work, and is available on GitHub for others to freely use or build upon. Here, we derive the biophysical model used in CyLaKS, illustrate the uses of the framework, and discuss two new forms of cooperativity that the framework has helped to uncover. The first is a micron-scale interaction between nanometer-sized motors, and the second is a novel form of active protein transport driven entirely by steric exclusion. These results offer new ways of understanding collective behavior of proteins within the cytoskeleton.

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Shane Fiorenza acquired his BS Physics degree at the West Chester University of Pennsylvania in 2016, and is currently a fifth-year graduate student at Betterton Group, the Department of Physics, CU Boulder. His research explores the physical mechanisms responsible for the self-assembly and length regulation of biological matter via computer simulations. To this end, he developed the Cytoskeleton Lattice-based Kinetic Simulator (CyLaKS). CyLaKS is a C/C++ kinetic Monte Carlo-Brownian Dynamics (kMC-BD) simulation framework designed to fill the large gap between atomistic simulations and coarse-grained cytoskeletal frameworks, which focus on larger-scale assemblies. He currently uses CyLaKS to study long-range coupling between molecular motors.