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Monte Carlo simulation of actin self-assembly XINJIANG LÜ, JAMES KINDT, Department of Chemistry and Cherry L. Emerson Center for Scientific Computation, Emory University — Using grand canonical Monte Carlo simulations we study the equilibrium properties of actin self-assembly. The statistics of actin polymerization is described by a mechanism involving monomer activation and chain propagation with bond association constants derived from experimental free energy parameters. For efficiency in representing systems of very long, stiff chains we use a coarse-graining based on spherocylinders. We will present results pertaining to the isotropic-nematic transition in this equilibrium polymer system.

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