309e Coarse-Graining the Actin Filament from Atomistic Simulations

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Actin filament is the essential component of the cytoskeleton, and is closely related to cell growth, cell locomotion, mitosis, and intracellular transportation. As the first step in building biophysical models of these cellular processes, a coarse-grained (CG) model of the actin cytoskeleton is developed. Each actin monomer in the filament is composed of four beads, and each bead represents a subdomain of the protein molecule. The intra-monomer interactions include three harmonic bonds, two angular potentials, and one dihedral angle. Therefore, important modes of the actin monomer, such as the propeller rotation and the open/close of the ATP cleft are captured in the CG model. Among actin monomers, harmonic springs are employed to describe their interactions. The parameters of the CG potentials are determined by reproducing the fluctuations of various internal coordinates in all-atom simulations using harmonic analysis. A self-consistent procedure has been developed for this purpose. It was found that by reproducing the internal coordinate fluctuations; the CG model can also reproduce the mechanical properties of the filament such as the persistence length. Therefore, the CG model presented in this work not only preserves the modes thermal fluctuations of the filament, but also its elasticity. Extension of this model to soft potentials will also be addressed.