Seminar

A Coarse-Grain Model For The Human Erythrocyte Membrane

By

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Castleman Building, Room 212

5:00-6:00 pm

Abstract:

We present novel coarse-grained models with high computational efficiency for simulating a variety of dynamic and topological problems involving biological membranes. The model is solvent-free and the inter-grain interaction potential is anisotropic. The model also allows free diffusion of membrane agents. By simultaneously invoking these three characteristics, the proposed method facilitates simulations that span much larger length-scales (~ μm) and time-scales (~ ms) than currently possible with other methods based on classical molecular dynamics models or other coarse-grain approaches. We also present a coarse-grained cytoskeletal dynamics simulation with breakable protein associations to elucidate the roles of shear stress, specific chemical agents, and thermal fluctuations in cytoskeleton remodeling. This cytoskeletal dynamics model offers a means to resolve long-standing questions regarding the extraordinary ability of Red Blood Cells to undergo reversible large deformation and fluidity. Such mechanical response cannot be consistently rationalized on the basis of fixed connectivity of the cell cytoskeleton

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[1] Dr. Lykotrafitis received his B.S., M.S. and Ph.D. degrees in Applied Mathematics and Physical Sciences from National Technical University of Athens, Greece. He subsequently received his second M.S. and Ph.D. degrees in Mechanical Engineering from Caltech studying dynamic frictional sliding modes along incoherent interfaces. Since 2006, he has been a postdoctoral fellow at MIT conducting experimental and computational studies of