Soft Living Active and Adaptive Matter

Chiral twisting in a bacterial cytoskeletal polymer affects filament size and orientation

Handuo Shi
Postdoctoral Fellow, Stanford University

Abstract:

In many rod-shaped bacteria, the actin homolog MreB directs cell-wall insertion and maintains cell shape, but it remains unclear how structural changes to MreB affect its organization in vivo. Here, we perform molecular dynamics simulations for *Caulobacter crescentus* MreB to extract mechanical parameters for inputs into a coarse-grained biophysical polymer model that successfully predicts MreB filament properties in vivo. Our analyses indicate that MreB double protofilaments can exhibit left-handed twisting that is dependent on the bound nucleotide and membrane binding; the degree of twisting correlates with the length and orientation of MreB filaments observed in vitro and in vivo. Extending the simulations to a longer time scale further reveal that MreB filaments can transition from multiple steady states, highlighting the dynamic nature of the protein filament. Taken together, our multiscale modeling correlates cytoskeletal filament size with conformational changes inferred from molecular dynamics simulations, providing a paradigm for connecting protein filament structure and mechanics to cellular organization and function.

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Time:
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About the speaker:

Dr. Handuo Shi is a James S. McDonnell Postdoctoral Fellow working with Dr. Justin Sonnenburg and Dr. KC Huang at Stanford University. Her research focuses on quantitative characterization and prediction of complex behaviors in biological systems. She is currently working on a large-scale, high-throughput chemical screen on in vitro bacterial communities derived from the human gut.

Handuo obtained her Ph.D. degree in Bioengineering at Stanford University. Her Ph.D. dissertation combines physical modeling with experimental validation to reveal the principles of bacterial morphogenesis under myriad environmental, genetic, and chemical perturbations.

For more information, contact: Kinjal Dasbiswas, Niranjan Sarpangala
kdasbiswas@ucmerced.edu, nsarpangala@ucmerced.edu